APS March Meeting 2015
San Antonio, Texas
http://www.aps.org/meetings/march/index.cfm
8:00AM A4.00001 Detergent Stabilized Nanopore Formation Kinetics of an Anthrax Protein
KELBY PETERSON, Utah State University — This summer research project funded through the Society of Physics Students Internship Program and The National Institute of Standards and Technology focused on optimization of pore formation of Protective Antigen protein secreted by Bacillus Anthracis. This experiment analyzes the use of N-tetradecylphosphocholine (FOS-14 Detergent) to stabilize the water soluble protein, protective antigen protein (PA63) to regulate the kinetics of pore formation in a model bilayer lipid membrane. The FOS-14 Detergent was tested under various conditions to understand its impact on the protein pore formation. The optimization of this channel insertion is critical in preparing samples of oriented for neutron reflectometry that provide new data to increase the understanding of the protein’s structure.

8:12AM A4.00002 Lipid membrane structure and dynamics in the presence of tamoxifen and antimicrobial peptides1. SAMUEL HEBENSTREIT, Colorado Mesa University, NAVAL KHADKA, JIANJUN PAN, University of South Florida — Lipids are organic molecules composed of hydrophobic fatty acid tails and hydrophilic head groups that can form a multitude of structures, including lipid vesicles, membranes, and micelles. By varying the ratios of poly(styrene sulfonate) chains and cationic peptides, and tamoxifen are incubated with the vesicles. Fourier transform infrared spectroscopy measurements are performed with and without antimicrobial peptide. A change in absorbance corresponding to the wavenumber ranges associated with the stretching of the carbonyl and phosphate groups is observed. Also, dye leakage assay is performed with vesicles composed of neutral and charged lipids. Calcein dye is enclosed within these vesicles in solution. Different concentrations of the active and inactive antimicrobial peptides, and tamoxifen are incubated with the vesicles. Concentration-dependent dye leakage is determined by measuring fluorescence intensity before and after the addition of the peptides and tamoxifen. Different leakage behavior is observed for the active and inactive peptides, and the lipid composition of the vesicle is found to have a large effect.

1Supported by an NSF grant

8:24AM A4.00003 Amphiplex Formation, SHANNON PETERSEN, Allegheny College, JENNIFER LAASER, TIMOTHY LODGE, University of Minnesota — Polymer-micelle complexes are currently under heavy investigation due to their potential applications in targeted drug delivery and gene therapy, yet the dynamics of the complex formation is still relatively unstudied. By varying the ratios of poly(styrene sulfonate) chains and cationic poly(dimethylaminoethyl methacrylate)-b-poly(styrene) micelles and the ionic strength of the solution, we created a variety of complex configurations of different sizes and charges. The complexes were characterized dynamic light scattering and zeta potential measurements which provided information regarding the hydrodynamic radius, distribution of sizes, and effective charge.

8:36AM A4.00004 Biomimetic Photonic Crystals based on Diatom Algae Frustules, JONATHAN MISHLER, Department of Physics, University of Arkansas, Fayetteville, ANDREW ALVERSON, Department of Biological Sciences, University of Arkansas, Fayetteville, JOSEPH HERZOG, Department of Physics, University of Arkansas Fayetteville — Diatom algae are unicellular, photosynthetic microorganisms with a unique external shell known as a frustule. Frustules, which are composed of amorphous silica, exhibit a unique periodic nano-patterning, distinguishing diatoms from other types of phytoplankton. Diatoms have been studied for their distinctive optical properties due to their resemblance of photonic crystals. In this regard, diatoms are not only considered for their applications as photonic crystals, but also for their use as biomimetic templates for artificially fabricated photonic crystals. Through the examination and measurement of the physical characteristics of many scanning electron microscope (SEM) images of diatom frustules, a biomimetic photonic crystal derived from diatom frustules can be recreated and modeled with the finite element method. In this approach, the average geometries of the diatom frustules are used to recreate a 2-dimensional photonic crystal, after which the optical field distribution and optical transmission through the photonic crystal are both measured. The optical transmission is then compared to the transmission spectra of a regular hexagonal photonic crystal, revealing the effects of diatom geometry on their optical properties. Finally, the dimensions of the photonic crystal are parametrically swept, allowing for further control over the transmission of light through the photonic crystal.

8:48AM A4.00005 Employing Multiple Spectroscopic Techniques Simultaneously to Observe Protein Unfolding, MICHAEL CROWE, BEN KELTY, JUSTIN LINK, Xavier University — A protein’s function is directly related to its native, folded structure. In order to study the structure of proteins, the unfolding process may be characterized. In our study, by using the spectroscopic techniques of circular dichroism (CD), absorption, and fluorescence simultaneously, we examined the unfolding of horse heart cytochrome c, a well-studied, model protein by gradually increasing the concentration of the chemical denaturant, guanidine hydrochloride. The signal changes from these modalities over the course of the unfolding reaction provide some of the thermodynamic properties like Gibbs free energy for insight into the stability of the protein. This allows us to compare the three techniques under the exact same conditions. The objective of this session is to present recent work in developing a protocol to observe the unfolding of cytochrome c using fluorescence, absorbance, and CD simultaneously.

9:00AM A4.00006 The Effect of Magnetic Fields on the Quorum Sensing-Regulated Luminescence of Vibrio fischeri, ADDIE BARRON, STEVE HAGEN, MINJUN SON. None — Quorum sensing (QS) is a mechanism by which bacteria communicate through the secretion and detection of extracellular signaling molecules known as autoinducers. This research focuses on the quorum sensing regulated bioluminescence of Vibrio fischeri, a marine bacterium that lives in symbiosis with certain fish and squid species. Previous studies of V. harveyi, a close relative of V. fischeri, indicate that a strong magnetic field has a positive effect on V. harveyi bioluminescence. However, the effect of magnetic fields on quorum-sensing-regulated luminescence is in general poorly understood. We grew V. fischeri in solid and liquid growth media, subject to strong static magnetic fields, and imaged the bioluminescence over a period of forty-eight hours. Luminescence patterns were analyzed in both the spatial and time dimensions. We find no indication that a magnetic field influences Vibrio fischeri luminescence either positively or negatively.

This research was funded by the grant number NSF DMR-1156737.

9:12AM A4.00007 Electron mobility in liquid-gated graphene biosensors, CHRISTINA HARMON, Linfield College, MORGAN BROWN, ETHAN MINOT, Oregon State University, MICHAEL CROSSER, Linfield College — We report measurements of the electron mobility in liquid-gated graphene. Graphene field-effect transistor (GFET) biosensors are more sensitive to changes in external fields when the mobility is high; therefore, increasing mobility will improve sensitivity. Mobility can be calculated from the ratio of sheet conductivity to carrier density. Sheet conductivity was measured using a van der Pauw geometry and carrier density was determined from measurements of the liquid-gate capacitance. We show that mobility improves after the graphene surface is cleaned by an annealing process.
9:24AM A4.00008 Detecting a Protein in its Natural Environment with a MOSFET Transistor\(^1\)

**Benjamin Perez\(^2\)**, The Society of Physics Students / NIST, Arvind Balijepalli\(^3\), NIST — Our group’s goal is to make a MOSFET transistor that has a nanopore through it. We want to have proteins flow through this device and examine their structure based on the modulation they cause on the current. This process does not harm the protein and allows the protein to be studied in its natural environment. The electric field and electric potential of a point charge were computed within a nano-transistor. The simulations were used to see if the point charge had enough influence on the current to cause a modulation. The point charge did cause a rise in the current making the modulation concept a viable one for medical applications. COMSOL metaphysics software was used to perform all simulations.

\(^1\)The Society of Physics Students internship program and NIST

\(^2\)This research was done at NIST through the Society of Physics Students internship program.

\(^3\)He worked as my mentor for my summer at NIST

9:36AM A4.00009 Topological Properties of Some Integrated Circuits for Very Large Scale Integration Chip Designs\(^1\)


\(^1\)The views expressed in this article are those of the author and do not reflect the official policy or position of the United States Air Force, Department of Defense or the U.S. Government.

9:48AM A4.00010 Exploration of Whispering Gallery Modes in an Optically Trapped Aerosol Droplet , Angela Ludvigsen, Lowell McCann, University of Wisconsin - River Falls — Optical traps use a laser beam to catch and hold small transparent objects. Past observations of optically trapped aqueous aerosol droplets have shown that the droplet moves between two or more stable positions depending upon the power of the trapping laser. It is hypothesized that this movement coincides with a resonance of the light with the droplet called a Whispering Gallery Mode. When the resonance occurs, additional forces act on the droplet. To investigate this behavior, Raman scattered light from the droplet is measured using a spectrometer while simultaneously recording the droplet’s position. The Raman spectrum exhibits a series of peaks that appear due to the very spherical shape of the droplet called Cavity Enhanced Raman Spectroscopy. The location and spacing of the peaks are related to the diameter and the optical properties of the droplet. In order to achieve an accurate determination of the radius from this spectrum, the magnitude of the electric and magnetic fields of the light scattered off the droplet are calculated. This allows for a precise measurement of the droplet’s radius at the moment that the droplet moves between stable positions.

10:00AM A4.00011 Measuring the Temperature of the Ithaca College MOT Cloud using a CMOS Camera, Jonathan Smucker, Bruce Thompson, Ithaca College — We present our work on measuring the temperature of Rubidium atoms cooled using a magneto-optical trap (MOT). The MOT uses laser trapping methods and Doppler cooling to trap and cool Rubidium atoms to form a cloud that is visible to a CMOS Camera. The Rubidium atoms are cooled further using optical molasses cooling after they are released from the trap (by removing the magnetic field). In order to measure the temperature of the MOT we take pictures of the cloud using a CMOS camera as it expands and calculate the temperature based on the free expansion of the cloud. Results from the experiment will be presented along with a summary of the method used.

10:12AM A4.00012 Investigation of Nanowire Thickness and Enhancement Characteristics , Cameron Saylor, Desalegn Debu, University of Arkansas Fayetteville, Eric Novak, Shippensburg University, Joseph Herzog, University of Arkansas Fayetteville — This work investigates of the effect of nanowire thickness on the optical enhancement of nanowire. We present a study that shows there is potential in altering the thickness of plasmonic structures to improve their optical field enhancement. The study was performed using a finite element method computational electromagnetic analysis, which allows for the thickness and width of the nanowire and wavelength of the incident light to be changed, and the corresponding effects on the optical enhancement characteristics of the structure to be measured. The nanowire was modeled using a two-dimensional cross-section that approximates the nanowire as being infinitely long, with the incident light polarized perpendicular to the length of the nanowire. Preliminary results suggest that lower nanowire thickness provide the highest optical enhancement. The effects of the material and thickness of the adhesion layer on the optical enhancement of the nanowire are also investigated.

10:24AM A4.00013 Nonlinear Interactions between Slender Structures and Axial Flow, Li Du, Nanjing University — For decades, dynamic behaviors of a slender structure with axial flow have been extensively studied. However, the governing equation based on expansions of small quantities is complicatedly-expressed and can be inappropriate as amplitude becomes considerably large. In this research, we are dedicated to finding an approach to study the nonlinear dynamics of a fluid-conveying slender strcture with arbitrary amplitude. By introducing the Intrinsic Coordinate, we find a concise way to describe the configuration of the system. Differential relations of such coordinate are studied and the rigorous nonlinear equation of motion is derived. Then rather than small-deflection approximation, linear dynamics are studied using Argand Diagram under a weaker condition named low-varying approximation. Nonlinear properties including Hopf bifurcation, limit-cycle motion and vibration frequencies are studied theoretically and experimentally.

10:36AM A4.00014 ABSTRACT WITHDRAWN
1: This work was part of the Society of Physics Students internship program.

Monday, March 2, 2015 2:30PM - 5:30PM –
Session D4 APS: Undergraduate Research/Society of Physics Students II
Mayor Cockrell Room 004 - Cortney Bougher, American Physics Society

2:30PM D4.00001 Photoresponsive memory device based on Graphene/Boron Nitride heterostructure
, SALMAN KAHN, JAIRO VELASCO JR, LONG JU, DILLON WONG, JUWON LEE, HSIN ZON TSAI, Department of Physics, University of California, Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, ALEX ZETTL, FENG WANG, MICHAEL CROMMIE, Department of Physics, University of California, Berkeley — Recent technological advancements have allowed the stacking of two dimensional layered material in order to create van der Waals heterostructures (VDH), enabling the design of novel properties by exploiting the proximal interaction between layers with different electronic properties. We report the creation of an optoelectronic memory device using a Graphene/Boron Nitride (hBN) heterostructure. Using the photo-induced doping phenomenon, we are able to spatially “write” a doping profile on graphene and “read” the profile through electrical transport and local probe techniques. We then utilize defect engineering to enhance the optoelectronic response of graphene and explore the effect of defects in hBN. Our work introduces a simple device architecture to create an optoelectronic memory device and contributes towards understanding the proximal effects of hBN on Graphene.

2:42PM D4.00002 High quality factor titanium nitride and aluminum resonators for increased superconducting qubit coherence
, N.E. FRATTINI, A. DOVE, D.M. TOYLI, S. HACOHEN-GOURCY, A. EDDINS, I. SIDDIQI, QNL, University of California, Berkeley — Superconducting qubits have successfully realized effective two-level quantum systems whose state can be read out by dispersive coupling to a linear resonator. Superconducting films which exhibit low loss in the microwave frequency regime at millikelvin temperatures and single photon excitation powers are an essential ingredient in realizing high-coherence qubits and high-fidelity readout. To explore the magnitude of these losses and their correlation with fabrication recipes, we prepare and characterize both lumped element and distributed element resonators derived from titanium nitride on silicon and aluminum on sapphire. We study the role of substrate annealing, film growth conditions, and lithographic technique on resonator quality factor.

2:54PM D4.00003 the Characteristic Phase Transitions of Co-doped BaFe2As2 Synthesized via Flux Growth
, C.H. SHEA, Ithaca College, Department of Physics and Astronomy, C. RONCAIOLI, C. ECKBERG, T. DRYE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, M.C. SULLIVAN, Ithaca College, Department of Physics and Astronomy, J. PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland — Since the discovery of a new family of type II superconductors in 2008, the iron pnictides, research has had suspicions that they might bear similar electronic properties to the well-known (but not easily understood) oxide superconductors. For this reason studies on this family of compounds has been of great interest to the materials science community. Our efforts have been aimed at single crystal growth and measurement of a particular member of this family, BaFe2As2. While this material is not superconducting at standard pressure, the partial substitution of cobalt on the iron site has been shown to suppress an anti-ferromagnetic phase transition occurring at lower temperatures allowing for the appearance of a superconducting phase. Transport and low field magnetization measurements taken on our samples show clean transitions, indicating Tc’s of up to 24 K in optimally doped samples. We will discuss the growth methods and temperature dependent phase transitions of this material at different cobalt concentrations.

3:06PM D4.00004 ABSTRACT WITHDRAWN

3:18PM D4.00005 Measurements of Viscosity and Dynamics of Thin Films of Organic Glass TPD via Hole Growth Wetting Studies
, KAREEM WAHID, University of Texas Pan American, YUE ZHANG, MU LI, ZAHRFAF KAKHRAI, Department of Chemistry, University of Pennsylvania — In this study, we aim to measure the viscosity of thin glassy films of the small organic molecule N,N′-bis[3-methylphenyl]-N,N′-diphenylbenzidine (TPD). Organic glasses such as TPD have various applications in organic light emitting diodes (OLED), and organic photovoltaics. An understanding of the origin for nano-scale properties (e.g. viscosity) would allow for better design of such devices in future applications. Viscosity is simple to measure in bulk systems but challenging at the nanometer scale. Dewetting experiments provide a simple and non-invasive method to measure viscosity in thin film systems. By following dewetting kinetics over time, we are able to identify material related viscous dissipation and substrate related fractional dissipation involved during dewetting. Both homogeneously and heterogeneously nucleated holes have been observed on TPD films of various thicknesses or various substrates. There is reasonable agreement between these observations and with full-slip dewetting models among heterogeneously nucleated holes. However, this is not observed in homogeneously nucleated holes. Careful substrate treatment and control of substrate properties influence the slip length and the dewetting dynamics.

1 This work was supported by funding from IARPA and ARO.

1 NSF grant DMR-1350044
3:30PM D4.00006 Monitoring Residual Solvent Additives and Their Effects in Solution Processed Solar Cells, DEREK M. FOGEL, Wake Forest University, JAMES I. BASHAM, NIST and Penn State University, SEBASTIAN ENGGMANN, SUJITRA J. POOKPANATANA, EMILY C. BITTLE, NIST, OANA D. JURCHESCU, Wake Forest University, DAVID J. GUNDLACH, NIST — High boiling point solvent additives are a widely adopted approach for increasing bulk heterojunction (BJH) solar cell efficiency. However, experiments show residual solvent can persist for hours after film deposition, and certain common additives are unstable or reactive. We report here on the effects of residual 1,8-diiodooctane on the electrical performance of poly[3-hexylthiophene-2,5-diyl] (P3HT): phenyl-C71-butyric acid methyl ester (PC71BM) BHJ solar cells. We optimized our fabrication process for efficiency at an active layer thickness of 220 nm, and all devices were processed in parallel to minimize unintentional variations between test structures. The one variable in this study is the active layer post spin drying time. Immediately following the cathode deposition, we measured the current-voltage characteristics at one sun equivalent illumination intensity, and performed impedance spectroscopy to quantify charge density, lifetime, and recombination process. Spectroscopic ellipsometry, FTIR, and XPS are also used to monitor residual solvent and correlated with electrical performance. We find that residual additive degrades performance by increasing the series resistance and lowering efficiency, fill factor, and free carrier lifetime.

3:42PM D4.00007 Solution Processed Polymeric Semiconductors for Carbon Nanotube-Enabled, Vertical, Organic Field Effect Transistors, ALEXANDER SCHACHTNER, Dept. of Physics, University of Oregon, NICHOLAS C. CUNNINGHAM, CHRISTOPHER C. SAMOUCHE, MAXIME G. LEMAITRE, ANDREW G. RINZLER, Dept. of Physics, University of Florida — Carbon nanotube-enabled, vertical, organic field effect transistors (CN-VFETs) based on the small molecule dinaphtho[2,3-b:2',3'-f]thieno[5,2-b]thiophene (DTNTT) have demonstrated high current, low-power operation suitable for driving active matix organic light emitting diode (AMOLED) displays [1]. This performance is achieved without the need for costly high-resolution patterning, despite the low mobility of the organic semiconductor, by employing sub-micron channel widths, defined in the vertical devices by the thickness of the semiconducting layer. Replacing the thermally evaporated small molecule semiconductor with a solution-processed polymer would possibly further simplify the fabrication process and reduce manufacturing cost. Here we investigate several polymer systems as wide bandgap semiconducting channel layers for potentially air stable and transparent CN-VFETs. The field effect mobility and optical transparency of the polymeric layers are determined, and the performance and air stability of CN-VFET devices are measured. 1. M. A. McCarthy et al. Science 2011 332, 570

5:34PM D4.00008 Synthesis and Characterization of Rare Earth Nanoparticles in a non-aqueous environment, E.J. PAREDES AULESTIA, R.H. FUKUDA, M.M. CASTRO DE LA TORRE, P.-C. HO, Physics, California State University Fresno, S. ATTAR, M. GOLDEN, Chemistry, California State University Fresno, D. MARCOSAN, USDA-ARS — Magnetic nanoparticles have several potential applications, such as in biomedicine and for magnetic information storage due to their reduced size and magnetization properties. We synthesize gadolinium and neodymium nanoparticles by applying the reverse micelle method. This method consists of using a surfactant with a large nonpolar-solvent-to-polar-solvent ratio to form spherical cages around a reactant. Most studies related to the reverse micelle method use water as the polar solvent, but the use of water is not suitable for our project since both Gd and Nd are highly reactive in water. Instead, we employ methanol as our polar solvent. Hexane and heptane are tested as nonpolar solvents. DDAB and AOT are used as surfactant molecules. A solution containing a reducing agent is then added to produce the desired Nd and Gd nanoparticles. Our samples are analyzed using light microscopy, SEM (Scanning Electron Microscopy) and EDX (Energy Dispersive X-ray). We found heptane, methanol and AOT produce Neodymium particles with diameters less than 5 micrometers. Heptane, methanol and DDAB yield Gadolinium particles with diameters less than 1 micrometer. The synthesis procedure is currently being revised, in order to produce cleaner samples and particles of smaller size.

4:06PM D4.00009 Atomic Structure of Grain Boundaries in Graphene, OTHO ULRICH, University of South Florida, Western Michigan University, JOSEPH GONZALEZ, KIEN NGUYEN CONG, IVAN OLEYNIK, University of South Florida — In its pristine form, graphene is one of the strongest materials measured, and possesses a wide range of technologically appealing characteristics. Several recent experiments have explored the mechanical properties of graphene which contains grains, some with contradictory results. To explore the atomic structure of grain boundaries in graphene, we employ a complex of computational approaches. A set of unit cells of graphene bicrystals with variable grain misorientation is generated by applying a conjugate gradient method with periodic boundary conditions using the SEDREBO potential for carbon-carbon interaction. Structures are classified by formation energy and atomic coordination, and identification of physically viable samples is achieved using these statistics. The defective regions constituting the grain boundaries are defined using the atomic energy distribution. Formation energies of any viable structures are normalized according to cell height and compared by formation energy and atomic coordination, and identification of physically viable samples is achieved using these statistics. The defective regions constituting the grain boundaries are defined using the atomic energy distribution. Formation energies of any viable structures are normalized according to cell height and compared by indexing misorientation angles. Lack of a functional relationship between misorientation angle and formation energy indicates a greater complexity in the mechanisms of the grain boundaries.

4:18PM D4.00010 Phase Boundaries of the Pseudogap Anderson Impurity Model, AARON MOHAMMED, Univ of South Florida, TATHAGATA CHOWDHURY, KEVIN INGERSENT, Univ of Florida — As the temperature of metals containing dilute concentrations of magnetic impurities reach very low temperatures, a phenomenon known as the Kondo effect takes place in which the resistance increases. This is due to the domination of spin-exchange processes that occur between the electrons of the metal and the electrons of the magnetic impurity near absolute zero. The Anderson model is a quantum impurity model that was developed in the 1960s to explain this phenomenon. It involves a single magnetic impurity tunnel-coupled to the conduction band of a metal. If the conduction band of this system contains a pseudogap, or a power-law decrease in the density of states around the Fermi energy, then quantum phase transitions will occur. The phase boundaries of the pseudogap Anderson impurity model have been previously approximated using mean field theory methods. Here, we focus on using the more accurate numerical renormalization group method to calculate the location of these boundaries. We then compare these numerical results with the predictions derived from the scaling approximations. The development of nanotechnology like quantum dots and STM have rekindled interest in the Kondo effect since it can now be studied within controlled settings.

4:30PM D4.00011 Intrinsic localized modes in antiferromagnetic sheets: the role of shape-dependent demagnetization fields, BENJAMIN KIMOCK, LARS ENGLISH, Dickinson College — We investigate numerically the role of global demagnetization fields on the formation of energy-localized patterns in two-dimensional sheets of antiferromagnetically-coupled, easy-axis spins. These global fields depend on the macroscopic shape of the lattice, and three scenarios can be delineated depending on whether the uniform mode is above, below or coincident with the long-wavelength spin waves in frequency. Each scenario leads to a different localization pathway and pattern. In the context of spin sheets, we can now also consider lattice anisotropies and their effects on the properties and interactions of intrinsic localized modes.

1. Supported by the NSF REU grant DMR-1156737. REU Site in Materials Physics at the University of Florida
Computational Electromagnetic Modeling of Optical Responses in Plasmonically Enhanced Nanoscale Devices Fabricated with Nanomasking Technique. ERIC NOVAK, Shippensburg University, DESALEGN DEBU, CAMERON SAYLOR, JOSEPH HERZOG, University of Arkansas — This work computationally explores plasmonic nanoscale devices fabricated with a recently developed nanomasking technique that is based on the self-aligned process. Computational electromagnetic modeling has determined enhancement factors and the plasmonic and optical properties of these structures. The nanomasking technique is a new process that is employed to overcome the resolution limits of traditional electron beam lithography and can also be used to increase resolution in photolithography fabrication as well. This technique can consistently produce accurate features with nanostructures and gaps smaller than 10 nm. These smaller dimensions can allow for increased and more localized plasmonically enhanced electric fields. These unique metal devices encompass tunable, enhanced plasmonic and optical properties that can be useful in a wide range of applications. Finite element methods are used to approximate the electromagnetic responses, giving the ability to alter the designs and dimensions in order to optimize the enhancement. Ultimately, we will fabricate devices and characterize the plasmonic properties with optical techniques, including dark-field spectroscopy, to confirm the properties with the goal of generating more efficient devices.

Trap State Introduction versus Band Gap Narrowing in Nitrogen-Doped La$_2$Ti$_2$O$_7$, BRANDON YOST, SCOTT CUSHING, NAINQIANG WU, ALAN BRISTOW, West Virginia University — Nitrogen doping was reported to extend lanthanum dittannate’s (LTO) La$_2$Ti$_2$O$_7$ absorption from 380 nm to 500 nm by narrowing the band gap without introducing trap states [1]. N-LTO holds promise for solar water splitting if, unlike in N-doped TiO$_2$, spectral coverage can be increased without decreasing carrier lifetimes and decrementing the overall performance. Therefore, in this presentation, the effect of N-doping on LTO is confirmed using transient absorption spectroscopy with a supercontinuum and THz probe. The supercontinuum probe reveals carrier evolution in both band edge and mid-gap defect states. By exciting above and below the band edge, the influence of N-doping on the density of trap states is directly compared to the band edge position. Further, comparison of dynamics measured with the supercontinuum and THz probes reveals which changes in lifetime correspond to increased mobility or increased trapping, showing how the shifted band edge modifies carrier dynamics, and that N-doping in LTO is an efficient strategy for solar energy harvesting.

Measurement of Specific Heat of Pr$_{1-x}$Nd$_x$Os$_2$Sb$_{12}$ from 11K-300K, TAYLOR MCCULLOUGH-HUNTER, SHOJI HISHIDA, PEI-CHUN HO, Physics Department, California State University, Fresno, BRIAN MAPLE, Physics Department, University of California, San Diego, TATSUYA YANAGISAWA, Physics Department, Hokkaido University, Japan — The filled skutterudite compound Pr$_{1-x}$Nd$_x$Os$_2$Sb$_{12}$ exhibits ferromagnetism at a Curie temperature near 1 K. Originally, Nd doped compounds of the form Pr$_{1-x}$Nd$_x$Os$_2$Sb$_{12}$ were developed to investigate the effect of ferromagnetism on the unconventional superconductivity and heavy fermion behavior of PrOs$_2$Sb$_{12}$. The specific heat of Pr$_{1-x}$Nd$_x$Os$_2$Sb$_{12}$ (where x = 0.25, 0.5, 0.75, 0.8, and 1) is measured at 11K-300K to investigate the compounds’ normal state properties. The specific heat is measured using relaxation calorimetry of finite heat pulse in a cryocooler system. Values of the electronic specific heat coefficient, $\gamma$, for these compounds are estimated to be 10-60 mJ/K$^2$-mol. This contrasts with previous low temperature measurements (<10K) of Nd$_x$Os$_2$Sb$_{12}$ with $\gamma$ approximately 520 mJ/K$^2$-mol.

Colossal Piezoresistance in strained La$_{0.67}$Sr$_{0.33}$MnO$_3$ thin films, MARIA VI-ITANIEMI, IN HAE KWAK, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — Piezoresistance is the change in electrical resistance as a function of strain. A known mechanism leading to piezoresistance is thermodynamic phase separation. It has been shown that the compound (La$_{1-x}$Pr$_x$)$_1$-$\chi$Ca$_x$MnO$_3$ (LPCMO) exhibits colossal piezoresistance (CPR) at low temperatures due to electronic phase separation. For use in many applications, such as sensors, materials must exhibit CPR near room temperature. A possible candidate compound is La$_{0.67}$Sr$_{0.33}$MnO$_3$ (LSMO) which has a Curie temperature of approximately 350 K. However, bulk LSMO single crystals do not show CPR since such samples are uniformly ferromagnetic and metallic with no phase separation. In this study, we examine the piezoresistance of ultrathin LSMO films grown on SrTiO$_3$ (STO) substrates using a three-point beam bending method to control the compressive and tensile strain. It has been suggested that the lattice mismatch strain due to the substrate induces phase separation in these thin films. We have observed CPR in such strained LSMO thin films even at room temperature.

Tuesday, March 3, 2015 4:30PM - 6:00PM – Session DA1 APS: Meet the APS Editors Reception

4:30PM DA1.00001 Meet the APS Editors Reception
8:00AM F4.00001 Light: A Spectrum of Utility, the 2014-2015 Society of Physics Students Science Outreach Catalyst Kit

MARK SELLERS, Rhodes College, KEARNS LOUIS-JEAN, Xavier University of Louisiana, SOCIETY OF PHYSICS STUDENTS COLLABORATION, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY COLLABORATION — The Science Outreach Catalyst Kit (SOCK) is a set of activities and demonstrations designed to bolster the outreach programs of undergraduate Society of Physics Students (SPS) chapters, creating the framework for a lasting outreach program. Targeted for students ranging from kindergarten to high school, the SOCK allows students to actively engage in hands-on activities that teach them scientific skills and allow them to exercise their natural curiosity. The 2014-2015 SOCK united themes from the 2014 International Year of Crystallography and the 2015 International Year of Light to explore how light is used as a tool every day. This presentation will discuss the contents of the SOCK, which contains a large assortment of materials, such as diffraction glasses, polarizers, ultraviolet flashlights, etc., and describe the research and development of the activities. Each activity explores a different light phenomenon, such as diffraction, polarization, reflection, or fluorescence. These activities will promote critical thinking and analysis of data.

1This work was supported by the Society of Physics Students summer intern program and by the National Institute of Standards and Technology.

8:12AM F4.00002 ABSTRACT WITHDRAWN —

8:24AM F4.00003 Capacitively-coupled differential position detection in the development of a high-sensitivity torsion balance

CHARLES RACKSON, ALEX WATT, WOO-JOONG KIM, Seattle University, SEATTLE UNIVERSITY TEAM — We report on the development of a high-sensitivity torsion balance using a capacitively-coupled Wheatstone Bridge. The torsion balance will be employed to measure the Casimir Force, with a particular emphasis on the surface patch effects that are ubiquitous on metallic surfaces. We will show that these effects also play a significant role in another class of experiments involving quantum-point contacts between two metal wires.

8:36AM F4.00004 Mapped grid methods for Numerov propagation

CHRISTOPHER MADRID, JUAN BLANDON, Angelo State University, GREGORY PARKER, University of Oklahoma — The Computational toll of solving the Schroedinger equation for certain atomic systems is sometimes prohibitively heavy. We present a grid-mapping method which decreases the number of points needed, and at the same time maintains or increases accuracy for three-atom scattering. By developing a hyperspherical mapping method for Numerov propagation, scattering cross-sections can be found for a large range of energies. This method is useful for systems with very shallow bound states where the mapping will give a large number of data points inside the potential well while decreasing the number of points at a large hyper-radius. The change in grid sizes is controlled by a mapping function that is easily modified. Results are shown for scattering in the HeH2 and HNe2 systems.

8:48AM F4.00005 Simulation of Planetary Formation using Python

JAMES BUFKIN, DAVID BIXLER, Angelo State University — A program to simulate planetary formation was developed in the Python programming language. The program consists of randomly placed and massed bodies surrounding a central massive object in order to approximate a protoplanetary disk. The orbits of these bodies are time-stepped, with accelerations, velocities and new positions calculated in each step. Bodies are allowed to merge if their disks intersect. Numerous parameters (orbital distance, masses, number of particles, etc.) were varied in order to optimize the program. The program uses an iterative difference equation approach to solve the equations of motion using a kinematic model. Conservation of energy and angular momentum are not specifically forced, but conservation of momentum is forced during the merging of bodies. The initial program was created in Visual Python (VPython) but the current intention is to allow for higher particle count and faster processing by utilizing PyOpenCl and PyOpenGl. Current results and progress will be reported.

9:00AM F4.00006 Effects of Turbulence on Cosmic Ray Propagation in Protostar Systems

DONOVAN HERBERT, MARCO FATUZZO, Xavier University, FRED ADAMS, University of Michigan — The magnetic field associated with young stellar objects is expected to have an hour-glass geometry, i.e. the magnetic field lines are pinched together in the equatorial plane surrounding the forming star but are subsumed smoothly onto a background field at large distances. In such a structure, incoming cosmic rays experience both a funneling effect, which acts to magnify the flux impinging on the circumstellar disk, and a magnetic mirroring effect that acts to reduce that flux. These effects nearly cancel out for simple underlying magnetic field structures with respect to the leading order. However, the environments surrounding young stellar objects are expected to be highly turbulent and, thus, act to complicate these effects. We consider here how the presence of magnetic field fluctuations affects the process of magnetic mirroring, and thereby changes the flux of cosmic rays striking the circumstellar disks. These results may have significant consequences for the ionization fraction of the disk, which in turn dictates the efficiency with which disk material can accrete onto the central object.

9:12AM F4.00007 Transverse distortion effects on the Kasteleyn and KDP transition in spin ice

CURTISLEE THORNTON, TRINANJAN DATTA, Georgia Regents University — Geometrically frustrated pyrochlore oxides containing a rare-earth ion and a transition metal ion form a network of corner-sharing tetrahedra. Prominent examples include Dy2Ti2O7 and Ho2Ti2O7. Magnetic frustration in these compounds suppresses the formation of a long-range ordered ground state resulting in an exotic phase of matter called spin ice. Elucidating the role of external perturbations such as pressure and magnetic field is an important step towards understanding the novel KDP and Kasteleyn phase transitions arising in these classical spin ice materials. Utilizing an analytical approach based on the Husimi tree approximation, we investigate the effects of both transverse and uniaxial pressure distortion of the spin ice tetrahedra on both the KDP and Kasteleyn transition in the presence of an external magnetic field. Compared to the uniaxial distortion scenario, we find that including the effects of transverse distortion leads to further suppression of magnetization and heat capacity in both the Kasteleyn and KDP cases.

1GRU Small Grants Program

9:24AM F4.00008 ABSTRACT WITHDRAWN —

9:36AM F4.00009 ABSTRACT WITHDRAWN —

9:48AM F4.00010 Super Atomic Molecular Orbitals of Variably Protonated Symmetric Molecules

TANNER LATTA, KYLE DRAKE, G.P. ZHANG, Indiana State Univ — The molecular structure of symmetric molecules creates conducive conditions for delocalized orbitals. The \( \pi \) bonding delocalizes the valence electrons away from the individual molecules. These delocalized valence electrons allow the symmetric molecules to adapt the characteristics analogous to that of an individual atom, creating Super Atomic Molecular Orbitals, SAMOs. The symmetric molecule is then comparable to that of an individual atom with its regular atomic orbitals. When these symmetric molecules are protonated in any form, there are notable changes in the shapes of the Super Atomic Molecular Orbitals. We use the Density Functional Theory with a grid mesh method to compute the wavefunctions of those SAMOs. Then we examine the Rydberg States of these symmetric molecules through the calculated Eigenstates, and find an important trend in the filling of the SAMOs as well as relationships between variably protonated symmetric molecules. This is potentially very useful to understanding the photovoltaic effect in the fullerene- based solar cells.

1Support by U.S. Department of Energy No DE-FG02-06ER46304
10:00AM F4.00011 Comparative Study of Wavelet Basis Set and Finite-Difference Time-Domain Methods for the Time Propagation of Quantum and Classical Systems, EWA NOWARA, IRWIN GOLDBERG, St. Mary’s University (San Antonio, Texas), BRUCE JOHNSON, Rice University, RICHARD LOMBARDINI, St. Mary’s University (San Antonio, Texas) — An extensive comparison in error accumulation between a grid point method, in particular finite-difference time-domain (FDTD), and a basis set method using Daubechies wavelets is presented in the modeling of electromagnetic (EM) pulses (classical) in inhomogeneous media and quantum (QM) wavepackets interacting with various potentials. It is demonstrated that the density of wavelet functions needed to attain a certain level of accuracy is far less than needed for grid points (FDTD) translating to savings in computational memory and processing. Since neighboring wavelet basis functions have overlapping support, fictitious wavelet projections created by derivative matching (T.A. Driscoll and B. Fornberg) will be used to handle Dirichlet boundary conditions in both the EM and QM cases in order to prevent rapid error growth.

10:12AM F4.00012 Temperature influenced higher order transverse mode in vertical-cavity surface emitting laser, KAI-WEI TU, YU-HENG WU, TSU-CHIANG YEN. None — This research discussed the transverse beam profile of VCSEL with variation of ambient temperature. In this experiment, the transverse mode profile presented a broken pattern when ambient temperature kept decreasing. On the other hand, the optical spectrum analyzer showed that the laser output appeared another frequency when the same approach applied. Therefore, an experiment was conducted by using grating in order to observe the separation of beam. The two separate and unstable spots showed on screen 10 meter away, indicating that the different wavelength really emerged in the output of laser. This result contributes to understanding the relationship between temperature modification and the transverse modes of VCSEL.

10:24AM F4.00013 Dissipative coherence of a superconducting qubit for microwave detection, SATCHER HSIEH, KATER MURCH, Washington University — Recent progress in coherent control and measurement of superconducting qubits has opened avenues to previously inaccessible regimes of metrology. Here we realize a detection scheme for microwave signals. Our scheme utilizes a superconducting transmon qubit coupled to a three-dimensional cavity. When subjected to a weak drive signal near resonance, the qubit equilibrates to a steady state coherence that arises from the competition between driven and dissipative dynamics. By measuring this steady state coherence with quantum state tomography, we map the quantum state to characteristics of the drive signal with shot noise limited resolution. We report detection figures of merit and discuss applications to itinerant microwave fields.

10:36AM F4.00014 Optimized reconstruction methods for imaging squeezed microwave states, ADITYA VENKATRAMANI, DAVID TOYLI, QNL, University of California, Berkeley, SAMUEL BOUTIN, DÉPARTEMENT DE PHYSIQUE, UNIVERSITÉ DE SHERBROOKE, ANDREW EDDINS, QNL, University of California, Berkeley, ALEXANDRE BLAIS, DÉPARTEMENT DE PHYSIQUE, UNIVERSITÉ DE SHERBROOKE, IRFAN SIDDIQI, QNL, University of California, Berkeley — Superconducting parametric amplifiers (paramps) are essential tools for quantum-limited measurement of superconducting qubits. A central feature of these devices is that they can ideally amplify information in one quadrature without adding noise while simultaneously squeezing fluctuations in the orthogonal quadrature. At microwave frequencies, moment-based reconstruction techniques are commonly utilized to image such squeezed states. Motivated by a desire to characterize and improve paramp squeezing performance, we have developed simulations to understand the application of these reconstruction techniques, with a focus on determining their performance at large signal gains where the amplifier output field becomes non-Gaussian. We make comparisons of this analysis to experimental data. We have also developed a complementary imaging method based on deconvolution techniques that is effective for high signal-to-noise ratios. This method benefits from a simple implementation and provides a best estimate for the output field Q function. We discuss experimental implementations of these techniques facilitated by the use of a broadband parametric amplifier.

10:48AM F4.00015 Toroidal moment contributions to the multiferroic acoustic susceptibility, ALEXANDER PRICE, TRINANJAN DATTA, Georgia Regents University — We consider the effects of toroidal moment corrections to the acoustic susceptibility tensor of a material that is simultaneously ferroelectric and a canted antiferromagnet (multiferroic). Using the Landau-Lifshitz equation of motion for the magnetization, the Landau-Khalatnikov relaxation equation for the electric polarization, and an equation of motion for the toroidal moment we analytically discuss experimental implementations of these techniques facilitated by the use of a broadband parametric amplifier.

2:00PM - 2:00PM —
Session H1 APS: Poster Session I (2:00 pm- 5:00 pm) Exhibit Hall C -

H1.00001 UNDERGRADUATE RESEARCH —

H1.00002 Electromagnetic cavities as an analog to chaos regularization of quantum tunneling rates, RACHEL OWEN, Western Washington University, JOHN RODGERS, University of Maryland — For double-well potentials separated by a tunneling barrier, it has been shown theoretically that quantum mechanical tunneling rates vary greatly with well geometry. Chaotic wells exhibit statistically smaller fluctuations in energy level splitting than those characterized by nonchaotic dynamics. This phenomenon (chaos regularization) can be analyzed by examining the statistical spread in symmetric and anti-symmetric wave states produced by tunneling. Exploiting the similarity of transverse electromagnetic waves in large cavities and quantum mechanical wave functions in symmetric double-wells, chaos regularization in electromagnetic structures was studied experimentally and numerically. The resonant frequencies in rectangular (integrable) and bowtie (chaotic) cavities coupled via short sections of cutoff waveguides were simulated using finite element code and measured using a vector network analyzer. The ensemble difference in the measured anti-symmetric and symmetric resonant frequencies squared (analogous to splitting in energy levels) showed remarkably good agreement with theory. In the rectangular cavity we observed quantized resonances spaced across a wide range of frequencies whereas in the bowtie cavity the resonances were grouped randomly close to the theoretical curve.
H1.00003 Quantifying the Relationship between Surface Hydrophobicity and Depletion Layer Thickness, JARED NUTTER, SHANNON PETERSEN, RYAN SAYKO, ADELE POYNOR, Allegheny College — When water comes into contact with an extended hydrophobic surface a uniform region of low density forms, called the depletion layer. This phenomenon has only been experimentally verified on surfaces with contact angles $>100^\circ$, but understanding how the thickness of the depletion layer changes with the hydrophobicity at intermediate contact angles is one of the underlying mechanisms behind several biological systems including colloidal self-assembly, protein folding, and fluid flow across membranes. We aim to quantify this relationship by using self-assembled monolayers of 1-octadecanethiol and 1-mercaptoundecanoic acid on gold to produce surfaces with contact angles between 55$^\circ$ and 107$^\circ$. We then use surface plasmon resonance spectroscopy to determine the thickness of the depletion layer formed for each surface.

H1.00004 Dependence of the Contact Angle on Self-Assembled Monolayer Production Method, BROOKE OLLANDER, RYAN SAYKO, JARED NUTTER, SHANNON PETERSEN, ADELE POYNOR, Allegheny College — When water is forced in contact with a hydrophobic surface, it attempts to reduce its contact area by forming a depletion layer. A depletion layer is defined as a nanometer scale low density region of water layers at the surface. To alter the hydrophobicity of the slide, self-assembled monolayers (SAMs) are formed by utilizing the following organothiol solutions: 1-mercaptoundecanoic acid (hydrophilic) and 1-octadecanethiol (hydrophobic). The contact angle of slides with different organothiol solution exposure times is measured using a homemade goniometer and ImageJ software.

H1.00005 Flow Rate In Microfluidic Pumps As A Function Of Tension and Pump Motor Head Speed, ANTHONY IRWIN, KRISTA MCBRIDE, Belmont University — As the use of microfluidic devices has become more common in recent years the need for standardization within the pump systems has grown. The pumps are ball bearing rotor microfluidic pumps and work off the idea of peristalsis. The rapid contraction and relaxation propagating down a tube or a microfluidic channel. The ball bearings compress the tube (occlusion) and move along part of the tube length forcing fluid to move inside of the tube in the same direction of the ball bearings. When the ball bearing rolls off the area occupied by the microfluidic channel, its walls and ceiling undergo restitution and a pocket of low pressure is briefly formed pulling more of the liquid into the pump system. Before looking to standardize the pump systems it must be known how the tension placed by the pumps bearing heads onto the PDMS inserts channels affect the pumps performance (mainly the flow rate produced). The relationship of the speed at which the bearings on the motor head spin and the flow rate must also be established. This research produced calibration curves for flow rate vs. tension and rpm. These calibration curves allow the devices to be set to optimal user settings by simply varying either the motor head tension or the motor head speed.

1 I would like to acknowledge the help and support of Vanderbilt University SyBBURE program, Christina Marasco, Stacy Sherod, Franck Bloch and Krista McBride.

H1.00006 Photoemission spectroscopy and X-ray diffraction analysis of 3D topological and Kondo insulators, PAVEL SHIBAYEV, Princeton University, HASAN GROUP TEAM — The advantage of studying 3D topological insulators (TIs), compounds that have attracted the attention of many in the condensed matter field, is the ability for their existence at room temperature and no magnetic fields, allowing both for resolving their band structure via angle-resolved photoemission spectroscopy (ARPES) and understanding electric transport and other properties via X-ray diffraction (XRD) and point-contact spectroscopy (PCS). A comprehensive quantitative analysis of Bi$_2$Se$_3$, a 3D TI, was carried out using these methods. The Bi$_2$Se$_3$ crystals were synthesized in-house at Princeton University. A first-principles calculation based on density functional theory, DFT, was performed using the Abinit software. The band structure of the crystal was then resolved via ARPES at the Advanced Light Source in LBNL, resulting in a surprisingly stark and clear single Dirac cone. A large band gap was confirmed, suggesting an increased potential for applications. In contrast, Kondo insulators are found in rare-earth based materials with 5-electron degrees of freedom. Photon energy dependent dispersion relationships and temperature dependence studies were performed on a Kondo candidate CeB$_6$ via ARPES, showing an even number of Dirac cones and a non-TI behavior. Analysis of I-V characteristics through PCS will follow, in addition to characterization via Bruker XRD for both compounds.

1 Research group led by Professor M. Zahid Hasan (Princeton University)

H1.00007 Structure Property Relationships in Imidazole-based Deep Eutectic Mixtures, LOGAN TERHEGGEN, TYLER COSBY, JOSHUA SANGÓRO, Univ of Tennessee, Knoxville — Deep eutectic mixtures of levulinic acid with a systematic series of imidazoles are measured by broadband dielectric spectroscopy, differential scanning calorimetry, and Fourier transform infrared spectroscopy to investigate the impact of steric interactions on charge transport and structural dynamics. An enhancement of dc conductivity is found in each of the imidazoles upon the addition of levulinic acid. However, the extent of increase is dependent upon the alky substitution on the imidazole ring. These results highlight the importance of molecular structure on hydrogen bonding and charge transport in deep eutectic mixtures.

H1.00008 Laser Induced Breakdown Spectroscopy of Metals, ANDRIA PALMER, CARLOS LAWHEAD, LASZLO UJJ, University of West Florida — Laser Induced Breakdown Spectroscopy (LIBS) is a very practical spectroscopy to determine the chemical composition of materials. Recent technical developments resulted in equipment used on the MARS Rover by NASA. It is capable of measuring the emission spectra of laser induced plasma created by energetic laser pulses focused on the sample (rocks, metals, etc.). We have develop a Laser Induced Breakdown Spectroscopy setup and investigated the necessary experimental and methodological challenges needed to make such material identification measurements. 355 and 532 nm laser pulses with 5 ns temporal duration was used to generate micro-plasma from which compositions can be determined based on known elemental and molecular emission intensities and wavelengths. The performance of LIBS depends on several parameters including laser wavelength, pulse energy, pulse duration, time interval of observation, geometrical configuration of collecting optics, and the properties of ambient medium. Spectra recorded from alloys (e.g. US penny coin) and pure metals will be presented.

1 Special thanks for the financial support of the Office of Undergraduate Research of UWF

H1.00009 Differential Conductance Measurements of MgB$_2$/I/Pb Heterojunctions and all-MgB$_2$ Junctions, DAVID CUSICK, Taylor University, MATTHEW ECKHARDT, Indiana Wesleyan University, WENQING DAI, QI LI, Pennsylvania State University, KE CHEN, DANIEL CUNNANE, Temple University, C.G. ZHUANG, None, X.X. XI, Temple University, MICHIO NAITO, Tokyo University of Agriculture and Technology, ROBERTO RAMOS, Indiana Wesleyan University — We present our work characterizing several types of Magnesium Diboride Josephson junctions, including MgB$_2$/I/Pb heterojunctions and all-MgB$_2$ junctions. We will report on the I-V and dI/dV-V data collected at various temperatures using both a cryocooler-based experimental platform between 2 and 20 Kelvin and using a $^3$He probe platform between 0.3 and 1.0 Kelvin. These were both developed by undergraduates in a liberal arts university. Using high-sampling rates with a 24-bit data acquisition card and access to a broad range of temperatures, we track and report energy gap distributions and temperature-dependent features of dI/dV peaks of MgB$_2$, comparing these with theoretical predictions.

1 R.C.R. acknowledges support from National Science Foundation Grant # DMR-1206561.

2 David Cusick is a Taylor University student interning at Indiana Wesleyan University.
H1.00010 Volume phase transition and corresponding change in composition of polymeric microgels. JANNA MINO, CHRISTIAN GUUNDER, KIRIL STRELETZKY, Cleveland State University — Temperature sensitive polysaccharide microgels and parent amphiphilic polymer solution were studied in parallel with Dynamic (DLS) and Static Light Scattering (SLS) spectroscopies. The microgels showed a reversible volume phase transition which was accompanied by a significant change in microgel volume and composition. Coupling DLS and SLS techniques on microgels and polymer solutions allowed to deduce microgel size, structure, molecular weight and a relative change in microgel water content during the volume phase transition. It also allowed comparing controlled dewetting transition in microgels with corresponding phase transition in parent polymer solution. Light scattering findings were tested with SEM imaging.

H1.00011 Synthesis and Characterization of Tetrathiafulvalene Derivatives, MARK BARTOLO, STEPHEN TSUI, Cal State Univ - San Marcos, ERIC REINHEIMER, Rigaku — We synthesize tetrathiafulvalene (TTF) derivative materials in an effort to identify conducting and magnetic properties. The doping of these TTF derivatives include tetracyanoethylene (TCNQ), 7,7,8,8-tetracyanoquinodimethane (TCNQ), and para-dinitrobenzene (pDNB). We examine these TTF containing donor-acceptor complexes through their structural and electronic transport characteristics.

H1.00012 Determination of stimulation focality in heterogeneous head models during transcranial magnetic stimulation (TMS) ERIK LEE, RAVI HADIMANI, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — Transcranial Magnetic Stimulation (TMS) is an increasingly popular tool used by both the scientific and medical community to understand and treat the brain. TMS has the potential to help people with a wide range of diseases such as Parkinson’s, Alzheimer’s, and PTSD, while currently being used to treat people with chronic, drug-resistant depression. Through computer simulations, we are able to see the electric field that TMS induces in anatomical human models, but there is no measure to quantify this electric field in a way that relates to a specific patient undergoing TMS therapy. We propose a way to quantify the focality of the induced electric field in a heterogeneous head model during TMS by relating the surface area of the brain being stimulated to the total volume of the brain being stimulated. This figure would be obtained by conducting finite element analysis (FEA) simulations of TMS therapy on a patient specific head model. Using this figure to assist in TMS therapy will allow clinicians and researchers to more accurately stimulate the desired region of a patient’s brain and be more equipped to do comparative studies on the effects of TMS across different patients.

H1.00013 Electronic Resonance Enhancement in Raman and CARS Spectroscopy: Surface Enhanced Scattering of Highly Fluorescent Molecules CARLOS LAWHEAD, LASZLO UJJ, University of West Florida — Surface enhanced Raman spectroscopy (SERS) is an extremely useful tool in increasing sensitivity of Raman spectroscopy; this technique significantly increases the signal from vibrational resonances which can overcome background fluorescences. Silver nanoparticles coated substrates and the silver nanoparticles in solution were used on a variety of fluorescent molecules in order to overcome sample complexities and measure the vibrational spectra. The possible enhancement of SERS using a coherent Raman (CARS) method was investigated, but enhancement factors due to Surface Enhanced CARS have yet to be verified. The instrument used was developed in the University of West Florida Physics Department utilized the second harmonic of a Nd:YAG laser to provide the excitation wavelength at 532 nm and is capable of both transmission and reflection Raman measurements.

H1.00014 Fluorescence and Bonding of Quantum Dots on DNA Origami Constructs MATTHEW KESSINGER, TIMOTHY CORRIGAN, Concord, DAVID NEFF, MICHAEL NORTON, Marshall University, CONCORD UNIVERSITY COLLABORATION, MARSHALL UNIVERSITY COLLABORATION — Semiconductor quantum dots (QDots) have historically been of interest to the scientific community since their creation for various applications ranging from solar energy to optical labeling. In this study, bioconjugated CdSe/ZnS core/shell QDots were synthesized and functionalized with 3-mercaptopropionic acid using both traditional ligand exchange as well as newly developed in situ functionalization techniques used to increase the quantum yield of the QDots. Their fluorescence and bonding to both gold as well as DNA origami were investigated for use in self assembled DNA constructs. It is believed that controlling the attachment and spacing of these nanoparticles on DNA origami could be used in a variety of optical labeling and sensing applications. Commercially available biotin and streptavidin functionalized quantum dots were also examined, and subject to the same experiments with gold nanoparticles as the MPA functionalized QDots.

H1.00015 Analysis of layer-by-layer thin-film oxide growth using RHEED and Atomic Force Microscopy ELI ADLER, M.C. SULLIVAN, Ithaca College, Department of Physics and Astronomy, ARACELI GUTIERREZ-LLORENTE, H. JORESS, A. WOLL, J.D. BROCK, Cornell High Energy Synchrotron Source, Cornell University — Reflection high energy electron diffraction (RHEED) is commonly used as an in situ analysis tool for layer-by-layer thin-film growth. Atomic force microscopy is an equally common ex situ tool for analysis of the film surface, providing visual evidence of the surface morphology. During growth, the RHEED intensity oscillates as the film surface changes in roughness. It is often assumed that the maxima of the RHEED oscillations signify a complete layer, however, the oscillations in oxide systems can be misleading. Thus, using only the RHEED maxima is insufficient. X-ray reflectivity can also be used to analyze growth, as the intensity oscillates in phase with the smoothness of the surface. Using x-ray reflectivity to determine the thin film layer deposition, we grew three films where the x-ray and RHEED oscillations were nearly exactly out of phase and halted deposition at different points in the growth. Pre-growth and post-growth AFM images emphasize the fact that the maxima in RHEED are not a justification for determining layer completion.

This work was funded by the Carver Charitable Trust.

H1.00016 Digital imaging of brain stimulation therapy with a custom made patient specific head model. Using this figure to assist in TMS therapy will allow clinicians and researchers to more accurately stimulate the desired region of a patient’s brain and be more equipped to do comparative studies on the effects of TMS across different patients.

This work was funded by the Carver Charitable Trust.

H1.00017 Enhanced Scattering of Highly Fluorescent Molecules. This work was supported by NIGMS MARC Grant GM-08807

**1** Work conducted at the Cornell High Energy Synchrotron Source (CHESS) supported by NSF awards DMR-1332208 and DMR-0936384 and the Cornell Center for Materials Research Shared Facilities are supported through DMR-1120296.
H1.00016 Developing a protocol for creating microfluidic devices with a 3D printer, PDMS, and glass. ROBYN COLLETTE, ERIC NOVAK, KATHRYN SHIRK, Shippensburg University of Pennsylvania — Microfluidics research requires the design and fabrication of devices that have the ability to manipulate small volumes of fluid, typically ranging from microliters to picoliters. These devices are used for a wide range of applications including the assembly of materials and testing of biological samples. Many methods have been previously developed to create microfluidic devices, including traditional nanolithography techniques. However, these traditional techniques are cost-prohibitive for many small-scale laboratories. This research explores a relatively low-cost technique using a 3D printed master, which is used as a template for the fabrication of polydimethylsiloxane (PDMS) microfluidic devices. The masters are designed using computer aided design (CAD) software and can be printed and modified relatively quickly. We have developed a protocol for creating simple microfluidic devices using a 3D printer and PDMS adhered to glass. This relatively simple and low-cost technique can now be scaled to more complicated device designs and applications.

H1.00017 Highly Porous Regenerated Cellulose Fiber Mats via the Co-Forcespinning of Cellulose Acetate for Separator Applications. ALEJANDRO CASTILLO, YUANBING MAO, University of Texas Pan-American Chemistry — Improvements in battery technology are necessary for the transition away from a fossil fuel based economy. An important bottle-neck in battery efficiency is the quality of the separator, which separates the cathode and anode to prevent a short-circuit while still allowing the ions in solution to flow as close to unobstructed as possible. In this work, solutions of cellulose acetate, polyvinylidifluorine (pvdf), and polyvinylpyrrolidone (pvp) dissolved in a 2:1 v/v acetone/dimethylacetamide solvent mixture were Forcespun to create nonwoven fiber mats of nanoscale diameter. These mats were then soaked in a NaOH solution so as to both strip the pvp from the fiber as well as regenerate cellulose from its acetate derivative for the purpose of creating high surface area, nonporous, hydrophile, and ionically conductive cellulose/pvdf nonwoven mats for the purposes of testing their suitability as battery separators.


H1.00019 Temperature dependence measurements for Cadmium Telluride (CdTe) solar cells. FERNANDA DUARTE, WEINING WANG, Department of Physics, Seton Hall University — Traditional silicon (Si)-based solar cells have been studied broadly and have already reached their maximum efficiency. However, their cost is relatively high, preventing them from being widely used. Unlike Si-based solar cells, Cadmium Telluride (CdTe) solar cells are considerably cheap, yet the record efficiency is still lower than that of traditional silicon-based solar cells. More studies are needed to understand and improve the efficiency of CdTe solar cells. In this work, we report our studies of the temperature dependence of CdTe solar cell parameters using the temperature-varying apparatus designed and built by us in-house. This temperature-varying apparatus will be incorporated with a solar cell testing station in order to measure the solar cell parameters while varying the temperature. The solar cell parameters will be measured at different temperatures (within a 100 K temperature range), and the effects of temperature on the open-circuit voltage, short-circuit current and efficiency of the solar cells will be reported. These results allow us to further understand the physics of CdTe solar cells and shine light on how to improve the efficiency of CdTe solar cells.

H1.00020 Systematic Studies of Phase Transitions in Thermo-Responsive Polymers Used in Targeted Drug Delivery. JANAE BRADLEY, Univ of Missouri - Columbia, DANIEL DENMARK, SARATH WITANACHCHI, University of South Florida — Thermo-responsive polymers such as poly-N-isopropylacrylamide (PNIPAM) can undergo reversible phase transitions in aqueous solutions under varying temperature. They are ideal candidates for the polymer shell of a targeted drug delivery capsule. Concentration and pH can affect the lower critical solution temperature (LCST) of the PNIPAM polymer and its physical properties. In this work, a systematic study of the factors that influence the LCST of the PNIPAM polymer mixed with Fe304 nanoparticles (MNPs) during thermal bath heating is presented. A series of PNIPAM solutions with various concentrations of PNIPAM with MNPs were prepared and characterized using scanning electron microscopy. In-situ transmission measurements were used to determine the LCST of PNIPAM concentrations. A systematic decrease in the LCST was observed as the concentration of PNIPAM was increased. In addition, the impact of pH on the LCST of PNIPAM was examined by increasing the basicity of the PNIPAM solutions by adding adjusted KOH pellets. An increase in the thermal stability of the LCST was observed when the basicity of the PNIPAM solution was increased. The results from this study provide valuable information towards using these thermo-responsive polymers in targeted drug delivery.

H1.00021 Superconducting Resonators: Protecting Schrodinger’s Cat. JOSE CHAVEZ, PHILIP MAUSKOFF, Arizona State University — Over the past decade, superconducting resonators have played a fundamental role in various novel astronomical detectors and quantum information processors. One example is the microwave kinetic inductance detector that is able to resolve photon energies by measuring shifts in its resonant frequency. Similar resonators have been integrated with superconducting qubits, specifically the transmon, to substantially improve quantum coherence times. The purpose of this investigation is to survey various resonant structures within the requirements of circuit quantum electrodynamics giving special attention to quality factors, TLS noise, and quasi-particle generation. Specifically, planar and three dimensional cavities with varying geometries and materials are characterized - primarily focusing on NbTiN and Nb.

H1.00022 Capacitance measurements of defects in solar cells: checking the model assumptions. JUSTIN DAVIS, THADDEUS COX, JENNIFER HEATH, Linfield College — Capacitance measurements of solar cells are able to detect minute changes in charge in the material. For that reason, capacitance is used in many methods to electrically characterize defects in the solar cell. Standard interpretations of capacitance rely on many assumptions, which, if wrong can skew the results. We explore possible alternate explanations for capacitance transitions, which may not be linked directly to defects, such as a non-ideal back contact, and series resistance.
H1.00023 Does a simple lattice protein exhibit self-organized criticality? — DANA GIBBON, ALISSA RUNYON, ARUN BAJRACHARYA, JOELLE MURRAY, Linfield College — There are many unanswered questions when it comes to protein folding. These questions are interesting because the tertiary structure of proteins determines its functionality in living organisms. How do proteins consistently reach their final tertiary structure from the primary sequence of amino acids? What explains the complexity of tertiary structures? Our research uses a simple hydrophobic-polar lattice-bound computational model to investigate self-organized criticality as a possible mechanism for generating complexity in protein folding and protein tertiary structures.

H1.00024 Development of TiO2-xwt%InVO4 Photocatalytic Nano-composites for Ambient Light Assisted Water Detoxification — SESA SRINIVASAN, Florida Polytechnic University, College of Innovation and Technology, JEREMIAH WILSON, Tuskegee University, Department of Physics, ERIC VICKERS, RYAN INTELLIGA, Florida Polytechnic University, College of Engineering — We have developed nano-composites of TiO2-xwt%InVO4 for environmental and biomedical research applications. TiO2 is commonly used as catalyst that utilizes the UV portion of the sun light spectrum to induce photo-oxidation and photo-reduction processes. We hypothesized that the combination of InVO4 and TiO2 will result in a material that will catalyze organic contaminants through photo-oxidation under visible light. We combined TiO2 with 2.4,6,8,10wt% of InVO4 via wet ball milling process. We have compared the various concentrations of InVO4 on TiO2 matrix by SEM, BET surface area analyzer, FTIR, XRD, and photodegradation of the organic contaminant Methyl Orange. After characterization we found that 4wt% InVO4+TiO2 mixture displayed the most promising characteristics for photo-oxidation under visible light. From the BET surface area analysis it showed the largest surface area out of the prior mentioned TiO2 = Xwt%InVO4 mixtures and a degradation amount equivalent to 50% of Methyl Orange contaminant over 7 hours under visible light. In conclusion, TiO2-xwt%InVO4 displayed evidence of photo-oxidation under visible light conditions. 1Authors would like to acknowledge the support from Sigma Pi Sigma and Society of Physics Students. National Science Foundation and Florida Energy Systems Consortium are gratefully acknowledged for the research and education grants.

H1.00025 Toward a Rb MOT for Undergrad Research and Advanced labs at Bridgewater State University — EDWARD DEVENEY, Bridgewater State University — The seminal paper for the undergraduate MOT appeared in AJP (63 (4), 1995) by C. Wieman, G. Flowers and S. Gilbert; ‘Inexpensive laser cooling and trapping experiment for undergraduate laboratories’. They wrote: “Because of this visual appeal and the current research excitement in this area, we felt that it was highly desirable to develop an atom trapping apparatus that could be incorporated into the undergraduate laboratory classes.” From our observations, it seems that while there are extraordinary examples of MOTs thriving in a few undergraduate labs, MOT experiments have yet to be widely incorporated into the undergraduate curriculum—likely because they are, in fact, not trivial to make. With the benefit of 20 years evolution since this 1st undergraduate MOT paper, we report the progress at BSU of constructing a 85Rb MOT that incorporates significant simplifications and straightforward techniques that include: using a single ECDL laser for both trapping and re-pumping (using an EOM to add FM sidebands) and combining a purchased stabilized HeNe with the ECDL in a Fabry-Perot Interferometer to correct and sufficiently stabilize the ECDL for trapping. When completed we will revisit the do-ability for the undergraduate research/advanced lab. The BSU MOT was planned with and is currently being built with the help and guidance of David DeMille and his research group at Yale University [including J. Barry Thesis, Yale].

H1.00026 Optical V-Band Observations of Active Galactic Nuclei — TAYLOR HUTCHISON, RAINA MUSSO, FRANCIS MACINNIS, MARK BOTTORFF, Western University — Students at Western University participated in an international observing campaign to study twelve active galactic nuclei (AGN). As part of this project, the students measured optical V-band light variations of four targets within the range of the Western University Fountainwood Observatory research telescope. Target images and a sample light curve of one target (NGC 5548) are presented.

H1.00027 ABSTRACT WITHDRAWN —

H1.00028 ABSTRACT WITHDRAWN —

H1.00029 ABSTRACT WITHDRAWN —

H1.00030 Origins of Nonlinearity in Superconductive Passive Circuits — SEAN HAMILTON, Grand Valley State University, STEPHEN REMILLARD, Hope College — The distinct origins of even and odd order nonlinear behavior in type II cuprate superconductors have yet to be fully elucidated. Microwave intermodulation distortion (IMD) was examined in a YBCO superconducting thin-film hairpin resonator at 840 MHz. Measurements of the temperature dependence of IMD near Tc support the view that the nonlinear Meissner effect is responsible for the occurrence of both 2nd and 3rd order IMD tones near Tc as well as their suppression in an applied magnetic field. However, at lower reduced temperatures (T/ Tc less than 0.95), where the influence of the nonlinear Meissner effect is less pronounced, 3rd order IMD is unaffected by a static magnetic field, while 2nd order IMD decays exponentially after a static magnetic field is removed with a temperature dependent time constant. It is apparent that the magnetically induced remnant vortex state contributes to the 2nd order nonlinearity, but not to the 3rd order nonlinearity, and that this effect is diminished close to Tc due to degradation of the remnant vortex state. 1This research was funded by the National Science Foundation under grant number DMR-1206149.

H1.00031 Measuring and Modeling the Plasma Temperature and Density in WIRX — MICHAEL MORKEN, DARREN CRAIG, Wheaton College (IL) — We develop a theoretical model and experimental techniques to provide a better picture of how the adjustable parameters such as the current, and electrode geometry affect the temperature and density of WIRX plasmas. Our model predicts the plasma temperature and density by balancing the Ohmic heating with convective losses. The Ohmic heating is measured directly as the product of the voltage drop between the electrodes and the plasma current. Temperature and density are measured independently using spectroscopic methods. Stark broadening of the H-β line is used to measure density. To measure the electron temperature of the plasma the line ratios of various hydrogen transitions were compared with the predictions of the Boltzmann thermal equilibrium model and the coronal equilibrium model. Preliminary experimental results are consistent with the plasma parameters predicted by our model. This work will be used to inform future modifications to the experiment with the intent of producing higher temperatures in WIRX plasma, making magnetic reconnection more probable. Work supported by US DOE.
H1.00032 Two Dimensional Intermodulation Distortion Scanning of Superconducting Filter Resonators, MICHAEL BISCHAK, STEPHEN REMILLARD, Hope College — Nonlinear superconducting conductivity produces distortion that has usually been measured globally across the entire sample. In order to fully understand the origin of nonlinearity, local methods must be used to examine specific points in the sample. The nonlinear Ohm’s law, $V = IZ(I)$ includes the current dependence in the impedance. The method in this work raster scans a magnetic loop probe across a sample. In order to address limited resolution, we reduced the size of the magnetic loop probe. Using the electromagnetic field solver, sonnet, two dimensional current simulations of superconducting microwave filters composed of Ti2Ba2CaCu2O8 or of YBa2Cu3O7 reveal microwave current which is bunched up at the corners and sides of the sample. Two dimensional images of third order intermodulation distortion made with the magnetic probe at the same corners and edges reveal elevated distortion in the same places. Using the magnetic probe, third order intermodulation was seen to come from the same corners and edges where the current is bunched. This research was funded by the National Science Foundation under grant number DMR-1260149.

H1.00033 Raman spectroscopy of single-walled carbon nanotubes of different lengths exposed to microwave radiation, P. BHATNAGAR, Angelo State Univ, S. FERGUSON, University of Texas - Dallas, G. SESTRIC, I. WRIGHT, S. WILLIAMS, Angelo State University — Carbon nanotubes have been observed to emit ultraviolet, visible, and infrared radiation when exposed to microwave fields. Although there is considerable controversy concerning the mechanism responsible for the emissions, the results of recently-performed experiments suggest that the emissions may be the result of field emission-induced luminescence. We have performed experiments in which both short (0.5 µm - 2 µm) and long (5 µm - 30 µm) single and double-walled carbon nanotubes were exposed to 2.46 GHz microwaves at a pressure of approximately $10^{-6}$ torr. A comparison of the spectra of the radiation emitted from the nanotubes suggests that the longer nanotubes emitted radiation of greater intensity than the shorter nanotubes, which is consistent with field emission-induced luminescence. Moreover, structural modification of the carbon nanotubes due to microwave irradiation has been studied using the Raman spectroscopy G-band and D-band intensities, which suggests that microwave irradiation at relatively low pressures results in a decrease in nanotube defects, especially in the case of the long nanotube samples.

H1.00034 Study of the angular distributions of X-rays emitted following L3 ionization of gold atoms by electron impact, I. WRIGHT, G. SESTRIC, S. FERGUSON, S. WILLIAMS, Angelo State University — Theoretical work suggests that when an atomic inner-shell vacancy with total angular momentum $j$ greater than 1/2 is created by interaction with a photon or charged particle the vacancy will be aligned due to the magnetic sublevels of the ion having nonstatistical populations. The experiments we performed, testing this theory, involved measurements of the angular distributions of gold L$_{\alpha}$, L$_{\beta}$, and L$_{\gamma}$ X-rays at forward angles in the range 0 degrees to 25 degrees emitted after being bombarded with 15 keV electrons. After corrections for absorption of the characteristic X-rays within the gold target, our results suggest that the angular distributions of the L$_{\alpha}$, L$_{\beta}$, and L$_{\gamma}$ X-rays are essentially isotropic, as no angular dependence was observed in our data outside of experimental uncertainties. However, the results of our experiments suggest that the angular distribution of the gold L$_{\gamma}$ X-rays may be weakly anisotropic.

H1.00035 A Study of Two Dimensional Electron Gas Using 2D Fourier Transform Spectroscopy¹, CARL MCINTYRE, Colorado Mesa University, JAGANNATH PAUL, DENIS KARAISKAJ, University of South Florida — The dephasing of FES was measured in a symmetrically modulation doped 12 nm single quantum well GaAs/AIGaAs two dimensional electron gas system using time integrated four wave mixing (TIFWM) and a two dimensional Fourier transform spectroscopy (2DFTS). At high in-well carrier densities of $\sim 4 \times 10^{11}$ cm$^{-2}$, many body effects that are prevalent and measurable with non-linear optical spectroscopy. Effects of exciton-exciton and exciton-phonon scattering events, exciton populations, and biexciton formation are detectable at these carrier concentrations. Homogeneous linewidths obtained from ZDF and TIFWM yield a zero Kelvin linewidth of 1.42 meV and an acoustic phonon scattering coefficient of 156 µ eV/K. These observations indicate a rapid increase in homogeneous linewidth with increased temperature.

¹NSF REU grant # DMR-1263066: REU Site in Applied Physics at USF

H1.00036 Analytically Evaluating Sums in Quantum and Statistical Physics Using Integral Transforms, JOHN VASTOLA, University of Central Florida — Evaluating sums analytically is a problem that is easy to pose and to give approximate solutions to, but that is difficult to exactly solve in general. Many results that are known are byproducts of Fourier analysis, which requires guessing that a series corresponds to a function. A more systematic method of evaluating sums using integral transforms is proposed which can reproduce many results obtained using other techniques. In particular, representing polynomials as Laplace transforms gives some nontrivial exact results. Some applications of the method are demonstrated, and extensions of the method using integral representations of frequently appearing functions are suggested. One useful representation of the gamma function is supplied, and used to provide both well-known and more obscure results. Interestingly, the application of this integral representation to evaluating sums suggests the introduction of a novel integral transform, which itself can be used to evaluate sums. Some of the transform’s properties are given, and its usefulness in other areas (like solving differential equations) is touched upon. Some physical problems involving the partition functions of statistical mechanics, and some infinite sums appearing in quantum mechanics, are considered.

H1.00037 In-air Rutherford Backscattering and Particle Induced X-ray Emission for Biophysics and Material Science Research, JAMES BECKER, None — Rutherford Backscattering (RBS) and Particle Induced X-ray Emission (PIXE) are methods of nondestructive analysis of elemental composition. Rebounding particles or emitted x-rays can be “collected” and then analyzed to reveal the number ratio of the elements in a sample. Due to the nondestructive feature of these processes, RBS and PIXE are useful in many diverse fields of study such as archaeology, art, and biology; however, these experiments usually require large, expensive particle accelerators and detectors. Instead, I am attempting to use a radioactive source, photodiodes, and computer software to perform the same methods at a fraction of the cost. I am exploring cost, time, and resolution benefits and losses of my approach versus the traditional accelerator-based approach.

H1.00038 Relativistic Quantum Mechanical Calculations on Alkali Atoms and Dimers from Cesium to Ununennium, CHUKVUNOSO ARINZE, WALTER ERMLER, University of Texas at San Antonio — Ab initio calculations using relativistic effective core potentials, and intermediate angular momentum coupling of electrons are carried out on the alkali metal atoms, and dimers from cesium through ununennium. A spin-orbit configuration interaction (SOCl) method is employed that includes a spin-orbit coupling operator and a relativistic effective core potential in the Schrodinger Hamiltonian operator. The energy levels from these calculation are found to reproduce the positions of the experimental spectral lines and predict lines not heretofore observed for both of these atoms.
H1.00039 Re-Examining Gravitational Tunneling Radiation when taking into account Quantum Gravity Effects

JOHN VALENTINE, TREVOR PRESCOTT, GARDO BLADO, Houston Baptist Univ — Although shown to theoretically exist, Hawking Radiation has yet to be detected. The paper entitled “Gravitational Tunneling Radiation” [1] by Mario Rabinowitz proposed a possible explanation by considering the gravitational tunneling effects in the presence of other bodies in the vicinity of the black hole. Rabinowitz showed that the power radiated (through gravitational radiation) by a black hole, $P_{BH}$, is related to the power generated by Hawking Radiation, $P_{SH}$ by $\frac{P_{SH}}{P_{BH}} \sim P_{SH}$ where $T$ is the gravitational tunneling probability. The presence of other bodies lowers the gravitational barrier which in turn increases the gravitational tunneling probability thereby decreasing the Hawking radiation, $P_{SH}$. In this paper, we examine the modification of $T$ in the presence of quantum gravity effects by incorporating the Generalized Uncertainty Principle.


H1.00040 A Novel Method of Line Detection using Image Integration Method

DANIEL LIN, BO SUN, Oregon State University — We developed a novel line detection algorithm based on image integration method. Hough Transformation uses spatial image gradient method to detect lines on an image. This is problematic because if the image has a region of high noise intensity, the gradient would point towards the noisy region. Denoising the noisy image requires an application of sophisticated noise reduction algorithm which increases computation complexity. Our algorithm can remedy this problem by averaging the pixels around the image region of interest. We were able to detect collagen fiber lines on an image produced by confocal microscope.

H1.00041 Exploring the Power Output of Small Wind Turbines in Urban San Antonio, Texas

JOSE CASILLAS, STEPHANIE SPERDUTI, ROSA CARDENAS, The University of the Incarnate Word — The means of transporting power from a centralized power plant by transmission lines has several disadvantages. Electricity transmission and distribution networks are costly, require long planning processes and are unsightly to residents. These networks are also susceptible to natural disasters creating massive disruptions to consumers. For these reasons distributed power sources such as solar panels and small wind turbines are becoming a more desirable and viable means of energy production. We report on the status of a study to determine the maximum output power of small wind turbines in urban San Antonio, Texas. Wind speed data along with power measurements from small wind turbines in urban San Antonio will be reported.

H1.00042 Analyzing Hurricane Sandy

ANGELYN CONVERTINO, STEPHAN MEYER, BECCA EDWARDS, Southwestern University — Post-tropical Storm Sandy underwent extratropical transition shortly before making landfall in southern New Jersey October 29 2012. Data from this system was compared with data from Hurricane Ike (2008) which represents a classic hurricane with a clear eye wall and symmetry after landfall. Storm Sandy collided with a low pressure system coming in from the north as the hurricane made landfall on the US East coast. This contributed to Storm Sandy acting as a non-typical hurricane when it made landfall. Time histories of wind speed and wind direction were generated from data provided by Texas Tech’s StickNet probes for both storms. The NOAA Weather and Climate program were used to generate radar loops of reflectivity during the landfall for both storms; these loops were compared with time histories for both Ike and Sandy to identify a relationship between time series data and storm-scale features identified on radar.

H1.00043 Using budget-friendly methods to analyze sport specific movements

LINDSAY JACKSON, SARAH WILLIAMS, DAVON FERRARA, Belmont University — When breaking down the physics behind sport specific movements, athletes, usually professional, are often assessed in multimillion-dollar laboratories and facilities. Budget-friendly methods, such as video analysis using low-cost cameras, iPhone sensors, or inexpensive force sensors can make this process more accessible to amateur athletes, which in-turn can give insight into injury mechanisms. Here we present a comparison of two methods of determining the forces experienced by a cheerleader during co-education stunting and soccer goalies while side-diving. For the cheerleader, accelerometer measurements were taken by an iPhone 5 and compared to video analysis. The measurements done on the soccer players were taken using FlexiForce force sensors and again compared to video analysis. While these budget-friendly methods could use some refining, they show promise for producing usable measurements for possibly increasing our understanding of injury in amateur players. Furthermore, low-cost physics experiments with sports can foster an active learning environment for students with minimum physics and mathematical background.

H1.00044 Porphyrin Induced Laser Deactivation of Trypsinogen-Trypsin Conversion

JOANNA PERIDO, Undergraduate Researcher, LORENZO BRANCALEON, Professor, PI — Pancreatitis is caused by the inflammation of the pancreas, where the digestive enzyme trypsin is activated from the precursor enzyme trypsinogen while still in the pancreas. The presence of trypsin in the pancreas causes auto-activation of trypsinogen, resulting in greater inflammation and auto-digestion of the pancreas. In severe cases, this cascade effect can lead to organ failure, diabetes, and pancreatic cancer. Our hypothesis is that if trypsinogen is prevented from auto-activating into trypsin, then this cascade can be stopped. We propose to do this by inducing conformational changes in trypsinogen when bound to a photoactive porphyrin dye. Porphyrins are comprised of four linked heterocyclic groups forming a flat ring, and bind well with proteins such as trypsinogen. In this study we used spectroscopic techniques to probe the binding of meso-tetrakis (4-sulfonatophenyl) porphyrin (TSP2) to trypsinogen in vitro, as a preliminary step to then prompt and characterize conformational changes of trypsinogen through irradiation. If conformational changes are detected the trypsinogen will be tested for trypsin inactivation. This investigation may provide promising initial results to the possible use of porphyrins as an inhibitor of the self-activation of trypsinogen into trypsin, and a potential inhibitor of pancreatitis.

H1.00045 Synthesizing new, high-temperature superconductors

CLAIRE WEAVER, Hofstra University, MEIGAN ARONSON, Brookhaven National Laboratory and Stony Brook University — Currently, there is no accepted theory behind type-II, high-temperature superconductors, but there is a distinct relationship between anti-ferromagnetism and superconductivity. Our research focuses on synthesizing new superconducting materials by observing the link between atomic structure and magnetic moments of anti-ferromagnetic compounds and attempting to reproduce the molecular physics of these known materials in new compounds. Consider the square-planar arrangement of the transition metal Fe in the Fe-pnictide superconductors of the ZrCuSiAs “11 11” and the ThCr$_2$Si$_2$ “122” structure types. We believe that the physics behind this superconductor, where Fe has d$^5$ valence electrons, contributes to the superconducting state, not the presence of Fe itself. For this reason, we are synthesizing materials containing neighboring transition metals, like Mn and Co, combined with other elements in similar crystal lattice arrangements, having ionization properties that hopefully impose d$^6$ valence electrons on the transition metals.

1This project was supported in part by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Science Undergraduate Laboratory Internships Program (SULI)
measure the vector correlations in the products of photo-initiated reactions. Simulations of different DC sliced imaging conditions using Simion 8.1 program — Vector correlations between parent molecule transition dipole moments, photofragment velocity angular momentum vectors, can provide valuable information, COLIN J. WALLACE, WEI WEI, SIMON W. NORTH, Texas A&M – College Station

the way for next-generation spectroscopies to investigate molecular structure. unqiue polarized light fields to study strong field ionization (SFI), which is the complementary process to HHG. Using a velocity map imaging photoelectron tabletop source of extreme ultraviolet (EUV) light, can be now extended to from linear to circular polarization. Here we present the first experiments using these Hua University — Recent experiments using two-color circularly polarized laser fields have demonstrated that high-harmonic generation (HHG), a versatile Solid State Institute and Physics Department, Technion and Department of Physics and Optical Engineering, Ort Braude College, XIAO-MIN TONG, Division

versus the phase step to fourth-order in the field. We show that the third-order polarization of the sample is sensitive to the single-photon transitions of IR-125. The sharp phase-step causes enhanced absorption of the high frequency components and a sharp narrow-band emission of low frequency. We calculate the frequency-dispersed nonlinear spectrum off-diagonal features into the stimulated emission spectra that are sensitive to the single-photon transitions of IR-125. The sharp phase-step introduces asymmetric diagonal and density functional theory calculations. Theoretical calculations show that only one adsorption configuration of terminal-bond CO (T-CO) is stable and that the bridge-bond CO is unstable. All the abundantly observed STM features due to CO adsorption can be identified as differently configured T-COs. The initial sticking probability of CO molecules on Si(001) at RT is estimated to be as small as ~ 1 x 10^-4 monolayer/Langmuir, which is significantly increased at high-temperature adsorption experiments implying a finite activation barrier for adsorption. Thermal annealing at 900 K for 5 min results in the dissociation of the adsorbed CO molecules with the probability of 60-70% instead of desorption, indicating both a strong chemisorption state and an activated dissociation process. The unique adsorption state with a large binding energy, a tiny sticking probability, and a finite adsorption barrier is in stark contrast with the previous low-temperature (below 100 K) observations of a weak binding, a high sticking probability, and a barrierless adsorption. We speculate that the low-temperature results might be a signature of a physisorption feature in the condensed phase.

Multidimensional stimulated emission with a single phase-shaped pulse, ARKAPRABHA KONAR, RACHEL GLENN, VADIM. V. LOZOVOY, MARCOS DANTUS, Michigan State University — Two-dimensional optical signals from a single-pulse excitation are experimentally and theoretically investigated as a function of a sharp spectral phase-step. The phase-step introduces asymmetric diagonal and off-diagonal features into the stimulated emission spectra that are sensitive to the single-photon transitions of IR-125. The sharp phase-step causes enhanced absorption of the high frequency components and a sharp narrow-band emission of low frequency. We calculate the frequency-dispersed nonlinear spectrum versus the phase step to fourth-order in the field. We show that the third-order polarization of the sample is sensitive to phase changes in the excitation spectrum and it is responsible for the observed narrowband feature in the experiments.

Spectroscopic Studies of Imidizolium and Pyridinium Based Ionic Liquids, RYAN BOOTH, JAIME STEARNS, Air Force Research Laboratory — Ionic liquids (ILs) have been shown to be extremely useful in areas ranging from chemical synthesis to energetic materials. Furthermore, ILs are thought to be a potential replacement for hydrazine as satellite propellants because a subset are hypergolic with nitric acid. While ILs are useful, however, there is a lack of understanding of the microscopic origins for their macroscopic properties (e.g. viscosity). An example of this is that [emim]^+][tf2N^-] is three times less viscous than its methylated counterpart [emim]^+][tf2N^-] and there is some discord regarding the reason. We have investigated the molecular properties of such IL pairs using UV and IR spectroscopy in the gas phase on both imidazolium and pyridinium-based ([pyr]^+][tf2N^-]) ILs. UV data show that the photophysics of [emim]^+][tf2N^-] is different than [emim]^+][tf2N^-] and there is a lack of evidence for the existence of a charge transfer (CT) state (as was seen in [emim]^+][tf2N^-]). Preliminary UV spectra for the [pyr]^+][tf2N^-] ILs show at least two distinct peaks in the region from 208-270 nm, which are tentatively established as CT states between the anion and cation. IR spectra deliver structural information for both sets of ILs and should provide insight into the correlation between microscopic and macroscopic properties.

Strong field ionization tomography with two-color circularly polarized femtosecond laser fields, MAITHREYI GOPALAKRISHNAN, CHRIS MANCUSO, DANIEL HICKSTEIN, PATRICK GRYCHTOL, RONNY KNUT, FRANKLIN DOLLAR, DIMITRY ZUSIN, CHRISTIAN GENTRY, EMRAH TURGUT, JENNIFER ELLIS, HENRY KAPTEYN, MARGARET MURNANE, JILA and Department of Physics, University of Colorado Boulder and NIST, OFFER KFIR, OREN COHEN, Solid State Institute and Physics Department, Technion, AVNER FLEISCHER, Solid State Institute and Physics Department, Technion and Department of Physics and Optical Engineering, Ort Braude College, XIAO-MIN TONG, Division of Material Science, Faculty of Pure and Applied Science, University of Tsukuba, MING-CHANG CHEN, Institute of Photonics Technologies, National Tsing Hua University — Recent experiments using two-color circularly polarized laser fields have demonstrated that high-harmonic generation (HHG), a versatile tabletop source of extreme ultraviolet (EUV) light, can be now extended to extend from linear to circular polarization. Here we present the first experiments using these uniquely polarized light fields to study strong field ionization (SFI), which is the complementary process to HHG. Using a velocity map imaging photoelectron spectroscopy and tomographic reconstruction techniques, we identify low-energy structures in the 3D photoelectron angular distributions that correspond to the rescattering of electrons with the ion. The observation of rescattering structures confirms the proposed explanation for HHG under two-color fields and paves the way for next-generation spectroscopies to investigate molecular structure.

DC Sliced Ion Imaging Study of Photodissociation Dynamics: Comparison between Conditions of Simulations and Experiments, COLIN J. WALLACE, WEI WEI, SIMON W. NORTH, Texas A&M — College Station — Vector correlations between parent molecule transition dipole moments, photofragment velocity angular momentum vectors, can provide valuable information about excited states symmetry, non-adiabatic dynamics and the forces and torques operating during fragmentation. Accurate molecular descriptions of photo-induced chemical reactions require detailed and experimental results which measure vector properties. Sliced velocity mapped ion imaging is a powerful method to measure the vector correlations in the products of photo-initiated reactions. Simulations of different DC sliced imaging conditions using Simion 8.1 program have performed to assist in the interpretation of experimental data. We have also recently re-assembled and modified a ion imaging apparatus and collected ion images of several photodissociation systems. Comparisons between these simulations and our experimental images will be presented. We are optimistic that our newly developed mathematical methods of extracting vector correlation information from sliced imaging anisotropy, will permit detailed study of a variety of benchmark dynamical systems.

ABSTRACT WITHDRAWN —
H1.00054 Applications of laser streaking at X-ray free electron lasers. GILLES DOUMY, Argonne Natl Lab, CHRIS ROEDIG, LOU DIMAUCO, Ohio State University, ADRIAN CAVALIERI, IVANKA GRIGIRAS, CFEL/University Hambourg, MICHAEL MEYER, XFEL, JOHN COSTELLO, Dublin University, WOLFRAM HELML, ANDREAS MAIER, REINHARD KIENBERGER, MPQ Garching, MARKUS ILLCHEN, NICK HARTMANN, RYAN COFFEE, CHRISTOPH BOSTEDT, SLAC — X-ray radiation has been long used to address selectively atoms and to yield structural information with atomic precision. The advent of X-ray Free Electron Lasers (XFEL) is revolutionizing the field of time resolved x-ray techniques. The availability of tunable pulses ranging from the soft to the hard x-ray region, and lasting only few tens of femtoseconds, or perhaps less, is enabling access to unprecedented temporal resolution. However, knowledge of the temporal properties of the x-ray pulses is poor, and synchronization to external sources introduces a timing jitter that dominates the fast dynamics and needs to be corrected for every shot. Using laser streaking techniques developed by the attosecond community, one can measure the pulse duration, and possibly improve the temporal resolution of pump probe experiments where electrons are collected to follow the processes by use of a self-referencing measurement. Illustration is presented following Auger decay in the time domain.

H1.00055 Ion Transport and Local Structural Dynamics in Analogous Quaternary Ammonium and Phosphonium-Based Room Temperature Ionic Liquids. ADAM HOLT, University of Tennessee, Knoxville — The ion transport and structural dynamics in a homologous pair of quaternary ammonium and phosphonium based room temperature ionic liquids (IL) ([EMIm][NTf2] and [EMIm][NO3]) is investigated using spectral intensity resolved ion mobility and fast scanning calorimetry. We have developed and proven this method using the ionic liquids [EMIm][NTf2] and [EMIm][NO3] at temperatures up to 750 K and in different atmospheres to distinguish between decomposition and evaporation. The atomic identity of the cation center has a pronounced effect on both long-range ion conduction as well as structural relaxation in these quaternary ILs. The dc conductivity is significantly higher in the phosphonium based IL. While the increase in dc conductivity can be attributed to a lower glass transition temperature, i.e. faster structural dynamics, of the phosphonium IL, we also have found the atomic identity of the cation center strongly influences the local secondary relaxations. The secondary relaxations in the ammonium IL exhibit an unexpected non-Arrhenius temperature dependence — in stark contrast to its phosphonium counterpart. In addition to structural dynamics, changes in the secondary relaxations suggest the differences in dc conductivity may also be attributed to a change in counter-ion coordination and could lead to a difference in the mesoscale aggregation of alkyl moieties which is known to exist in these ILs. Therefore, subtle changes of inter-ionic interactions have a direct consequence on local, structural, and long-range dynamics in these analogous ILs.

H1.00056 Determination of Volatility of Ionic Liquids at the Nanoscale by means of Ultra-Fast Scanning Calorimetry – the Method. MATHIAS AHRENBERG, Institute of Physics, University of Rostock, Germany, MARTIN BECK, Faculty of Mechanical Engineering, University of Rostock, Germany, CHRISTIN SCHMIDT, SERGEY P. VEREVKIN, Institute of Chemistry, University of Rostock, Germany, OLAF KESSLER, Faculty of Mechanical Engineering, University of Rostock, Germany, UDO KRAGL, Institute of Chemistry, University of Rostock, Germany, CHRISTOPH SCHICK, Institute of Physics, University of Rostock, Germany — We present a new method for the determination of the vapour pressure of low volatile compounds using differential fast scanning calorimetry. We have developed and proven this method using the ionic liquids [EMIm][NTf2] and [EMIm][NO3] at temperatures up to 750 K and in different atmospheres to distinguish between decomposition and evaporation. It was demonstrated that evaporation is still the dominating process of mass loss even at temperatures 100 K above the onset of decomposition as measured with common techniques, e.g. TGA. Since the method allows very high heating rates (up to 106 K/s), much higher temperatures can be reached in the measurement of the vapour pressure as compared to common devices without significant decomposition of the ionic liquid. Furthermore, this method represents an improvement of the boiling point estimation of ILs due to the large accessible temperature range of mass loss rate determination.

H1.00057 Morphological and Chemical Analysis of Degraded Single Junction Amorphous Silicon Module. GILBERT OSAYEMWENRE, Fort Hare — Photovoltaic solar modules have different defects and degradation characteristic modes. These defects/degradation modes normally heats up some regions in the PV module, depending on the degree and size of the localised heat or hot spot, the localized heat can rise above the temperature limit of the module thereby cause damage to the structural orientation. The presence of severe defect and degradation correlates with high temperature gradients that usually results in morphological damage especially under outdoor conditions. The present study investigates the effect of defect/degradation on the surface morphology of the single junction amorphous silicon modules (a-Si:H) during outdoor deployment. The observed structural damage was analysed using scanning electron microscope (SEM) and energy dispersion X-ray (EDX) to ascertain the elemental composition. Results show huge discrepancies in the chemical composition of the affected region, the presence of high concentration of carbon and oxygen was found in the affected region.

H1.00058 Cross-relaxation quenching of x-ray excited luminescence in Eu-activated phosphors. JOSEPH PACOLD, Lawrence Berkeley National Laboratory, DEVON MORTENSEN, University of Washington, WILLIAM REICHLIN, Central Washington University, ZOU FINFROCK, Argonne National Laboratory, ANTHONY DIAZ, Central Washington University, GERALD SEIDLER, University of Washington — Compounds, molecules, and nanoparticles containing lanthanides as primary constituents or as dopants are widely used in applications including luminescent dyes and lighting phosphors. Recent work has shown that x-ray spectroscopy methods can be used to monitor the sequence of excited states that leads to luminescence in lanthanide materials. Here, we use x-ray spectroscopy methods to identify a nonradiative process that quenches the emission of excited state of Eu3+ in the phosphors YVO4:Eu3+, Eu3+:YVO4:B3+:Eu3+ and YVO4:Eu3+. Taking advantage of the high flux (up to 2 × 1012 photons/second) and focusing capability (beam FWHM 5 μm) of a modern synchrontron beamline, we observe saturation of the XEOL yield at high x-ray flux densities. The saturation effect is interpreted with a kinetic model in which pairs of excited Eu ions undergo an Auger-like cross-relaxation. This effect is well documented in the literature on cathode-ray phosphors, and allows us to estimate the excited fraction of Eu3+ ions. We discuss applications of this method to the broader problem of studying energy transfer in luminescent materials, as well as technical implications for future x-ray spectroscopy studies that require high flux.

H1.00059 Inner-shell photoionization and core-hole decay of Xe and XeF2. ANTONIO PICÓN, C. STEFAN LEHMANN, Argonne National Laboratory, RALF WEHLITZ, University of Wisconsin, LAN CHENG, JOHNN F. STANTON, University of Texas — Molecular effects on inner-shell photoionization and core-hole decay are explored by comparing cross sections and partial ion yields of Xe and XeF2 from Xe 3d and F 1s subshells in the 660-740 eV range. The Xe 3d–f continuum shape resonances dominate the total cross sections, but prominent resonances appear in the XeF2 cross section due to excitation of Xe 3d and F 1s electrons to the lowest unoccupied molecular orbital (LUMO), a delocalized anti-bonding MO. Relativistic coupled-cluster calculations were performed to identify the subshell ionization thresholds, the LUMO resonances and their oscillatory strengths. Comparison of the Xe charge state distributions of the atom and molecule show a general shift to lower charge states in XeF2. The measurements support a model of core-hole decay in which charge is redistributed from Xe to the F ligands and energetic F ions are produced by Coulombic fragmentation.

1Supported by the Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, Office of Science, US Dept of Energy, Contract DE-AC02-06CH11357.
and illustrate the interference effects significant gap between the largest flux loop and the rest of them. On the kinetic level, we found that multiple kinetic paths between quantum states emerge between major states and increasing the mean value of the flux. A limit-cycle mode emerges when the underlying flux-landscape becomes funnelled with a the flux-landscape. Improving the voltage and electronic coupling in general facilitates the quantum transport by reducing the population landscape barriers non-equilibrium curl quantum flux which leads to the detailed-balance-breaking and time-irreversibility. The multi-loop structure of the flux emerges which forms the population landscape contribution which mainly governs the equilibrium part of dynamics while the anti-symmetric part of the driving force generates the acceptor energy transfer. We found two driving forces for the non-equilibrium quantum dynamics. The symmetric part of the driving force corresponds to a population and flux landscape theory for general non-equilibrium quantum systems. We illustrated our theory by modelling the quantum transport of donor-acceptor energy transfer in non-equilibrium quantum systems.
however the location of Ni is one of the tasks of this kind of catalyst.

2 type of material belongs to a novel family of catalysts specially designed for ultra-low sulfur production from straight-run gas oil (SRGO), cycle oil, coker gas techniques. The used catalysts was a state-of-the-art commercial nickel-molybdenum alumina-supported formulation, including organic agent modifier. This most important role in the catalytic activity. We studied an industrial NiMo/Alumina sulfide catalyst highly active by using aberration-corrected HAADF-STEM reactions, like hydrodenitrogenation and HDS. One of the main issues in these catalysts is to understand the mechanism of the reaction, where MoS$_2$, WATHEQ AL-BASHEER, Department of Physics, King Fahd University of Petroleum & Minerals, SAID AL AZAR, Basic Sciences Department, Dar Al Ioom University — $R(+)\cdot 3$-methylcyclopentanone ($R$3MCP) is a chiral ketone which can exist in as many as five conformers with two dominant conformers at room temperature; equatorial-methyl and axial-methyl. Density Functional Theory (DFT) calculations of the optimized geometries of $R(+)\cdot 3$-methylcyclopentanone ($R$3MCP) individual dominant conformers were performed in 10 common solvents of wide polarity range, under the framework of polarizable continuum model (PCM). DFT correlation function type B3LYP using a powerful basis set (aug-cc-pVDF) yielded different linear correlation between solvent polarity and $R$3MCP equatorial and axial conformers Gibbs free and zero-point energies, entropies, vibrational modes frequencies, in addition to heat capacity resulting from translational, electronic, rotational and vibrational motion. Furthermore, DFT calculations of the $R$3MCP equatorial and axial conformers electric dipole and quadrupole moments components in 3D were also carried out and found to have a linear correlation with solvent polarity and cavitation energy. An observed trend for the standard Gibbs energies for the rotational equilibrium of $R$3MCP to be strongly solvent dependent will be presented.

H1.0068 1 D Simulation of Capacitively Coupled Water Vapor Plasma, ZIANE KECHIDI$^1$, None, A.H. BELBACHIR TEAM, M. ANNOUN COLLABORATION, W.W. GRAHAM COLLABORATION — The results of a 1D simulation of a capacitively coupled water vapor discharge is reported. The simulated plasma consists of two electrodes separated by gap distance of 1 mm operating at 13.56 MHz with 26 species and 62 dominant reaction channels. The input parameters under which the plasma can be created is explored and space and time profiles of the electron densities are presented. The model finds that plasma ignition cannot be obtained in the present configuration and at pressures of greater than 0.1 atmosphere. The model has also been used to demonstrate the impact of rotational and vibrational excitation of water molecules in suppressing electrical breakdown.

H1.0069 Charge Conservation in BDG Formalism and its Effect in Calculating Berry Phase of Transporting a Localized BDG Quasiparticle around a Vortex in Superfluids/Superconductors, YIRUO LIN, TONY LEGGETT, University of Illinois at Urbana-Champaign — We examine charge conservation in BDG formalism and discuss the consequence of violating the charge conservation in Berry phase calculation of transporting a localized BDG quasiparticle around a vortex in superfluids/superconductors. We calculate explicitly the Berry phase in a model system in which the vortex is replaced by a 1D annulus ring geometry with quantized superfluid center-of-mass winding number and a localized Zeeman field is imposed to trap a quasiparticle with definite spin orientation.

H1.0070 Parahydrogen Induced Polarization by Pairwise Replacement on Pt and Ir Nanoparticles, CLIFFORD BOWERS, RONGHUI ZHOU, EVAN ZHAO, WEI NEAL, HELENA WEAVER, Univ of Florida - Gainesville — Parahydrogen Induced Polarization (PHIP) is a robust and scalable method for production of bulk quantities of hyperpolarized fluids. The symmetrization order inherent in parahydrogen is transformed via symmetry breaking hydrogenation reaction into NMR-observable hyperpolarization. Spin polarization of order unity can be obtained. A key requirement of PHIP is pairwise hydrogenation by addition of H atoms originating from the same H$_2$ molecule. PHIP using supported metal catalysts is a promising recent development because it exploits the advantages over homogeneous and supported metal complexes. The present work demonstrates a new PHIP mechanism involving the pairwise replacement of parahydrogen into propane (the substrate) over TiO$_2$ supported Ir and Pt nanoparticle catalysts. Analysis of the stereoselectivity of the pairwise replacement process is facilitated by density matrix spectral simulations. The cis and trans dispositions of the symmetric order give strikingly different PHIP spectra. The observed stereoselectivity of the pairwise replacement step, together with control experiments, rule out an alternative mechanism involving dehydrogenation of free propane over the catalyst.

H1.0071 Promoting alkali and alkaline-earth metals on MgO for enhancing CO2 capture by first-principles calculations, HYOSEOK KIM, WON BO LEE, KIWOONG KIM, Sogang Univ — The CO2 capture properties of Alkali (Li, Na, K, Rb, Cs) and Alkaline-earth metals (Be, Ca, Sr, Ba) promoted MgO sorbents are investigated by first principles density functional theory on the basis of PW91/GGA augmented with DFT+D2. Calculated Adsorption energy on the metal-promoted MgO sorbents is higher than Pure MgO sorbents, except for the Na-promoter. These results indicate that the CO2 capture capacity is improved by metal promotion. Li, Ca, Sr and Cs were identified as adequate promoters among 9 metals, considering bind stability and regenerability.

H1.0072 Diffusion of a particle on a static rugged energy landscape with spatial correlations, BIMAN BAGCHI, SAIKAT BANERJEE, Indian Institute of Science — Despite the broad applicability of the problem, we have limited knowledge about the effect of ruggedness on diffusion at a quantitative level. Every study seems to use the expression of Zwanzig [Proc. Natl. Acad. U.S.A, 85, 2029 (1988)] who derived the effective diffusion coefficient, $D_{eff} = D_0 \exp (-\beta \varepsilon^2)$. We introduce and study two models of Gaussian random energy surface; a discrete lattice and a continuous field. Our simulations show that Zwanzig’s expression overestimates diffusion in the uncorrelated Gaussian random lattice. The disparity originates from the presence of “three-site traps” (TST) on the energy landscape — which are formed by the presence of deep minima flanked by high barriers on either side. Using mean first passage time (MFPT) formalism, we derive a general expression for the effective diffusion coefficient, $D_{eff} = D_0 \exp (-\beta \varepsilon^2) [1 + \text{erf}(\beta \varepsilon/2)]^{-1}$ in the presence of TST. In presence of spatial correlation we derive a more general form of the expression, which reduces to Zwanzig’s form in certain limits. We characterize the same using non-Gaussian order parameter, and show that this “breakdown” scales with ruggedness following an asymptotic power law. The breakdown of Zwanzig’s elegant expression was perhaps anticipated but was not clearly demonstrated earlier.

H1.0073 New insights in the characterization of HDS industrial catalysts by HAADF-STEM, PAZ DEL ANGEL, ARTURO PONCE, JOSEFINA ARELLANO, MIGUEL J. YACAMAN, Universidad de Texas, San Antonio, MARTHA HERNANDEZ-PICHARDO, Instituto Politecnico Nacional, J. ASCENCION MONTOYA, JOSE ESCOBAR, Instituto Mexicano del Petroleo — Hydrodesulfurization (HDS) catalysts are of great importance in the petroleum industry. Transition metal sulfides catalysts of Ni(Co)Mo(W)/Al$_2$O$_3$ are widely used for hydrodesulfurizing reactions, like hydrodenitrogenation and HDS. One of the main issues in these catalysts is to understand the mechanism of the reaction, where MoS$_2$ plays the most important role in the catalytic activity. We studied an industrial NiMo/Alumina sulfide catalyst highly active by using aberration-corrected HAADF-STEM techniques. The used catalysts was a state-of-the-art commercial nickel-molybdenum alumina-supported formulation, including organic agent modifier. This type of material belongs to a novel family of catalysts designed for ultra-low sulfur production from straight-run gas oil (SRGO), cycle oil, coker gas oil, or their combinations at operating conditions of commercial interest in hydrodesulfurizing units at industrial scale. Aberration corrected HAADF-STEM allowed to observe the nanostructure and location of MoS$_2$ and its interaction with the alumina. The results indicate that the MoS$_2$ is highly dispersed on the alumina, however the location of Ni is one of the task of this kind of catalyst.
and theoretical works suggest that it is due to the adsorbed Cl atoms. We test this hypothesis and show that adsorbed Cl atoms only lead to a p-type character

potential candidate for highly sensitive and selective gas sensors, a clear identification of the source of the p-type doping is not achieved. Recent experimental

carbon nanotubes (CNTs) is investigated using first-principles self-interaction corrected density functional theory. Although the system has been studied as

Dublin 2, Ireland, UDO SCHWINGENSCHLOGL, PSE Division, KAUST, Saudi Arabia — The microscopic origin of the p-type doping of AuCl

MURAT, PSE Division, KAUST, Saudi Arabia, IVAN RUNGGER, STEFANO SANVITO, School of Physics, AMBER and CRANN Institute, Trinity College,

we find that the molecule consisting of donor and acceptor mimics a pn-junction, whereas the tandem setup does not behave as a pn-pn junction, rather like a

study a tandem setup for the representative optimized rectifier, finding that it significantly improves the rectification behavior of the molecular diode. Moreover,

increasing donor groups using self-interaction corrected density functional theory combined with the non-equilibrium Green's function method. In particular, we

H1.00074 Effective Reaction Coordinates in Competitive Nucleation of Gold Nanoclusters1. CLETUS ASUQUO, RICHARD BOWLES, Dept. Chemistry, University of Saskatchewan — Many materials exhibit crystal polymorphism such that they can freeze to form a variety of different structures under the same conditions. Which structure is formed, and how, is determined by the nucleation kinetics that includes the creation of a critical embryo for the new phase. In classical nucleation theory, the embryo size is usually used as the sole order parameter to describe the reaction coordinate, but this does not always contain sufficient information to describe the formation of the different phases observed in a competitive nucleation process. We present an evaluation of the transition path sampling algorithm to the simulation of transition paths in a competitive process, as well as the development of a multiple paths maximum likelihood analysis used to obtain accurate reaction coordinates for the different transitions. The new techniques are used to study competitive nucleation in gold nanoclusters where non-crystalline structures such as icosahedra, decahedra and face-centered cubic crystals can form. The reaction coordinates, and analyses of the nucleation pathways, give new insights to how correlated local structures arrange to form more complex structures on longer length scales. In particular, we show that the formation of the tetrahedral subunits are important

1We thank NSERC for financial support and Compute Canada for computational resources.

H1.00075 Structural Properties of Finite MoS2 Nanowires, SHAYLYN CLARK, Department of Physics & Astronomy, The University of Texas at San Antonio, ANDRES SALGADO, University of Texas - Pan American, LUCAS FERNANDEZ-SEIVANE, Dept. of Physics, Universidad de Oviedo, XOCHITL LOPEZ-LOZANO, Department of Physics & Astronomy, The University of Texas at San Antonio — Molybdenum disulfide (MoS2) has been one of the most important catalysts used in refineries worldwide for hydrodesulfurization over the past century. In the last decade, and with the advent of nanotechnology, there has been a special interest in MoS2 nanostructures due to their high potential as novel nanocatalysts. The study of the properties of these systems is of fundamental interest for the experimental design of their catalytic activity and efficiency. In this work, we have performed ab initio density-functional calculations (DFT) to investigate the structural properties of finite MoS2 nanostructures. All the models here presented were based on newly experimentally observed morphologies in MoS2 industrial catalysts using high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) images. We simulated STEM images of the theoretical models to compare it with the experimental ones. In contrast with infinite models, the finite models prefer a rippled/twisted structure morphology over the planar or helical ones. The rippled/twisted models appear to be structurally more stable.

H1.00076 Theoretical DFT Study of Homonuclear and Binary Transition-Metal Dimers1, ALVARO POSADA-AMARILLAS, Dept. de Investigacion en Fisica, Universidad de Sonora, ALVARO POSADA-BORBON, Dept. de Fisica, Universidad de Sonora — A DFT study of homonuclear, and heteronuclear Pd-M, Pt-M (M=Cu, Ag, Au, Ni) and Pt-Pd neutral dimers is presented using different XC functionals and basis sets. Bond length and vibrational frequencies were determined for ground state configurations. Doublet and triplet states were obtained for heteronuclear dimers while dissociation energy exhibits unambiguous dependency on the HF exchange term. Electronic configurations were determined for Pt-Ag (Σ) and Pt-Ni (3Σ) dimers. Hybrid functionals provide results in close agreement with experimental data for Pt-Ni, Pt-Pd, and Pd-Ni dimers. The hybrid mPW1PW91 functional predicts a dissociation energy value for Pt-Cu dimer of about 3.3 eV, consistent with experimental information. Overall PBE and B3PW91 are reliable functionals to predict bond lengths and harmonic frequencies of heteronuclear dimers.

1CONACY-T-Mexico is acknowledged for funding project No. 180424.

H1.00077 An integral method to compute Helmholtz free energies of crystalline solids1, ZHIYUE LU, CHRISTOPHER JARZYNSKI, University of Maryland at College Park — We describe a method to compute the Helmholtz free energy of a crystalline solid by direct evaluation of the partition function. In the many-dimensional conformation space of all possible arrangements of N particles inside a periodic box, the energy landscape consists of localized islands corresponding to different solid phases. Calculating the partition function for a specific phase involves integrating over the corresponding island. Introducing a natural order parameter that quantifies the net displacement of particles from lattices sites, we write the partition function in terms of a one-dimensional integral along the order parameter, and evaluate this integral using umbrella sampling. We validate the method by computing free energies of both face-centered cubic (FCC) and hexagonal close-packed (HCP) hard sphere crystals with a precision of 10-3 k_BT per particle.

1This research is supported by the National Science Foundation (USA) under grants CHE-0841557 and DMR-1200971.

H1.00078 The effect of excitonic interactions on singlet fission dynamics in crystalline tetracene1, CHUNFENG ZHANG, BO ZHANG, RUI WANG, Nanjing University, MIN XIAO, University of Arkansas — Singlet fission in organic semiconductors is interesting for its potential application in boosting the efficiency of solar conversion. Singlet-singlet annihilation induced by excitonic interactions has been regarded as a process that competes against singlet fission in high-density regime. In this work, we conduct a systematic transient optical study to investigate the density-dependent singlet fission dynamics in crystalline tetracene. Surprisingly, the transient absorption data indicate the rate of singlet fission is actually increased with increasing the excitation density [1], which is further supported by probing the quantum beating between the manifold states of triplet pairs following Burdett’s approach. Our result suggests it is necessary to re-examine the role of excitonic interactions to uncover the physical mechanism underlying singlet fission in crystalline tetracene. [1] Zhang et al., J. Phys. Chem. Lett. 5, 3462 (2014). [2] Burdett & Bardeen, J. Am. Chem. Soc. 134, 8597(2012).

1This work is supported by National Science Foundation of China and “973” project.

H1.00079 A Single Diblock Molecular Diode, TOBECHUKWU JOSHUA OBODO, ALTYNEBEK MURAT, UDO SCHWINGEN-SCHLÖGL, PSE Division, KAUST, Saudi Arabia — We investigate the rectification behavior of the diblock dipyrromethyldiphenylmolecule and its derivatives with increasing donor groups using self-interaction corrected density functional theory combined with the non-equilibrium Green’s function method. In particular, we study a tandem setup for the representative optimized rectifier, finding that it significantly improves the rectification behavior of the molecular diode. Moreover, we find that the molecule consisting of donor and acceptor mimics a pn junction, whereas the tandem setup does not behave as a p-n junction, rather like a p-n-p-n junction. Our results help explain the mechanism behind the experimentally observed rectification behavior of the molecule.

H1.00080 AuCl3 Functionalized Carbon Nanotubes: Origin of the p-Type Doping, ALTYNEBEK MURAT, PSE Division, KAUST, Saudi Arabia, IVAN RUNGGER, STEFANO SANVITO, School of Physics, AMBER and CRANN Institute, Trinity College, Dublin 2, Ireland, UDO SCHWINGENSCHLÖGL, PSE Division, KAUST, Saudi Arabia — The microscopic origin of the p-type doping of AuCl3 functionalized carbon nanotubes (CNTs) is investigated using first-principles self-interaction corrected density functional theory. Although the system has been studied as potential candidate for highly sensitive and selective gas sensors, a clear identification of the source of the p-type doping is not achieved. Recent experimental and theoretical works suggest that it is due to the adsorbed Cl atoms. We test this hypothesis and show that adsorbed Cl atoms only lead to a p-type character for very specific concentrations and arrangements, which furthermore are not the lowest energy configurations. We therefore propose and investigate alternative mechanisms while considering all possible configurations and concentrations. In particular, we study the possible formation of different conformations of AuCl3 as well as the effect of the adsorbate concentration. As a result, we find that especially AuCl4 molecules bind strongly to the CNT and that they lead to an electron transfer to the nanotubes and thus a shift of the Fermi energy below the valence band maximum. We conclude that the origin of the p-type doping in AuCl3 functionalized CNT is due to the adsorption of AuCl4 molecules.
H1.00081 First-Principles Investigations of Lead-Free Formamidinium Based Hybrid Perovskites, ALTYNEB K. MURAT, UDO SCHWINGENSHÖGL, PSE Division, KAUST, Saudi Arabia — Hybrid organic-inorganic perovskite solar cells have recently emerged as the next-generation photovoltaic technology. Most of the research work has been focused on the prototype MAPbI₃ perovskite (MA = Methylammonium = CH₃NH₃⁺) and its analogues that have lead to power conversion efficiencies in excess of 15%. Despite the huge success, these materials are still non-optimal in terms of optical absorption where the bandgaps are greater than 1.6 eV as well as the toxicology issue of lead. Thus, investigation and development of lead-free perovskites with bandgaps closer to optimal, allowing greater spectral absorption, is of great interest. In this work, we perform first principles calculations to study the structural, optical, and electronic properties of new derivatives of MAPbI₃ in which the organic MA cation is replaced by other organic amines of similar size such as Formamidinium (FA) and/or the Pb cation replaced by similar elements such as Sn. In particular, we investigate the role and effect of FA and Pb cations on the electronic and optical properties and analyze to which extend the bandgaps can be tuned.

H1.00082 Dye attached fullerene and P3HT complexes, AMANDA GARNICA, LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — We study the electronic structure of C60 fullerenes functionalized with thiophe-diketo-pyrolypopyrro-thiophene based chromophores using density functional theory combined with large polarized basis sets. These chromophores have electron donor character and thus the functionalization of the fullerene produces donor-acceptor (DA) systems. We examine in detail the effect of the linker and the addition site on the electronic structure of the fullerenes. We further study how the charge transfer excited states of these DA complexes and also that of the complexes of these functionalized fullerenes with the poly(3-hexylthiophene-2,5-diyl) (P3HT) are studied using the perturbative J-SCF method. The exciton binding energies in the functionalized fullerene-P3HT complexes are found to be smaller compared to similarly prepared phenyl-C61-butyric acid methyl ester (PCBM)-P3HT complex.

1Support from DOE (DE-SC0002168) and NSF (DMR-1205302) is acknowledged.

H1.00083 Electronic structure and charge transfer excitation energies of three endohedral fullerene-ZnTPP/ZnPc dyads, FATEMEH AMERKHEIRABADI, LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, The University of Texas at El Paso — Organic donor-acceptor (D-A) moieties make up the main component of organic photovoltaics (OPVs). It has been proved that the open circuit voltage of these devices which is a parameter in efficiency determination, is directly related to the charge transfer excited states of the D-A pairs. Fullerenes having lots of interesting acceptor properties and porphyrins as well as phthalocyanines possessing intriguing donor characteristics, are shown to be promising nominees. In this work, we computationally analyze three donor-acceptor dyads of Zn-tetraphenyl porphyrin and Zn- phthalocyanine with novel endohedral fullerenes: Sc₂[N@C₆₀]ZnTPP, Y₂[N@C₆₀]ZnTPP and Sc₂[N@C₆₀]ZnPc. The Sc₂[N@C₆₀] and Y₂[N@C₆₀] belong to a particular class of fullerenes called trimplalctic nitride endohedral fullerenes where the trimplalctic nitrides form the endohedral units. Density functional theory, as implemented in NRLMOL code, is used to study the electronic structure and the related properties of these D-A complexes. The charge transfer excitation energies are calculated using the perturbative delta self-consistent field method recently developed in our group. We find that the CT excitation energies are larger for endohedr fulleren based dyads compared to similar C₆₀ based dyads.

H1.00084 Current flow in biased bilayer graphene: the role of sublattices, CARLOS PAEZ, Universidade Estadual de Campinas-FCA, DARIO BAHAMON, MackGraphe -Graphene and Nano-Materials Research Center, Mackenzie Presbyterian University, ANA PEREIRA, Universidade Estadual de Campinas-FCA — We investigate here how the current flows over a bilayer graphene in the presence of an external electric field perpendicularly applied (biased bilayer). Charge density polarization between layers in these systems is known to create a layer pseudospin, which can be manipulated by the electric field. Our results show that current does not necessarily flow over regions of the system with higher charge density. Charge can be predominantly concentrated over one layer, while current flows over the other layer. We find that this phenomenon occurs when the charge density becomes highly concentrated over only one of the sublattices, as the electric field breaks layer and sublattice symmetries for a Bernal-stacked bilayer. For bilayer nanoribbons, the situation is even more complex, with a competition between edge and bulk effects for the definition of the current flow. We show that, in spite of not flowing trough the layer where charge is polarized to, the current in these systems also defines a controllable layer pseudospin.

H1.00085 PHYSICS EDUCATION —

H1.00086 Visualizations of Illinois Educational Data, CACEY STEVENS, The James Franck Institute and Department of Physics, University of Chicago, MICHAEL MARDER, Department of Physics, The University of Texas at Austin, SIDNEY NAGEL, The James Franck Institute and Department of Physics, University of Chicago — We examine data from scores on standardized exams taken by students in the state of Illinois. In order to analyze the factors affecting school performance in mathematics, we represent the data through visualizations, an approach commonly used to identify patterns in studies of physical systems. Exam scores for different schools are shown to depend on program type, location, and poverty concentration. For most schools in Illinois, test scores decline linearly with increased poverty concentration. However, schools in Chicago show deviations from the linear trend. For any given poverty level, schools in Chicago perform better than those in other communities of Illinois. We also compare different school types, such as neighborhood, magnet, and charter programs, at each grade level. The city’s selective enrollment programs show notably superior achievement at the high school level. This is less pronounced at earlier grades.

H1.00087 Lab-in-a-box @ school: Exiting hands-on experiments in soft matter physics, KARIN JACOBS, MARTIN BRINKMANN, FRANK MÜLLER, Experimental Physics, Saarland University, Saarbruecken, Germany — Soft materials like liquids and polymers are part of everyday life, yet at school, this topic is rarely touched. Within the priority program SPP 1064 ‘Nano- and Microfluidics’ of the German Science Foundation, we designed an outreach project that allows pupils (age 14 to 18) to perform hands-on experiments (www.labinabox.de). The experiments allow them e.g. to feel viscosity and viscoelasticity, experience surface tension or see structure formation. We call the modus operandi ‘subjective experiments’ to contrast them with the scientifically objective experiments, which pupils often describe as being boring. Over a dozen different experiments under the topic ‘physics of fluids’ are collected in a big box that travels to the school. Three other topics of boxes are available, ‘physics of light’, ‘physics of liquid crystals’, and ‘physics of adhesion and friction’. ‘Subjective experiments’ especially catch the attention of girls without disadvantaging boys. Both are fascinated by the hands-on physics experience and are therefore eager to perform also ‘boring’ objective experiments. Moreover, before/after polls reveal that their interest in physics has greatly advanced. The project can easily be taken over and/or adapted to other topics in the natural sciences.

1Financial support of the German Science Foundation DFG is acknowledged.

H1.00088 QUANTUM INFORMATION, CONCEPTS AND COMPUTATION —
H1.00089 Approach to solving spin-boson dynamics via non-Markovian quantum trajectories
ZENG-ZHAO LI, Beijing Computational Science Research Center, CHO-TUNG YIP, Hong Kong Polytechnic University, HAI-YAO DENG, Hong Kong Polytechnic University and National Institute for Materials Science, MI CHEN, Fudan University, TING YU, Stevens Institute of Technology, J. Q. YOU, Beijing Computational Science Research Center, CHI-HANG LAM, Hong Kong Polytechnic University — We develop a systematic and efficient approach for numerically solving the non-Markovian quantum state diffusion equation for an open quantum system that can be strongly coupled to an environment. As an important application, we consider a real-time simulation of a spin-boson model in a strong coupling regime that is difficult to deal with using conventional methods. We show that the non-Markovian stochastic Schrödinger equation can be efficiently implemented as a real-time simulation for this model, so as to give an accurate description of spin-boson dynamics beyond the rotating-wave approximation.

H1.00090 Relation between Full Counting Statistics and the flow of Shannon entropy, MOHAMMAD ANSARI, YULI NAZAROV, Kavli Institute for nanoscience, Delft University of Technology — We show that microscopic theory of counting statistics that is applicable for many quantum noise analysis, has an internal and fundamental correspondence to the Renyi entropy flow in the quantum system. This analogy reveals an interesting step towards understanding quantum thermodynamics. We also further extend the formulation for the flows of entropy using full counting statistics and determine novel quantum terms in the statistical moment measurements.

H1.00091 Coherent control of multipartite excitonic entanglement in quantum dot arrays, JUAN E. ROLON, JOAQUIN E. DRUT, University of North Carolina at Chapel Hill — We propose a coherent control scheme for multipartite entanglement of exciton states in optically driven quantum dot arrays (QDAs) coupled by charge tunneling and resonant energy transfer (RET) processes. An adiabatic manipulation of the entanglement dynamics is devised by pulse shaping and time-dependent electric field sweeps. By varying the inter-dot distance and number of quantum dots (QDs) comprising the QDA, the excitonic qubit manifolds are obtained by a Feshbach projection over the resulting multilevel exciton configurations. We identify regimes in which the dynamics is confined to decoherence-free excitonic qubit manifolds taking into account spontaneous recombination and non-Markovian effects introduced by a phonon bath. We present results for entanglement monotonies and measures such as the entanglement of formation and entanglement entropy for different QDA geometries and carrier injection conditions. Our results indicate that in spite of the effects of phonon-assisted relaxation, entanglement can be optimized and transferred between QDs by the controlled interplay of system geometry, pulse shaping, RET and carrier tunneling.

H1.00092 Anisotropic exchange coupling in a nanowire double quantum dot with strong spin-orbit coupling, RUI LI, J.Q. YOU, Beijing Computational Science Research Center — A spin-orbit qubit is a hybrid qubit that contains both orbital and spin degrees of freedom of an electron in a quantum dot. Here we study the exchange coupling between two spin-orbit qubits in a nanowire double quantum dot (DQD) with strong spin-orbit coupling (SOC). We find that while the total tunneling in the DQD is irrelevant to the SOC, both the spin-conserved and spin-flipped tunnelings are SOC dependent and can compete with each other in the strong SOC regime. Moreover, the Coulomb repulsion between electrons can combine with the SOC-dependent tunnelings to yield an anisotropic exchange coupling between the two spin-orbit qubits. Also, we give an explicit physical mechanism for this anisotropic exchange coupling.

H1.00093 Spin decoherence of mobile impurity in a one dimensional spin bath, TRITHEP DEVAKUL, ADRIAN FEIGUIN, Northeastern University — We study the spin decoherence of a mobile impurity interacting locally with a one dimensional spin bath. In contrast to the central spin model, where a single central spin interacts with the bath via long ranged interactions, our model considers only local exchange interactions, while allowing the impurity to move to neighboring sites via hopping $t$. We consider a spin-$1/2$ impurity, and study the decoherence, tracing over the position degree of freedom. In the large $t$ limit, the delocalized impurity behaves identically to a localized spin interacting with the bath, same as a central spin. This model allows one to treat a spin coupling problem which inherently builds up long-range entanglement within the bath — instead as a Hamiltonian with only local interactions. Numerical calculations are done at various regimes of parameters, and comparison with the central spin model is discussed.

H1.00094 Finite-temperature reservoir engineering and entanglement dynamics, SERGII FE-DORTCHENKO, Université Paris Diderot, ARNE KELLER, Université Paris-Sud 11, THOMAS COUDREAU, PEROLA MILMAN, Université Paris Diderot — We propose experimental methods to engineer reservoirs at arbitrary temperature which are feasible with current technology. Our results generalize to mixed states the possibility of quantum state engineering through controlled decoherence. Finite-temperature engineered reservoirs can lead to the experimental observation of thermal entanglement—the appearance and increase of entanglement with temperature—to the study of the dependence of finite-time disentanglement and revival with temperature, quantum thermodynamical effects, and others, enquiring the comprehension of temperature-dependent entanglement properties. Our proposal is discussed in detail in two model systems, consisting of different modes of a single photon and a trapped-ion system.

H1.00095 Reproducing the D-Wave Entanglement Results in Candidate Models, TAMEEM ALBASH, University of Southern California, ITAY HEN, FEDERICO SPEDALIERI, Information Science Institute, DANIEL LIDAR, University of Southern California — The demonstration of entanglement on the D-Wave devices [1] relies on the assumption that the populations derived from measurement correspond to energy eigenstate populations of the quantum Hamiltonian. We therefore ask whether leading model candidates for the D-Wave devices are able to reproduce this entanglement signature. We focus our work on a quantum adiabatic Markovian master equation (ME) [2] and a Monte Carlo rotor model (SSSV) [3]. We show that the ME reproduces both the energy spectrum and the thermal state populations of the quantum Hamiltonian extremely well, hence agreeing with the experimental results. SSSV on the other hand fails to reproduce either, a consequence of the absence of discrete energy states in this model.


H1.00096 Using the SLUG as a First Stage, Low Noise Microwave Amplifier for Superconducting Qubit Readout, EDWARD LEONARD JR., TED THORBECK, SHAOJIANG ZHU, ROBERT MCDERMOTT, Univ of Wisconsin, Madison — The SLUG (Superconducting Low-inductance Undulatory Galvonometer) microwave amplifier is a large bandwidth, high saturation power, high gain, and low noise microwave element designed as a first stage cryogenic amplifier for dispersive readout of superconducting qubits. High forward gain is paired with simultaneous high reverse isolation such that bulky, expensive cryogenic circulators and isolators might be eliminated from the microwave readout chain. Here we present recent experimental data on SLUG gain, noise, and reverse isolation. We achieve gain over 10 dB at 7 GHz across a band of several hundred MHz, with system added noise of order one photon. For appropriate flux bias of the device, reverse isolation is better than -20 dB. These qualities make the SLUG a very desirable first stage amplifier for a scalable superconducting qubit readout.
Dynamic nuclear polarization of nitrogen-vacancy centers in diamond. Wen-Hui Hu, Beijing Computational Science Research Center, Nan Zhaoh Collaborations — Single nitrogen-vacancy (NV) centers in diamond triggered the research for wild applications in quantum information processing and quantum metrology. One of the most important advantages of the NV centers is the long coherence time of the center electron spins. Dynamic nuclear polarization (DNP) has been introduced as an efficient method to protect the spin coherence. The coherence time $T_2^*$ should have been prolonged of two orders theoretically, nevertheless less than one order in experiments. In this work, we theoretically study the DNP process in a high-purity diamond, where the dipole-dipole hyperfine interaction between the center electron spins and the bath $^{13}$C nuclear spins is dominant. The simulations show that the saturated polarization of the nuclear bath depends on the spin-lock period and the efficiency of the initialization laser, accompanied with the magnitude of the external magnetic field. The polarization saturation comes from the capability of the polarization transfer and the equilibrium of probability distribution between the polarized and unpolarized states.

Phase noise of a cavity electromechanical oscillator at millikelvin temperatures. Junho SuH, SungWan Cho, Sang Goon Kim, Seung-Bo Shim, Korea Research Institute of Standards and Science — The frequency stability of a mechanical resonator is an important factor in its application to quantum information technology. We investigate the phase noise in a self-oscillation of a micromechanical resonator, parametrically driven by a superconducting microwave resonator at millikelvin temperatures. Possible physical origins of the noise are also discussed.

Investigation of the thermal motion and mode coupling in a micromechanical resonator. Seung-Bo Shim, SungWan Cho, Sang Goon Kim, Korea Research Institute of Standards and Science, Sung Un Cho, Yun Park, Seoul National University, Junho SuH, Korea Research Institute of Standards and Science — We have investigated the thermal motion and mode coupling in a micromechanical resonator. The mechanical resonator was designed for dielectric gradient force actuation scheme. The laser reflection measurement method enabled multi-mode detection of the thermal motion up to $5^{th}$ mode at room temperature. With these multi-modes, we could investigate the energy transfer between first and second mode by applying mechanical sideband signals. We have utilized the second mode as a phonon cavity and observed the coupling and interaction between two modes. Here, we will discuss about the room temperature mechanical mode detection method and mode coupling effect in the micromechanical resonator.

Construction of a Confocal Fluorescence Microscope to Image Nitrogen Vacancy Centers. Jordan Stroman, James Griffin, Gary Harris, Howard University — Long term atomic memory can be achieved using nitrogen vacancy centers (NV). Howard University is optimizing the process of creating nitrogen vacancy centers using hot filament chemical vapor deposition (HFCVD). In order to provide reliable feedback concerning the presence, concentration, and orientation of these color centers, an optical system capable of performing confocal laser scanning fluorescence microscopy has been constructed. This system consists of a 200mw laser that emits light with a wavelength of 532nm. This light is focused on a sample using a Nikon Oil Objective Lens with a numerical aperture of 1.3. The system can be used in a piezoelectric stage with a resolution of 20nm in the $x$, $y$, and $z$ direction. This optical system can confirm and locate NV centers with a resolution of 200nm.

Digital quantum simulation of Heisenberg spin systems in circuit QED. Markus Oppliger, Yves Salathe, Muntu Mondal, Johannes Heinsoo, Philipp Kurpiers, Anton Potočnik, Stefan Filip, Andreas Wallraff, ETH Zurich, Switzerland, Antonio Mezzacapo, Urtzi Las Heras, Lucas Lamata, Enrique Solano, University of the Basque Country, Bilbao, Spain — A Quantum simulator realized by a well-controlled quantum system allows to simulate a wide range of complex quantum systems that are very difficult to study with classical computing. We use a promising quantum simulator based on circuit quantum electrodynamics (QED) to digitally simulate the isotropic Heisenberg XYZ interaction between two spin 1/2 particles. Since the XYZ interaction does not occur directly in the Jaynes-Cummings Hamiltonian, the interaction is decomposed into a set of single- and two-qubit gates. The resulting evolution of the quantum state is analyzed by state tomography for different interaction times after each step. As our approach can be generalized further, this experiment is a first step towards simulating large spin systems in a circuit QED architecture.

High-fidelity quantum memory utilizing inhomogeneous nuclear polarization in a quantum dot. Wenkui Ding, Anqi Shi, Wuhan University, Jianqiang You, Beijing Computational Science Research Center, Wenxian Zhang, Wuhan University — We numerically investigate the encoding and retrieval processes for a quantum memory realized in a semiconductor quantum dot, by focusing on the effect of inhomogeneously polarized nuclear spins whose polarization depends on the local hyperfine coupling strength. We find that the performance of the quantum memory is significantly improved by the inhomogeneous nuclear polarization, as compared to the homogeneous one. Moreover, the narrower the nuclear polarization distribution is, the better the performance of the quantum memory is. We observe the performance improvement to the full harnessing of the highly polarized and strongly coupled nuclear spins, by carefully studying the encoding and decoding process. Our results shed new light on the implementation of a quantum memory in a quantum dot.

A photon-photon quantum gate using a multilevel atomic system. Yuuki Tokunaga, NTT SC Labs. — We propose a method for a quantum gate between photons assisted by a multilevel atomic system. The atomic system is supposed to be in a cavity or a one-dimensional waveguide. The system can transfer a quantum state between a photon and the atom, and also works as a quantum gate for consecutively input photons. This system could be used for a building block for a universal quantum computation. We also discuss the characteristics of such quantum gates with several different multilevel systems.

Riemannium nucleus and quantum solution to the Riemann hypothesis (RH). Carlos FIGUEROA-NAVARRO, Departamento de Ingeniería Industrial, Unidad Regional Centro, Universidad de Sonora, Julio Campos-García, Departamento de Ciencias de la Salud, Unidad Cajeme, Universidad de Sonora, Martin Molinar-Tabares, Organismo de Cuenca Noroeste, Comisión Nacional del Agua, Lamberito Castro-Arce, Departamento de Física e Ingeniería, Universidad Regional Sur, Universidad de Sonora — Is there an energy spectrum according to the center electron spins? This raises the question whether physical systems whose spectrum is the Riemann zeta function; ie, is there a spectrum of resonances of a nucleus that are the zeros of the zeta function? The renowned RH is basically preceded by the Euler principle, the Euler product and the Gauss theorem. The best mathematical interpretation is the one that threw Riemannian revolution. RH holds that the nontrivial zeros of the zeta function keep the harmony of primes, but this is not fully tested. There are two possibilities: The RH can be true, then the primes have harmony, but if false, they nest in the chaos. The idea of this is important for studying models of quantum chaos is getting stronger in the last decade. These investigations lead us to believe that a highly mathematical problem becomes a physical problem; because according to Hugh Montgomery and Michael Berry the variations of the zeros, with drums and quantum billiards, can provide a physical model for explain the primes. In this paper, we generate the Mount Riemann by using Mathematica and we get the profile that relates the prime numbers with the zeros of the zeta function; also we explain how quantum helps to explain the famous old problem known as the conjecture of Riemann.
H1.00105 Distribution of quantum Fisher information in asymmetric cloning machines¹, XING XIAO, YAO YAO, Beijing Computational Science Research Center, LEI-MING ZHOU, Key Laboratory of Quantum Information, University of Science and Technology of China, XIAOGUANG WANG, Zhejiang Institute of Modern Physics, Department of Physics, Zhejiang University — An unknown quantum state cannot be copied and broadcast freely due to the no-cloning theorem. Approximate cloning schemes have been proposed to achieve the optimal cloning characterized by the maximal fidelity between the original and its copies. Here, from the perspective of quantum Fisher information (QFI), we investigate the distribution of QFI in asymmetric cloning machines which produce two nonidentical copies. As one might expect, improving the QFI of one copy results in decreasing the QFI of the other copy, roughly the same as that of fidelity. It is perhaps also unsurprising that asymmetric phase-covariant cloning outperforms universal cloning in distributing QFI since a priori information of the input state has been utilized. However, interesting results appear when we compare the distributabilities of fidelity (which quantifies the full information of quantum states), and QFI (which only captures the information of relevant parameters) in asymmetric cloning machines. Unlike the results of fidelity, where the distributability of symmetric cloning is always optimal for any d-dimensional cloning, we find that any asymmetric cloning outperforms symmetric cloning on the distribution of QFI for d ≤ 18, whereas some but not all asymmetric cloning strategies could be worse

¹supported by the NNSFC (Nos. 11247006, 11025527 and 11475146), the National 973 program(No. 2012CB921602)

H1.00106 Quantum Information in Biological Systems, SHANTILIL GORADIA, Retired — We can derive strong coupling and also recover Newtonian gravity with a quantum mechanical approach implicitly implying the variation of universal constant of gravity on a cosmic scale. Since constancy of G does not lead to cosmological constnat, we derive 137 (described as the hand of God by Feynman) as a natural logarithm of the age of the universe in Planck times (10E60). Since we use Boltzmann equation on his tomb to do that, we describe that equation as the heart of God! Since otherwise, no theory including the string theory can so far come up with 137 mathematically. Maximum potential ON and OFF signals of interactions of 10E60 ever since the big bang could provide the fundamental basis of information system in the universe including in biology, implying the sperm of a man carries the genetic information of the male which combined with the genetic information of a female egg decides the characteristics of the offspring. We may never know the exact language of nature. We speculate the string theory may be able to step in to show some deeper light in that direction.

H1.00107 Two-Slit Particle Experiment and the CMB, ALFRED PHILLIPS JR., Source Institute — Both Einstein and Feynman discussed the difficulty of understanding the two slit experiment for particles. We show a connection between this experiment and the Cosmic Microwave Background. We have not yet determined whether this new connection necessitates a modification of metrics such as that of Robertson-Walker or how much light this new connection sheds on the dark energy (cosmological constant) problem.

H1.00108 MATTER AT EXTREME CONDITIONS —

H1.00109 RKKY and Dzyaloshinsky-Moriya Interaction in the Electron Gas, MOHAMAD MAHDI VALIZADEH, SASHI SATPATHY, Department of Physics & Astronomy, University of Missouri, Columbia, MO 65211, USA — We illustrate the origin of the Dzyaloshinsky-Moriya interaction term 1 2 between two localized spins embedded in a solid by considering the example of the electron gas with spin-split bands, which serves as a simple pedagogical model for the understanding of this interaction. In this case, where symmetry is broken, the magnetic interaction acquires the Dzyaloshinsky-Moriya term in addition to the well-known RKKY interaction term 1 2 , so that the net interaction has the form J = J 1 2 + D 1 2 . For the standard electron gas with spin degenerate states, the DM term vanishes yielding the well known RKKY interaction results. Explicit expressions for the magnitudes of the interactions are obtained for the electron gas in two and three dimensions. This simple model serves as a pedagogical example for the origin of the Dzialoshinski-Moriya interaction in a system with broken time-reversal symmetry.

H1.00110 Chromium based Spins under Compressions, YUEJIAN WANG, ILIAS EFTHIMIOPOULOS, Oakland University, THOMAS AHEARN, Oakland, VLADIMIR TSURKAN, JOACHIM DEISENHOFER, ALOIS LOIDL, University of Augsburg — The Chromium (Cr) based spins, ACr2X4, represent a prototype system for the study of magnetism in solid [1]. More recently, multiferroicity has been found in members of this series [2]. However, the origin of the ferroic properties is not well understood; Given the strong interplay between structural and ferroic properties in this system, the structural evolution induced by pressure may shed light on the multiferroicity [3]. High-pressure X-ray diffraction and Raman spectroscopic studies have been conducted on ZnCr2Se4 and ZnCr2S4. The study elucidated the phase transformation of these spinels under high pressures by the X-ray data and the complementary information from Raman spectra. In the meantime, the unit cell volumes as well as the lattice parameters versus pressures of each individual series [2]. However, the origin of the ferroic properties is not well understood; Given the strong interplay between structural and ferroic properties in this system, the structural evolution induced by pressure may shed light on the multiferroicity [3]. High-pressure X-ray diffraction and Raman spectroscopic studies have been conducted on ZnCr2Se4 and ZnCr2S4. The study elucidated the phase transformation of these spinels under high pressures by the X-ray data and the complementary information from Raman spectra. In the meantime, the unit cell volumes as well as the lattice parameters versus pressures of each individual series [2]. However, the origin of the ferroic properties is not well understood; Given the strong interplay between structural and ferroic properties in this system, the structural evolution induced by pressure may shed light on the multiferroicity [3]. 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H1.00111 SURFACES, INTERFACES AND THIN FILMS —

H1.00112 Directed Chemical Transport and Separation by Hydrogel Films containing Static and Dynamic Chemical Potential Gradients, TSUNG-HAN TSAI, CHUNJIE ZHANG, HYUN-JUN KOO, PAUL V. BRAUN, University of Illinois at Urbana-Champaign — Materials that can manipulate the anisotropic molecular transport through built-in chemical potential gradients offer new opportunities to process chemical agents. Different from electrophoresis and microfluidics, here the chemical potential gradients, which provide the driving forces for molecular transport, are incorporated in the diffusion media. The autonomous systems can independently control the anisotropic flux of molecules and thus do not need external inputs such as electric fields and flowing carrier phases. As model systems, we used hydrogels containing static and dynamic built-in chemical potential gradients in asymmetric cloning machines which produce two nonidentical copies. As one might expect, improving the QFI of one copy results in decreasing the QFI of the other copy, roughly the same as that of fidelity. It is perhaps also unsurprising that asymmetric phase-covariant cloning outperforms universal cloning in distributing QFI since a priori information of the input state has been utilized. However, interesting results appear when we compare the distributabilities of fidelity (which quantifies the full information of quantum states), and QFI (which only captures the information of relevant parameters) in asymmetric cloning machines. Unlike the results of fidelity, where the distributability of symmetric cloning is always optimal for any d-dimensional cloning, we find that any asymmetric cloning outperforms symmetric cloning on the distribution of QFI for d ≤ 18, whereas some but not all asymmetric cloning strategies could be worse

H1.00113 A density functional theory investigation of select transition metal dichalcogenides, RODRICK KUATE DEFO, Physics Department, Harvard University, GEORGIOS TRITSARIS, SEAS, Harvard University, SHIANG FANG, EFTHIMIOS KAXIRAS, Physics Department, Harvard University — As a result of the extensive work done on graphene, leading to advances in sample preparation, optical detection, and transfer and manipulation of 2D materials, there has been a resurgence of interest in layered materials from which single sheets can be extracted, such as molybdenum disulfide. Particularly intriguing is the fact that layered MoS2 transitions from an indirect band gap in the bulk to a direct band gap in the monolayer opening up the possibility of optoelectronic applications. These results have been verified using density functional theory and, further, dependence of the band gap on lattice strain has been investigated. This dependence is crucial in understanding emergent properties of compounds consisting of MoS2 layered with other materials where there is a lattice mismatch. MoSe2, MoS2, MoS2, WSe2 and WS2 have also been studied. Finally, dielectric functions have also been obtained for these compounds to explore the effect particularly of the asymmetric atom configurations on polarization of the material.
H1.00114 Monomer Adsorption on 6-Atoms Wide Zigzag (111) Terraces1, ALAIN PHARES, Villanova University, DAVID GRUMbine, Jr, St. Vincent College — We study monomer adsorption on six-atoms wide, zigzag (111) terraces, with first- (V), second- (W), and third-neighbor (U) interactions, specializing to repulsive first-neighbors. All possible crystallization patterns, or phases, that may exist are expected to occur at relatively low temperatures. Under these conditions, the energy phase diagram is three-dimensional and depends on the dimensionless variables, \( v = \mu/|V|, u = U/|V|, \) and \( w = W/|V| \). The chemical potential energy of the monomers, \( \mu \), in the medium to which the terrace is exposed depends on the pressure, if the medium is a gas, or the concentration if the medium is solution. There are 95 phases, or crystallization patterns, of the adsorbates with coverages ranging from 1/5 to 8/9. In particular, we find that there are 10 distinct 1/2, 2/3, and 4/9 coverage phases, and 9 distinct 1/3 coverage phases.

1Work supported in part by NICS supercomputing grant # CHE040001.

H1.00115 Interplay between Self-Assembled Structures and Energy Level Alignment of Benzene-diamine on Au(111) Surfaces1, GUO LI, Lawrence Berkeley Natl Lab, JEFFREY NEATON, Lawrence Berkeley Natl Lab; UC-Berkeley; Kavli Energy NanoSciences Institute at Berkeley — Using van der Waals-corrected density functional theory (DFT) calculations, we study the adsorption of benzene-diamine (BDA) molecules on Au(111) surfaces. We find that at low surface coverage, the adsorbed molecules prefer to stay isolated from each other in a monomer phase, due to the inter-molecular dipole-dipole repulsions. However, when the coverage rises above a critical value of 0.9nm\(^2\), the adsorbed molecules aggregate into linear structures via hydrogen bonding between amine groups, consistent with recent experiments [Haxton, Zhou, Tamblyn, et al, Phys. Rev. Lett. 111, 265701 (2013)]. Moreover, we find that these linear structures at high density considerably reduces the Au work function (relative to a monomer phase). Due to reduced surface polarization effects, we estimate that the resonance energy of the highest occupied molecular orbital of the adsorbed BDA molecule relative to the Au Fermi level is significantly lower than the monomer phase by more than 0.5 eV, consistent with the experimental measurements [DellAngela, Kladnik, and Cossaro, et al., Nano Lett. 10, 2470 (2010)].

H1.00116 Benzene Derivatives Adsorbed to the Ag(111) Surface: A Binding Site Study, DANIEL MILLER, SCOTT SIMPSON, NINA TYMINSKA, EVA ZUREK, University at Buffalo, ZUREK GROUP TEAM — Dispersion corrected Density Functional Theory (DFT) calculations were employed to study the interaction of benzenes mono and disubstituted with functional groups encompassing a region of the activated/deactivated spectrum. Benzene substituted with weak activating or deactivating groups like methyl and fluoro, respectively, do not have a strong site preference for adsorption to the Ag(111) surface. Strong activating (CN) and deactivating (NO\(_2\)) groups, on the other hand, have a distinct site preference. The nitrogen in the former prefers to lie above a silver atom (top site), but in the latter an Hhcp site of the Ag(111) surface is favored. Benzene derivatives with classic activating groups donate electron density from the highest occupied molecular orbital (HOMO) of the molecule to the surface, and those functionalized with deactivating groups withdraw electron density from the surface into orbitals that are unoccupied in the gas phase. In the case of disubstituted benzene, the strong activating/deactivating groups control the site preference and other groups assume sites that are, to a large degree, dictated by their positions on the benzene ring. Surface adsorption alters the relative stabilities of the ortho, meta and para positional isomers of disubstituted benzenes.

H1.00117 Quasi-1D States Confined in a Self-Assembled Organic Super-Lattice of TTF-TCNQ on Ag(111)1, SEOKMIN JEON, Oak Ridge National Laboratory (ORNL), PANCHAPAKESAN GANESHE, BOBBY SUMPTER, ORNL, JORGE IRIBAS CERDÁ, Instituto de Ciencia de Materiales de Madrid, PETRO MAKSYMOVYCH, ORNL, CNMS TEAM, ICMC-CSC TEAM — Organic charge transfer complexes (CTC) have drawn much attention due to their potential applications to conducting or semiconducting organic thin films and contacts in devices. TTF-TCNQ is a historic organic CTC with one of the highest conductivity values among numerous organic conductors. As a two-component molecular material, TTF-TCNQ in a low-dimension form on a surface naturally creates monolayer super-lattices with corrugated electrostatic potential and adsorbate-induced strain. Generally this will lead to strong confinement of the surface states, although the detailed response of the surface electronic structure remains to be understood. We investigated TTF-TCNQ monolayer films grown on Ag(111), Au(111) and Ag(100) surfaces using STM/STS at 4.3 K. Confinement of sp-derived surface states was indeed ubiquitous, including spontaneous formation of quantum dots and quasi-1D bands. The small periodicity of the lattice caused a complete depopulation of the surface states, with charge upshift of the band minimum — much stronger effect than normally observed in assemblies. This also allows us to infer the height of the confining potential using 1D Kronig-Penney model and critically assess the long-standing problem of molecule-surface charge transfer.

1A portion of this research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility

H1.00118 Adsorption of pentacene on (100) vicinal surfaces: role of coordination, surface chemistry and vdW effects1, JERONIMO MATOS, ABDEKADER KARA, University of Central Florida — In contrast to low miller index surfaces, vicinal surfaces are characterized by steps and step edges that not only present an interesting atomic landscape for the adsorption organic molecules, but also a unique electronic structure resulting in part from the low coordinated atoms at the step edges. The adsorption of pentacene on the stepped (511), (711), (911) surfaces (respectively 3, 4 and 5-atoms wide terraces of Cu and Ag (coincidence transition metals); Pt (reactive transition metal); and Ni (reactive, magnetic transition metal) are studied using density functional theory, in order to investigate the support effects arising from differing surface chemistry. We compare the adsorption energy, adsorption geometry and electronic structure predicted by the PBE functional with those obtained from one of the optimized vdW-DF methods: optB88-vdW.

1Work supported by the U.S. Department of Energy Basic Energy Science under Contract No DE-FG02-11ER64243

H1.00119 Electron configuration and correlation effects in organometallic molecules from constraint density functional theory, KENJI NAWA, KOHIJI NAKAMURA, TORU AKIYAMA, TOMONORI ITO, Mie University, MICHAEL WEINERT, University of Wisconsin-Milwaukee — Interest in single organometallic molecule and that adsorbed on solid surfaces has rapidly increased because of possible novel applications. For molecules with transition metals (TM), the \( d \)-electron configuration is an essential aspect of their electronic and magnetic properties, and correlation effects can not be excluded. Here, we investigate systematically the electron configuration and correlation effects for prototypical organometallic molecules of tridimensional metallocene (TMCP) and planer phthalocyanine (TMPC). Calculations were carried out based on the constraint density functional theory (DFT) by using the full-potential linearized augmented plane wave method that incorporates an on-site Coulomb interaction correction \( U \). We find that these correlation effects play a key role in determining the ground state of the organometallic molecules. The calculated ground states of TMCPs, where TM = Cr, Mn, Fe, Co, and Ni, obtained by constraint DFT with \( +U \) reproduce the experimentally determined structures of \( 3E_2g, 6A_1g, 1A_1g, 2E_2g, \) and \( 3A_2g \), respectively. Results for the TMPC will be also presented.

H1.00120 MAGNETISM —
H1.00121 Structural and Magnetic Properties of Mn$_{1.5}$X$_{0.5}$Sn (X = Cr, Mn, Fe, Co) Melt-spin Ribbons

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H1.00122 Noncollinear ferromagnetic easy axes in spin valves induced by oblique deposition

V. NAIK, Department of Natural Sciences, University of Michigan-Dearborn, Dearborn, Michigan, 48128, R. NAIK, Department of Physics and Astronomy, Wayne State University, Detroit, Michigan, 48202 — Magnetic hyperthermia (MHT) using magnetic nanoparticles (MNPs) is a promising technique for cancer therapy. The dominant mechanism of heat generation in MHT using superparamagnetic MNPs is the Néel relaxation in response to an applied ac magnetic field. The efficiency of heating depends on the particle size, particle size distribution and the intrinsic magnetic properties of the MNPs. In this study, we have prepared Fe$_3$O$_4$ (8-14 nm) and Co$_{60}$Fe$_{30}$O$_{70}$ (10 nm) MNPs by the co-precipitation method and characterized using XRD, TEM, Zeta potential and DC magnetometry measurements. The MNPs are found to be polydispersed and form stable colloidal suspensions in weakly basic solutions (zeta potential ~ 20 mV) with their hydrodynamic radii ranging from 80 to 120 nm. The specific power loss (SPL) was determined as a function of temperature using MHT measurements (140-235 Oe and 188-375 kHz) by incorporating heat losses due to nonadiabatic sample conditions. The SPL values at 298 K measured with 235 Oe and 375 kHz range from 20-95 W/g for the MNPs, and SPL monotonically decrease with increasing in temperature. The results are in agreement with the linear response theory. Details of the measurement and analyses will be presented.
H1.00126 Anatomy of Dzyaloshinskii-Moriya Interaction at Co/Pt Interfaces\(^1\), HONGXIN YANG, Spintec/INAC, Grenoble France, STANISLAS ROHART, ANDRE THIAVILLE, LPS, Universit Pariss-Sud, CNRS UMR 8502, F-91405 Orsay, France, ALBERT FERT, Unit Mixte de Physique CNRS/Thales, 91767 Palaiseau and Universit Pariss-Sud, 91405 Orsay, France, MAIRBEK CHISHIEV, Spintec/INAC, Grenoble France — Dzyaloshinskii-Moriya Interaction (DMI)\(^1\) was recognized to play a crucial role at ferromagnetic (FM)/heavy metal (NM) interfaces to create magnetic skyrmions\(^2\). DMI also plays an essential role for fast domain wall dynamics driven by spin-orbit (SO) torques\(^3\). Here, we clarify the main features and microscopic mechanisms of DMI in Co/Pt bilayers by ab initio. We find that large antilocalization DMI of the bilayers has a predominant contribution from DMI pair couplings between spins of interfacial Co layer. This DMI between interface Co spins is directly related to the change of SO energy in the adjacent Pt when Co spin chirality is reversed. DMI does not extend significantly into other Co layers and is very weak between the proximity-induced spins in Pt. It was suggested\(^4\) that DMI at FM/NM interfaces is directly related to the proximity induced moment in NM. However, we find the opposite result, i.e. Pt moment reduction slightly increases the DMI\(^5\). \(^1\) I. E. Dzialoshinskii, Sov. Phys. JETP 5, 1259 (1957); T. Moriya, Phys. Rev. 120, 91 (1960). \(^2\) A. Fert et al. Nat. Nanotech. 8, 152 (2013). \(^3\) A. Thiaville, et al, Europhys. Lett. 100, 57002 (2012). \(^4\) K. Ryu et al, Nat. Nanotech. 8, 527 (2013). \(^5\) H. Yang et al, submitted

H1.00127 Theory of damping for the standing spin waves, IRINA BARIAKHTAR, Boston College, USA, VICTOR BARIAKHTAR, Institute of Magnetism, Ukraine — It is well known, that the thin magnetic films exhibit dependency of the magnetic dispersion on the wave vector. This is due to the fact that in films with their thickness comparable to the exchange length, the wave vector of the spin waves becomes of the order of the exchange length because of the boundary conditions for magnetization. These kinds of thin films were studied at first by Kittel \(^1\). The standing spin waves are characterized by the fact, that under certain conditions they do not correlate to an alternating magnetic field within or outside the film \(^2\). The damping theory for the standing spin waves was not well studied yet. This problem appears interesting, since the distance between the neighboring standing spin waves increases with increasing number of frequency as \(n\), and the attenuation increases with a mode number increase as \(n^4\). In other words, high-frequency modes of the standing spin waves can be created if the exchange relaxation mechanism is valid. The standing spin waves properties are being well studied experimentally lately \(^3\). The authors would like to compare their theoretical results to the experimental data.

\(^1\) Phys. Rev. 110, 1295 (1958).

H1.00128 Controlling strain anisotropy in iron-palladium thin films using perovskite-oxide substrates, RENEE HARTON, VLADIMIR STOICA, ROY CLARKE, University of Michigan — In this study, iron-palladium (FePd) thin films were deposited on (100) barium-titanate (\(BaTiO_3\)) and (100) strontium-titanate (\(SrTiO_3\)) substrates. Both \(BaTiO_3\) and \(SrTiO_3\) have a perovskite crystal structure and exhibit similar structural phases, such as tetragonal and cubic, at various temperatures. In contrast to \(SrTiO_3\), \(BaTiO_3\) exhibits ferroelectric and piezoelectric behavior in all of its structural phases except the cubic phase. In the tetragonal phase, the strain anisotropy of \(BaTiO_3\) is two-fold about the in-plane c-axis, while in the cubic phase the epitaxial strain in the substrate plane is four-fold. In this investigation, the effect of strain on the magnetism and structure of FePd/\(SrTiO_3\) and FePd/\(BaTiO_3\) heterostructures was studied using the Magneto-Optic Kerr Effect (MOKE), Atomic Force Microscopy (AFM) and X-Ray diffraction (XRD) analysis to investigate the correlation between the magnetic anisotropy, morphology and structure of the FePd films.

H1.00129 Synthesis of magnetic GdC\(_2\) nanoparticles using cavitation plasma, RAKESH CHAUDHARY, ALI R. KOYMEN, Department of Physics, The University of Texas at Arlington — Gadolinium dicarbide (GdC\(_2\)) nanoparticles were synthesized using Gd electrodes in toluene. Gd nanoparticles are formed in plasma caused due to collapse of cavitation bubbles using ultrasonication in electric field between Gd wire electrodes. The presence of a single phase of GdC\(_2\) nanocrystals have been determined by X-Ray Diffraction (XRD) and High Resolution Transmission Electron Microscopy (HRTEM). The GdC\(_2\) nanoparticles have tetragonal crystal structure. Transmission Electron Microscopy (TEM) shows that the nanoparticles range in size of 4-45 nm in diameter. Magnetization measurements performed using a Superconducting Quantum Interference Device (SQUID) magnetometer shows GdC\(_2\) nanoparticles are paramagnetic in nature. To the best of our knowledge, this is the first synthesis of GdC\(_2\) in single phase form, allowing further characterization of physical properties.

H1.00130 Magnetic and Structural characterization of Co nanowires using advanced electron microscopy techniques\(^1\), JESUS CANTU-VALLE, FRANCISCO RUIZ-ZEPEDA, JOHN EDER SANCHEZ, FERNANDO MENDOZA-SANTOYO, ARTURO PONCE, University of Texas at San Antonio, UTSAA TEAM — We report the magnetic imaging and crystalline structure of high aspect ratio cobalt nanowires. Experimental results of magnetization reversal in cobalt nanowires are presented to illustrate the functionality of the in situ magnetization process through the manipulation of the objective lens. By making use of this applicability, we measure the magnetization and show experimental evidence of the magnetic flux distribution in polycrystalline cobalt nanowires using off-axis electron holography. The retrieved phase map can distinguish the magnetic contribution from the crystalline contribution with high accuracy. To determine the size and orientation of the grains within the Co nanowires, PED-assisted orientation mapping was performed. Finally, the magnetic analysis performed on individual nanowires was correlated with the crystalline orientation map, obtained by PED-assisted crystal phase orientation mapping. The large shape anisotropy determines the major magnetization direction rather than the magneto-crystalline anisotropy in the studied nanowires. The combination of the two techniques allowed us to directly visualize the effects of the crystallographic texture on the magnetization of the nanowire.

\(^{1}\)The authors would like to acknowledge Dr. B.J.H. Studler for providing the samples and financial support from NSF PREM #DMR 0934218, CONACYT, #215762 and Department of Defense #64756-RT-REP.

H1.00131 Magnetic properties of Ru-Ti doped Strontium hexaferrite nanocrystalline particles, ABDEL ALSMADI, Kuwait University, S. MAHMOOD, University of Jordan, I. BSOU, Al-Boyt University — We carried out a systematic study on the effect of the substitution of Ti\(^{4+}\) and Ru\(^{4+}\) ions for Fe\(^{3+}\) ions on the magnetic properties of the strontium ferrite \(SrFe_{12-x}Ru_xTi_{0.5}O_{19}\) nanoparticles with \(0 \leq x \leq 1\), using vibrating sample magnetometry, electrical resistivity, and Mössbauer spectroscopy. A clear irreversibility between the zero-field-cooled and field-cooled curves was observed below room temperature and the zero-field-cooled magnetization curves displayed a broad peak at a temperature \(T_M\). These results were discussed within the framework of random particle assembly model and associated with the magnetic domain wall motion. The resistivity data show some kind of a transition from insulator to perfect insulator around \(T_M\). With Ru-T substitution at \(T = 5\) K, the saturation magnetization showed small variations were slightly increased up to \(x = 0.2\) and then starts to decrease for \(x\) between 0.2 and 0.5, while the coercivity decreased monotonically, recording a reduction of about 93% at \(x = 0.4\). These results were discussed in light of the single ion anisotropy model and the cationic distributions based on the results of the Mössbauer spectroscopy data.
H1.00132 Doping controlled spin reorientation in dysprosium-samarium orthoferrite single crystals. SHIXUN CAO, WEIYAO ZHAO, BAOJUAN KANG, JINCANG ZHANG, WEI REN, Shanghai University — As one of the most important phase transitions, spin reorientation (SR) in rare earth transition metal oxides draws much attention of emerging materials technologies. The origin of SR is the competition between different spin configurations which possess different free energy. We report the control of spin reorientation (SR) transition in perovskite rare earth orthoferrite Dy$_{1-x}$Sm$_x$Fe$_3$O$_5$, a whole family of single crystals grown by optical floating zone method from $x=0$ to 1. Temperature dependence of the magnetizations under zero-field-cooling (ZFC) and field-cooling (FC) processes are studied. We have found a remarkable linear change of SR transition temperature in Sm-rich samples for $x>0.2$, which covers an extremely wide temperature range including room temperature. The $a$-axis magnetization curves under FC process bifurcated from and then jump down to that of warming process (ZFC and FCW curves) in single crystals when $x>0.5-0.9$, suggesting complicated 4f-3d electron interactions among Dy$^{3+}$-Sm$^{3+}$, Dy$^{3+}$-Fe$^{3+}$, and Sm$^{3+}$-Fe$^{3+}$ sublattices of diverse magnetic configurations for material physics and design. The magnetic properties and the doping effect on SR transition temperature in these single crystals might be useful in the spintronics device application.

3This work is supported by the National Key Basic Research Program of China (Grant No. 2015CB921600), and the National Natural Science Foundation of China (NSFC, Nos. 51372149, 50932003, 11274222)

H1.00133 Crystal structure and magnetic properties of 5d double perovskite oxide Sr$_2$EuOsO$_6$. JIANFENG HE, National Institute for Materials Science (NIMS), HAI L. FENG, Max Planck Institute for Chemical Physics of Solids, YAHUA YUAN, YOSHIHIRO TSUJIMOTO, KAZUNARI YAMAURA, National Institute for Materials Science (NIMS), SUPERCONDUCTING PROPERTIES UNIT, NATIONAL INSTITUTE FOR MATERIALS SCIENCE TEAM, GRADUATE SCHOOL OF CHEMICAL SCIENCES AND ENGINEERING, HOKKAIDO UNIVERSITY TEAM, MATERIALS PROCESSING UNIT, NATIONAL INSTITUTE FOR MATERIALS SCIENCE TEAM — Polycrystalline Sr$_2$EuOsO$_6$ has been synthesized with high-pressures and temperatures. It crystallizes in a monoclinic double perovskite structure and shows an antiferromagnetic-like transition at $51\,K$ in a magnetic susceptibility measurement. The transition has been further characterized by specific measurements and electrical resistivity measurements. The results are compared with the magnetic properties of Ba$_2$EuOsO$_6$ [1] and other double perovskite oxides containing Os(V) atom. We will discuss role of spin-orbit coupling and spin polarization on the gapped electronic structure of Sr$_2$EuOsO$_6$ and other related compounds.


H1.00134 Thermal fluctuations in novel artificial spin ice. HENRY STOPPEL, ERIK OSTMAN, UU, AARON STEIN, CFN, UNNAR ARNALDS, UI, VASSILIOS KAPAKLIS, BJORGVIN HJORVARSSON, UU, UU TEAM1, CFN COLLABORATION2, UI COLLABORATION3 — Artificial spin ice (ASI) is used as a model material to investigate frustrated systems. The square and kagome ASI has been extensively investigated since there discovery. Novel ASI structures like the Shakti lattice, have been proposed and already realized. In this structure what is not an admixture of natural magnetic materials the lattice topology leads to a high degree of degeneracy. We present here the results of Photoemission electron microscopy (using XMCID) to image the magnetization of nano-islands in a Shakti ASI. By using a three layer of Pd-Fe-Pd we can tune the Curie temperature of our magnetic material by varying the thickness of the Fe-layer. Beside a statistical analysis of the frozen-in ground state, we present also a temperature series, in which we could visualize the two energy levels of the small and large islands and due to this the different blocking temperatures for these islands. This comparison of these measurements with previous measurements on squared ASI give us a better understanding of the magnetic ordering and the thermal fluctuations in the novel Shakti ASI.

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H1.00135 Negative magnetization and exchange bias in Y$_1$-xPr$_x$CrO$_3$ with (0>x>0.3). E. VERDIN, Departamento de Fisica, Universidad de Sonora, A. DURAN, Centro de Nanociencias y Nanotecnología-UNAM, F. MORALES, E. ESCUDERO, Instituto de Investigaciones en Materiales-UNAM — Rare earth orthochromites compounds with perovskite structure have attracted great interest because their potential applications as data storage and spintronics. We report studies of the crystalline structure, thermal, and magnetic properties performed in the compound Y$_{1-x}$Pr$_x$CrO$_3$ with 0<x<0.3. We found changes in the specific heat and in the magnetization when the Pr atoms are substituted in the compound. The antiferromagnetic transition, $T_N$, increases when the Pr atoms are introduced into the compound which is clearly observed by specific heat and magnetization measurements. We also found an exchange bias and magnetization reversal when the magnetization-temperature (M-T) curves were measured in field cooled mode (FC). All those changes are attributed to the influence of the Dzialoshinskii-Moriya indirect interaction that we related to the octahedral distortion, because the Pr substitution affecting the Cr-O bond lengths.

3This work was partially supported by DGAPA-UNAM, IN103213, IN10014, CONACyT-Mexico, project 129293, BISSNANO, and by the Institute of Sciences project PICCO 11-7, Distrito Federal, Mexico.

H1.00136 Neutron diffraction study on the phase diagram in muliferroic DyFeO$_3$. JINCHEN WANG, JUANJUAN LIU, JIEMING SHENG, Renmin Univ of China, ZHYING ZHAO, XIA ZHAO, XUEFENG SUN, University of Science and Technology of China, SERGEY DANIILKIN, Australian Nuclear Science and Technology Organisation, WEI BAO, Renmin Univ of China — The discovery of the muiferroic effect in perovskite DyFeO$_3$ opens the door to a new field of study with magnetic-electric coupling. In this low temperature and high magnetic-field single-crystal neutron diffraction study, we determined the magnetic phase-diagram of DyFeO$_3$. Although the weak ferromagnetic phase of Fe spins has been suggested to be instrumental to the strong multiferroic effect in current experimental and theoretical works, the multiferroic effect is observed only in the phase area where the applied magnetic field breaks the long-range ordered (LRO) AF order of the Dy ions into a short-range order (SRO). Our results suggest the mechanism of the remarkably strong multiferroic effect in the prototype rare-earth orthoferrite DyFeO$_3$ ought to be investigated through the interplay between the weak ferromagnetism of Fe and the antiferromagnetic SRO of Dy spins.

H1.00137 Engineering magnetic properties and microstructure of La$_2$CoMnO$_6$ thin films by tailoring the oxygen stoichiometry. BENJAMIN MARTINEZ, REGINA GALCERAN, CARLOS FRONTERA, LLUIS BACELLS, JOSE CISNEROS-FERANDEZ, ICMAB-CSIC, JAUME ROQUETA, JOSE SANTISO, ICN2-CSIC, ALBERTO POMAR, FELIP SANJUANMIECE, ICMAB-CSIC, ADVANCED MATERIALS CHARACTERIZATION TEAM, THIN FILMS GROWTH TEAM — We report on the magnetic and structural properties of ferromagnetic-insulating La$_2$CoMnO$_6$ thin films grown on top of (001) STO substrates by means of RF sputtering technique. Insulating ferromagnets are of interest because of the exchange splitting of the bands allowing obtaining tunnel barriers with different height for spin-up and spin-down carriers. Belonging to the perovskite family, this material can be easily integrated in spintronic devices, such as magnetic tunneling junctions and spin filters, with upgraded and distinctive functionalities. An exhaustive structural analysis, by using synchrotron X-ray diffraction, allows identifying a close correlation between the film composition and their magnetic properties. Both Curie temperature and the features of the hysteresis loops turn out to be dependent on the oxygen stoichiometry. In situ annealing conditions allow tailoring the oxygen content of the films, therefore controlling their microstructure and magnetic properties. On the other hand, transport measurements confirm the insulating character of the films.

3We acknowledge financial support from the Spanish MINECO (MAT2012-33207).
H1.00138 Magnetic and thermoelectric properties of Fe$_{3-x}$Co$_x$O$_4$ thin films and CoFe$_2$O$_4$/Fe$_3$O$_4$ superlattices. QUANG NGUYEN VAN, University of Ulsan, Korea. MELY CHRISTIAN, Institute of Physics and Chemistry for Materials of Strasbourg, UMR 7504 UDS-CNRS, Strasbourg, France, ANH TUAN DUONG, YOOLEMI SHIN, RHIH S. H, MINH HAI NGUYEN THI, SUNGLAE CHO, University of Ulsan, Korea — Microcrystalline ferrites are used as a medium for the magnetic storage and as a sensor of information. Magnetite, Fe$_3$O$_4$, is a ferrimagnet with a cubic inverse spin structure and exhibits a metal-insulator, Verwey, transition at about 120 K. It is predicted to possess as half-metallic nature, ~100% spin polarization, and high Tc (~580 K). Cobalt ferrite, Co$_3$O$_4$, is one of the most important members of the ferrite family, which is characterized by its high Hc, moderate magnetization, and very high magneto-crystalline anisotropy. Here we report on the magnetic and thermoelectric properties of Fe$_{3-x}$Co$_x$O$_4$ (x = 0 to 1) thin films and CoFe$_2$O$_4$/Fe$_3$O$_4$ superlattices grown on MgO (100) by MBE. XRD and RHEED patterns confirmed the inverse spinel structure of the Fe$_3$O$_4$ films. Magnetic properties of the Fe$_{3-x}$Co$_x$O$_4$ films are markedly sensitive to the Co content. The Verwey transition was disappeared in Co-doped films. A negative MR curve with butterfly shape was observed with low Co content but disappeared for the samples with x = 0.8 and 1. Seebeck coefficients increased with Co concentration; -70 µV/K for x=0 and -220 µV/K for x=1. We will also discuss on the relationship between magnetic and thermoelectric characteristics in CoFe$_2$O$_4$/Fe$_3$O$_4$ superlattices with the modulations of 5, 10, and 20 nm.

H1.00139 Magnetic and electrical properties on possible room temperature hybrid multiferroic BaTiO$_3$/La$_{2/3}$Sr$_{1/3}$MnO$_3$. JOHN EDWARD ORDOÑEZ, MARÍA ELENA GÓMEZ, WILSON LOPERA MUÑOZ, Universidad del Valle, Cali, Colombia. PEDRO ANTONIO PRIETO, Center of Excellence on Novel Materials — CENM, Cali, Colombia. THIN FILM GROUP TEAM, CENTER OF EXCELLENCE ON NOVEL MATERIALS — CENM, Cali, Colombia. — We addressed to deposit the ferromagnetic phase of the La$_{1-x}$Sr$_x$MnO$_3$ and the ferroelectric BaTiO$_3$ for possible hybrid multiferroic heterostructure. We have optimized the growth parameters for depositing BaTiO$_3$(BTO) / La$_{2/3}$Sr$_{1/3}$MnO$_3$(LMO) / (001) SrTiO$_3$ by sputtering RF and DC, respectively, in pure oxygen atmosphere and at a substrate temperature of 830°C. Keeping fixed the magnetic layer thickness (t$_{BTO}$=40 nm) and varying the thickness of the ferroelectric layer (t$_{BTO}$ = 20, 40, 80, 100 nm). We want to point out the influence of the thicknesses ratio (t$_{BTO}$/t$_{LMO}$) on electrical and magnetic properties. From x-ray diffraction (XRD) analysis, we found the bragg peaks for LSMO maintain its position but BTO peak shifted to lower Bragg angle indicating a strained BTO film. Magnetization and polarization measurements indicate a possible multiferroic behavior in the bilayers. Hysteresis loop measurements of bilayers show ferromagnetic behavior.

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H1.00140 Magnetization fluctuation in FeB nanomagnets under asymmetric magnetization-potential. SHINJI MIWA, Osaka Univ., HIZO KUBOTA, KAY YAKUSHIJI, AIST, SHOTA ISHIBASHI, Osaka Univ., TAKESHI SARUYA, AKIO FUKUSHIMA, SHINJI YUSA, AIST, YOSHIHIGE SUZUKI, Osaka Univ. — Thermal fluctuation of magnetizations gives understandings of physics in magnetic materials and noise in magnetic devices. It is theoretically calculated using the Fokker-Planck equation and the fluctuation-dissipation theorem, [1] and is experimentally characterized using magnetoreisitive devices [2]. In the present study, the magnetization-fluctuation under asymmetric magnetization potential has been investigated. Magnetic tunnel junctions (MTJs) [CoFeB(3 nm)/ MgO(1 nm)/ FeB (2 nm)] were employed to conduct the study. The FeB layer (120 nm in a diameter) is a magnetic free layer whose magnetic anisotropies are B mT (in-plane) and 97 mT (perpendicular). The asymmetric magnetization-potential was prepared using magnetic field application (110 mT) tilted from the film normal (10 deg.). [3] Unlike the first-order response to the thermal fluctuation, [2] the second-order response is identified as a Lorentzian power spectrum whose peak appears at 0 Hz. To derive the analytic formula, fourth-order moments are calculated using the quasi-normality hypothesis (⟨ABCD⟩ = ⟨AB⟩ ⟨CD⟩ + ⟨AC⟩ ⟨BD⟩ + ⟨AD⟩ ⟨BC⟩). As a results, the obtained formula quantitatively reproduces the experiment.


2This work was supported by JSPS KAKENHI (No. 23226001).

H1.00141 Exchange interaction reduction as a precursor to laser-induced demagnetization in ferromagnets. GUOPING ZHANG, YIHUA BAI, Indiana State University. THOMAS F. GEORGE, University of Missouri-St. Louis. — Laser-induced femtosecond demagnetization in a ferromagnet presents an opportunity to develop all-optical ultrafast magnetic storage devices, but its underlying mechanism is under intense debate. The controversy has been on the first several hundred femtoseconds, where the spin moment is reduced sharply up to 50% or higher, but the optically accessible electrons are very few. This apparent contradiction is puzzling. Here we show that a small number of excited electrons is enough to trigger a strong band structure relaxation. In all of the three 3d ferromagnets investigated here, this band relaxation sharply reduces the exchange splitting and spin moment. For fcc Ni, for every electron excited, the spin moment can be reduced by 0.23 µ$_B$ to trigger a strong band structure relaxation. In all of the three 3d ferromagnets investigated here, the optically accessible electrons are very few. This apparent contradiction is puzzling. Here we show that a small number of excited electrons is enough to trigger a strong band structure relaxation. In all of the three 3d ferromagnets investigated here, this band relaxation sharply reduces the exchange splitting and spin moment. For fcc Ni, for every electron excited, the spin moment can be reduced by 0.23 µ$_B$ to trigger a strong band structure relaxation. In all of the three 3d ferromagnets investigated here, the optically accessible electrons are very few. This apparent contradiction is puzzling. Here we show that a small number of excited electrons is enough to trigger a strong band structure relaxation. In all of the three 3d ferromagnets investigated here, this band relaxation sharply reduces the exchange splitting and spin moment. For fcc Ni, for every electron excited, the spin moment can be reduced by 0.23 µ$_B$ or more. Our first-principles calculation, free of fitting parameters of any kind, finally explains the experimental findings and presents a paradigm for future experiments.

1 Solely supported by the U.S. Department of Energy under Contract No. DE-FG02-06ER46304. The work was done on Indiana State University’s quantum cluster and high-performance computers and used resources of NERSC at BNL.

H1.00142 A mechanical analogy for spin currents and torques. YAROSLAV BAZALIY, University of South Carolina. — We map the problem of spin-transfer torques in nanostructures with diffusive spin currents on a mechanical problem involving elastic strings connecting points of attachment that slide along the fixed straight rails. The obtained mechanical analogy provides a qualitative understanding of the effects of spin relaxation on spin torques, and of the phenomenon of sign-changing angular dependence [1-3] of the efficiency factor g(θ).


1 Supported by NSF grant DMR-0847159.
H1.00143 Ultra Low Energy Switching of Ferromagnet with Perpendicular Anisotropy on Topological Insulator by Voltage Controlled Magnetic Anisotropy1, BAHMINAM GHOSH, TANMOY PRAMANI, RIK DEY, URMIMAALA ROY, LEONARD REGISTER, SANJAY BANERJEE, Microelectronics Research Center, Univ of Texas at Austin — We propose and demonstrate, through simulation, an ultra low energy memory device on a topological insulator thin film. The device consists of a thin layer of Fe deposited on the surface of a topological insulator, \( \text{Bi}_2\text{Se}_3 \). The top surface of Fe is covered with MgO so that the ferromagnetic layer has perpendicular anisotropy. Current is passed on the surface of the topological insulator which switches the magnetization of the Fe ferromagnet through strong exchange interaction, between electrons contributing to the surface current on the \( \text{Bi}_2\text{Se}_3 \) and the d electrons in the ferromagnet, and spin transfer torque due to shunting of current through the ferromagnet. Voltage controlled magnetic anisotropy enables ultra low energy switching. Our micromagnetic simulations, predict switching time of the order of 2.4 ns and switching energy of the order of 0.16 fJ for a ferromagnetic bit with thermal stability of 90 k\(_B\)T. The proposed structure combines the advantages of both large spin torque from topological insulators and those of perpendicular anisotropy materials.

1This work is supported by NRI SWAN and NSF NASCENT Center.

H1.00144 Capturing the Magnetic and Structural Phase Transition of Ferurh through Extreme Ultraviolet Light1, DMITRIY ZUSIN, PATRICK GRYCHTOL, CHRISTIAN GENTRY, MARGARET MURNANE, HENRY KAPTEYN, JILA, University of Colorado, Boulder, CO 80309, SOPHIE CANTON, Max-Lab, Lund University, SE-223 63 Lund, Sweden, RONNY KNUT, JUSTIN SHAW, HANS NEMBACH, THOMAS SILVA, Electromagnetics Division, National Institute of Standards and Technology, Boulder, CO 80305, ALEJANDRO CEBALLOS, CATHERINE BORDEL, PETER FISCHER, FRANCES HELLMAN, University of California, Berkeley, CA 94720 — The temperature dependent transition from the anti-ferromagnetic to the ferromagnetic phase in FeRh is accompanied by a modification of its crystal lattice. The interplay between the magnetic and the structural transition is a matter of strong debate. It is important to better understand the mechanism(s) of the transition since it can be induced by femtosecond laser pulses and, unlike slower (nanosecond) magnetic phase transitions, does not seem to be limited by heat transfer. In this work, we use extreme ultraviolet light generated by a tabletop high harmonics source to perform element-selective investigations of the temperature-dependent magneto-optical response of a thin film FeRh sample. We study the optically induced phase transition using two ultrafast pump-probe spectroscopy approaches: by monitoring the time-resolved transversal magneto-optical Kerr effect (T-MOKE) and the transient change in reflectivity.

1PF acknowledges support from BES MSD DOE # DE-AC02-05-CH11231 and LFRIR program (# 2012K1A4A305565) through NRF Korea funded by MEST, and JILA from DOE # DE-FG02-09ER4665.

H1.00145 The effects of shape anisotropy and exchange coupling on spin precession frequencies in exchange coupled Co/Cu/Pt trilayers1, SAM KERAMATI, UDAY SINGH, SETH KURFMAN, CH. BINEK, S. ADENWALLA, Univ of Nebraska - Lincoln — Ultrafast high-power laser systems have successfully opened up the field of magnetization dynamics, studying subpicosecond laser-induced spin precession dynamics, demagnetization processes and magnetization reorientation. Here we investigate laser-induced magnetization dynamics in a series of photolithographically patterned microstructures of exchange coupled trilayers of Co/Cu/Pt grown on Si substrates. The microstructures have different shape anisotropies as well as different exchange coupling parameters. The latter determines the magnetization state, varying from ferromagnetically to anti-ferromagnetically coupled. We explore how the different spin precession frequencies of the constituent exchange coupled magnetic layers with unequal relaxation times can trade-off with the differing shape anisotropies. The key physical point is that the precession frequency of ferromagnetic materials and their damping parameter vary with the effective field which depends on both the shape anisotropy, and exchange coupling, while their corresponding effects can be modulated through the action of the intense pump beam. Precession frequency maps of the behavior of the exchange coupling parameter of the samples with respect to their shape anisotropy and their laser-induced modulated precession frequencies will be generated through a pump-probe experiment to address the above-mentioned objective of our work.

1This work is supported by NSF Grant No. 1409622 and MRSEC DMR-0820521.

H1.00146 Electron Irradiation Induced Modification of Ferromagnetism in (Ga,Mn)As1, JIA LUO, GANG XIAO, Department of Physics and Key Laboratory for Radiation Physics and Technology of Ministry of Education, Sichuan University — The ferromagnetism properties of diluted magnetic semiconductor (Ga,Mn)As firstly improved by energetic electron irradiation, through a sequence of irradiation doses. We did a systematic study of magnetization as a function of temperature and additional magnetic field. SQUID measurements demonstrate the \( T_c \) of all (Ga,Mn)As film increased from 40K to 60K after irradiation. At the same time, electron irradiation improved the crystal quality and electric properties. The irradiation process decreases the resistance by a factor of 1/2 in the range of 10K to 50K, and transforms (Ga,Mn)As samples from insulator behavior to metallic behavior. SIMS and transport measurements confirm that the rearrangement of Mn interstitials plays a key role in the improvement of ferromagnetism properties. We infer that electron irradiation paves a new path to room-temperature ferromagnetism of (Ga,Mn)As.

1Natural Science Foundation of China (NSFC) Grant Nos. 1140414111004142, and 1174212

H1.00147 ABSTRACT WITHDRAWN —

H1.00148 Dynamics of bright and dark localized excitonic magnetic polarons in CdMnTe spin glass compound, YURIY GNATENKO, PETRO BUKIVSKII, YURIY PIARYATINSKI, Institute of Physics of National Academy of Science of Ukraine — The measurements of the magnetic properties of spin glass (SG) system indicate that the magnetic relaxation is characterized by a broad range of times below \( T_f \). Here, for the first time, we have investigated time-resolved photoluminescence spectra of Cd\(_{1-x}\)Mn\(_x\)Te SG compound at the temperature below the freezing temperature \( T_f \). This enables us to study the dynamics of different localized excitonic magnetic polarons (LEMPs) at \( T = 0.7 T_f \) excited in the crystal regions where various microscopic magnetic spin states (MMSs) are formed. It was found that there is a broad distribution of the lifetimes of the LEMPs which have different lifetimes but same energies. It was also found that the decay process of the PL exciton band intensity is described by the Kohlrausch—Williams—Watts stretched exponential function which describes the recombination processes which correspond to the emission of the LEMPs formed in the crystal region of the finite clusters as well as the infinite cluster. These complex dynamical phenomena, observed for Cd\(_{1-x}\)Mn\(_x\)Te at low temperatures, reflect the spatially heterogeneous dynamics in the SG system which is due to the presence of different MMSs below \( T_f \).
**H1.00149** Ferruquadrupolar phase of the Heisenberg model with bilinear and biquadratic interactions\(^1\)  
ANTONIO PIRES, Universidade Federal de Minas Gerais — The Heisenberg antiferromagnet with bilinear and biquadratic exchange interactions has been studied using several techniques. In contrast to bilinear interactions models, quantum spin models with biquadratic interactions present a phase diagram qualitatively different from their classical counterparts, as for instance nonmagnetic phases such as the quadrupolar phase. In this work I will study the ferruquadrupolar phase of the \( S = 1 \) Heisenberg model with bilinear and biquadratic exchange interactions on the square lattice using a SU(3) Schwinger boson formalism in a mean field approximation. This nonmagnetic phase is characterized by a finite quadrupole moment. I will calculate the quadrupole moment and the static spin structure factor for several values of the parameters involved in the model. The results obtained will also be compared with the ones obtained from other theories.

\(^1\)I acknowledge support from CNPQ

**H1.00150** Effect of Zn substitution on the magnetic properties of Skyrmion \( \text{Cu}_2\text{OSeO}_4 \).  
TIEN-YU WEI, HUNG-CHENG WU, KAKARLA DEVI CHANDRASEKHAR, HUNG-DUEN YANG, Natl Sun Yat Sen Univ, NATIONAL SUN YAT-SEN UNIVERSITY TEAM — There is a considerable interest in the new magnetic state, the “Skyrmion state (A-phase),” whose magnetic properties have a remarkable characteristic as a vortex-like spin orientation. The polycrystalline \( (\text{Cu}_1-x\text{Zn})_2\text{OSeO}_4 \) \((x = 0 \text{ to } 0.20)\) samples were synthesized using solid state reaction method and studied by X-ray diffraction, X-ray absorption spectra and magnetic measurements. Variation of lattice constant with Zn doping follows the Vegard’s law which signifies the successful substitution of Zn in place of Cu up to \( x \) less than 0.20. The Cu L\(_2,3\) spectra show 2+ valence state for all samples. The Curie temperature decrease with Zn doping indicate the ferrimagnetic ordering is gradually suppressed. Moreover, we have notice another magnetic phase for the doping level \( x \) between 0.05 and 0.2, whose magnetic transition also shifted to low temperature for higher Zn doping. The H-T magnetic phase diagrams of the samples from ac susceptibility have been established with increasing Zn doping. The explanations for the observations of doping effects on the A-phase of Skyrmion \( \text{Cu}_2\text{OSeO}_4 \) will be discussed.

**H1.00151** Effect of Ni substitution on the magnetic properties of Skyrmion \( \text{Cu}_2\text{OSeO}_4 \).  
CHUNG-LUN HUANG, HUNG-CHENG WU, KAKARLA DEVII CHANDRA SEKHAR, HUNG-DUEN YANG, Natl Sun Yat Sen Univ, NATIONAL SUN YAT-SEN UNIVERSITY TEAM — Chiral magnetic lattice of \( \text{Cu}_2\text{OSeO}_4 \) exhibits such kind of unique magnetic ordering where spins form the vortex like ordering called as Skyrmion. In this paper, the effects of isovalent ion doping on the Skyrmion phase of \( \text{Cu}_2\text{OSeO}_4 \) were presented. Polycrystalline \( (\text{Cu}_1-x\text{Ni})_2\text{OSeO}_4 \) \((x = 0.0 \text{ to } 0.1)\) samples were prepared by solid standard-state methods. Temperature and magnetic field dependent AC and DC magnetic measurements were performed. The Curie temperature decreases obviously with increasing Ni concentration by using ac susceptibility \((\chi_{ac}-T)\). Systematic H-T phase diagrams indicating the effects of Ni doping are established and will be discussed.

**H1.00152** High pressure and doping effect on the magnetic properties of \( \text{CaMn}_2\text{O}_4 \).  
KUN-JU HSIEH, HONG-CHEN WU, KAKARLA D. CHANDRA SEKHAR, HUNG-DUEN YANG, Natl Sun Yat Sen Univ, NATIONAL SUN YAT-SEN UNIVERSITY TEAM — Polycrystalline \( \text{Ca}_1-x\text{Sr}_x\text{Mn}_2\text{O}_4 \) \((x = 0.05, 0.10, 0.15, \text{ and } 0.20)\) compounds were synthesized using solid state reaction method. Samples were characterized by X-ray diffraction and magnetization measurements. The lattice constants \((a, b, \text{ and } c)\) determined by Rietveld refinement increases with Sr substitution. \( \text{CaMn}_2\text{O}_4 \) shows antiferromagnetic transition \( T_N \) near 220 K due to the Mn(III)-O-Mn(III) superexchange interaction. High-pressure effect on the \( T_N \) of \( \text{CaMn}_2\text{O}_4 \) has been investigated using piston-cylinder high-pressure apparatus designed for MPMS-XL7 magnetometer. It is found that the \( T_N \) increases with applying pressure up to 17.7 kbar at a rate of 0.487(22) K/kbar and decreases with higher Sr content.

**H1.00153** Exact Diagonalization of a Quantum Ising Model with Long-Range Interactions.  
SHANNA MUEHE, THOMAS GUINN, Univ of West Florida, C.C.-JOSEPH WANG, None, CHRISTOPHER VARNEY, Univ of West Florida — Due to the rapid advance of quantum spin simulators in ultra-cold ions, the varying interaction for spin models in two-dimensional lattices have become feasible for experimental exploration for exotic states of collective states of multiple spins. It is particularly interesting for the case of a triangular lattice with antiferromagnetic interaction between spins. When the Ising spin-spin interaction is uniform and restricted between nearest neighbors, the spins are geometrically frustrated. When the system interaction becomes long ranged, the geometric frustration is lost but the spins are frustrated by the long-range interaction. In the latter case, the underlying orders present in the ground state are unclear and understanding these states in finite spin systems is crucial for the benchmarking of experimental observations. Here, we investigate the quantum dilopar Ising model with exact diagonalization to analyze the ground state, order parameters, and excitations and provide a baseline for comparison with experiments.

**H1.00154** Exchange interaction between \( J \)-multiplets.  
NAOYA IWAKARA, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven — The crystal-field levels in lanthanides and other metal complexes with unquenched orbital momentum originate from the ground atomic \( J \)-multiplet. It was long believed that the exchange interaction between \( J \)-multiplets is basically described by Heisenberg form, \( J_1 \) \(-\) \( J_2 \). In this work, Anderson’s superexchange model is applied for analytical derivation of exchange interaction between arbitrary \( J_1 \) \(-\) \( J_2 \) \( J \)-multiplets \((1)\). The structure and the energy spectrum of the obtained exchange Hamiltonian are significantly different from those of a Heisenberg Hamiltonian. Besides, it is also found that the \( 1/U \) approximation \((2)\) is not applicable for the description of exchange spectrum, since it gives qualitatively different predictions compared to the present treatment. Similar results are obtained for the exchange interaction between \( J \)-multiplet \((J_1)\) and isotropic magnetic center \((S_2)\).


**H1.00155** The origin of magnetic ordering in quasi-two-dimensional quantum magnets \( \text{Cu}(en)(\text{H}_2\text{O})_2\text{SO}_4 \).  
ALZBETA ORENDACOVA, P.J. Safarik University, Park Angelinum 9, 041 54 Kosice, Slovakia, LUCIA BARANOVA, Technical University of Kosice, Vysokeškolska 4, 042 00 Kosice, Slovakia, ROBERT TARASENKO, MARTIN ORENDAC, ALEXANDER FEHER, P.J. Safarik University, Park Angelinum 9, 041 54 Kosice, Slovakia, RUDOLF SYKORA, DOMINIK LEGUT, VSB-Technical University of Ostrava, 17. listopadu 15, Ostrava 70833, Czech Republic — A comparative analysis of magnetic properties of \( \text{Cu}(en)(\text{H}_2\text{O})_2\text{SO}_4 \) \((en = \text{C}_6\text{H}_5\text{N}_2)\) \((1)\) and \( \text{Cu}(en)(\text{Cl}_2)(en = \text{C}_6\text{H}_5\text{N}_2)\) \((2)\) has been performed to search for the origin of magnetic ordering observed in \((1)\) at \( T_c = 0.9 \) K while hidden in \((2)\). Previously, both materials were approximated by a quasi-two-dimensional \((2d)\) spin \(1/2\) Heisenberg model on the square lattice with effective intralayer and interlayer coupling \( J/\beta = K = 3 \) and \( J' = 10^{-3}J \), respectively. The first principles calculations revealed in \((1)\) a spatial anisotropy of exchange coupling within a layer, \( J_1/J_2 = 0.15 \), in agreement with a provoking data set to 3D behavior. Considering only effect of interlayer coupling, \( T_c = 0.8 \) K was evaluated, while \( T_c = 0.85 \) K, when a weak Ising-like spin anisotropy, \( \Delta = 0.015 \) was introduced into Heisenberg layers. The effects of spin and spatial anisotropy on the ordering of \((1)\) and the absence of a phase transition in \((2)\) are discussed.

\[1\] Supported by CFNT MVEP, ITMS26220120005, APVV 0132-11, SK-CZ-2013-0083, CZ.1.07/2.3.00/30.0055, and CZ.1.05/1.1.00/02.0070.
H1.00156 Thermodynamic properties of a layered $S = 7/2$ Heisenberg magnet Gd(OH)CO$_{3}$,1 M. Orendac, M. Ulcny, E. Cizmar, A. Orendacova, J. P. Safarik University, Park Angelinum 9, 040 01 Kosice, Slovakia, Y. Cong Chen, Zhaoshan Meng, Mingliang Tong, Sun Yat-Sen University, Guangzhou, 510275, P. R. China. — Thermodynamic quantities and ESR spectra of Gd(OH)CO$_{3}$ (I) are reported. The material may be considered to consist of weakly coupled layers with potentially triangular arrangement of exchange paths within each layer. Different bridging groups and distances among Gd$^{3+}$ ions may be responsible for spatial anisotropy of magnetic coupling. Preliminary analysis of magnetic susceptibility using Curie-Weiss law yielded $\theta = -1.05$ K indicating weak antiferromagnetic coupling and consequently, spin frustration in (I). More detailed simultaneous analysis of specific heat, susceptibility and magnetization studied down to nominally 0.45 K revealed non-negligible role of single-ion anisotropy. Using the model of weakly interacting S=7/2 trimer, the gross features of measured data may be explained while assuming single-ion anisotropy $D/k_B \approx 0.6$ K and effective intratramer magnetic coupling $|J/k_B| \approx 0.3$ K. The obtained $D$ value reasonably reproduces the position and shape of ESR line. The performed analysis suggests that magnetism in (I) is governed predominantly by crystal field effects and frustration plays a minor role.

1Supported by ITMS26220120005 and VEGA I/0143/13.

H1.00157 The structural, electronic and magnetic properties of Ga$_8$-xMn$_x$As$_8$ clusters,1... Gangu Xu Gu, Gang Xiang, College of Physical Science and Technology, Sichuan University — We systematically investigate the ground-state magnetic properties of Ga$_8$-xMn$_x$As$_8$ clusters (x = 0, 2, 4, 6, 8) within the framework of density functional theory (DFT) using a strategy that successively adopts the particle swarm optimization (CALYPSO) code and fixed spin-moment (FSM) method. The results show that for Ga$_8$-xMn$_x$As$_8$ in the ground states or low-lying isomers, Mn atoms tend to assemble at the core of the clusters and the ferrimagnetic Mn-Mn couplings are identified for Ga$_8$-xMn$_x$As$_8$ (x = 4, 6, 8), while Ga$_8$As$_8$ and Ga$_6$Mn$_2$As$_8$ are nonmagnetic. The possibility of multiple ground states of Ga$_8$-xMn$_x$As$_8$ (x = 4, 6, 8) is also demonstrated. The binding energy and LUMO-HOMO gap analysis show that Ga$_8$-xMn$_x$As$_8$ clusters with large x are more likely synthesized and exhibit stronger chemical reactivity.

1the Natural Science Foundation of China (NSFC) Grant No. 11174212

H1.00158 Quantum oscillations of the mechanical forces in rotating molecular magnets,1... Kwang-Hee Kim, Sejong University — We study a rotating nanomagnet that exhibits beat structure of the quantum forces. We show that such forces are originated from tunneling between two entangled states of spin and mechanical angular momentum. They can be observed in the presence of a static magnetic field gradient with ac magnetic field and disappear on increasing total angular momentum and parameter which depends on the moment of inertia and the tunnel splitting.

H1.00159 Uniaxial-pressure dependence of the magnetization dynamics in the high-symmetry single-molecule magnet Mn$_{12}$-MeOH,1... James H. Atkinson, Department of Physics, University of Central Florida, Orlando, FL, and the Department of Physics, Amherst College, Amherst, MA, Lakshmi Bhaskaran, Stephen Hill, National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, FL, Yury Myasoedov, Eli Zeldov, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel, Jonathan F. Bredl, Department of Physics, Amherst College, Amherst, MA, Adeline Fournet, George Christou, Department of Chemistry, University of Florida, Gainesville, FL — The single-molecule magnet [Mn$_{12}$O$_{12}$(O$_2$CCH$_3$)$_{16}$(CH$_3$OH)$_4$]CH$_3$OH ("Mn$_{12}$-MeOH") is a high-symmetry sibling of the Mn$_{12}$-Acetate SMM that offers a prime opportunity to explore the consequences of molecular symmetry. A previous study [1] has shown that applied pressure induced changes in the Mn$_{12}$-Acetate’s anisotropy parameters. Here we present the results of a study in which uniaxial pressure was applied to a crystalline sample of Mn$_{12}$-MeOH in order to examine how the pressure affects the quantum tunneling of magnetization at low temperature. We find that the pressure induces an increase in the resonant tunneling rate manifested as a change in the height of the tunneling steps in the magnetic hysteresis. These results suggest that pressure is altering symmetry-breaking terms in the molecule’s spin Hamiltonian, giving rise to increased tunneling.


H1.00160 Phase transitions of a quantum chain with four-spin interactions in longitudinal and transverse magnetic fields, B. Boechat, J. Florencio, A. Sagui, Universidade Federal Fluminense, O. F. de Alcantara Bonfim, University of Portland — We study the ground-state properties of a spin-1/2 model on a chain containing four-spin Ising-like interactions in the presence of both transverse and longitudinal magnetic fields. We use entanglement entropy and finite-size scaling methods to obtain the phase diagrams of the model. Our numerical calculations reveal a rich variety of phases and the existence of multi-critical points in the system. We identify phases with both ferromagnetic and anti-ferromagnetic orderings. We also find periodically modulated orderings formed by a cluster of like-spins followed by another cluster of opposite like-spins. The quantum phases in the model are found to be separated by either first or second order transition lines.

H1.00161 Quantum criticality in a magnetic chain with two- and four-spin interactions in a transverse field, O. F. de Alcantara Bonfim, University of Portland, A. Sagui, B. Boechat, J. Florencio, Universidade Federal Fluminense — We use entanglement entropy and finite-size scaling methods to investigate the ground-state properties of a spin-1/2 Ising chain with two-spin $(J_1)$ and four-spin $(J_2)$ interactions in a transverse magnetic field ($H$). We concentrate our study on the unexplored critical region $B = 1$ and obtain the phase diagram of the model in the $(J_1-J_2)$ plane. The phases found include ferromagnetic (F), antiferromagnetic (AF), as well as more complex phases involving spin configurations with multiple periodicity. The system presents both first and second order transitions separated by tricritical points. We find an unusual phase boundary on the semi-infinite segment $(J_4 < -1, J_2 = 0)$ separating the F and AF phases.

H1.00162 Unusual Phase Transitions in Single Crystals of Gd$_{3}$Si$_{1.5}$Ge$_{7.7}$ and Gd$_{3}$Si$_{1.4}$Ge$_{7.6}$, R. L. Hadimani, Iowa State Univ, Y. Mekhikov, Polish Academy of Science, D. L. Schlager, T. A. Lograsso, K. W. Dennis, R. W. McCallum, Ames Laboratory, US Dept. of Energy, D.C. Jiles, Iowa State Univ, Iowa State University COLLABORATION, POLISH ACADEMY OF SCIENCE COLLABORATION, Ames Laboratory, US Dept. of Energy — We have studied the magnetic properties of Gd$_{3}$(Si$_{1.5}$Ge$_{7.7}$) and Gd$_{3}$(Si$_{1.4}$Ge$_{7.6}$) whose compositions fall in the mixed phase regions of orthorhombic I and orthorhombic II phases. The samples were estimated to be 383 K for Gd$_{3}$Si$_{1.5}$Ge$_{7.7}$ and 365 K for Gd$_{3}$Si$_{1.4}$Ge$_{7.6}$. These temperatures are much higher than the expected second order phase transition temperature of the orthorhombic II phase (280 K). This may be due to the presence of the orthorhombic I phase in larger volume fraction.
H1.00163 Evidence for a magnetic metallic R phase in Vanadium dioxide VO$_2$ , HUI XING, PAYAM TAHERI, PEIHONG ZHANG, HAO ZENG, Department of Physics, The State University of New York at Buffalo — Vanadium dioxide VO$_2$ has garnered extensive research interests for over decades due to its metal-insulator transition (MIT) around 340 K (Ref. 1). Much is known for the physics behind the MIT (including a correlated structural transition and the involvement of several intermediate states). On the other hand, the magnetic property across the MIT is much less known. Although there are no fundamental arguments against the possibility of forming local magnetic moments in VO$_2$, so far, only the M2 phase has been confirmed to possess local magnetic moments. However, our temperature-dependent magnetic susceptibility measurements of VO$_2$ show a sudden jump at the MIT, which cannot be attributed to a simple Pauli susceptibility from conducting electrons. In a recent paper, we pointed out local magnetic moments may form in the metallic R phase. The formation of local moment would naturally explain the extremely high magnetic susceptibility of VO$_2$ above the phase transition temperature. We further discuss the magnetoresistance (MR) measured across the MIT, which shows different magnitude and field dependence in M1 and R phase, including the MR in the metallic phase suppressed to lower temperature in a VO$_2$ electric double layer transistor device using ionic liquid as gate dielectrics. 1. F. J. Morin, Phys. Rev. Lett. 3, 34 (1959). 2. Xun Yuan et al., Phys. Rev. B 86, 235103 (2012).

H1.00164 Control of proliferation rate of N27 dopaminergic neurons using Transcranial Magnetic Stimulation orientation, YIWEN MENG, RAVI HADIMANI, VELLAREDDY ANANTHARAM, ANUMANATHA KANTHASAMY, DAVID JILES, None — Transcranial magnetic stimulation (TMS) has been used to investigate possible treatments for a variety of neurological disorders. However, the effect that magnetic fields have on neurons has not been well documented in the literature. We have investigated the effect of different orientation of magnetic field generated by TMS coils with a monophasic stimulator on the proliferation rate of N27 neuronal cells cultured in flasks and multi-well plates. The proliferation rate of neurons would increase by exposed horizontally adherent N27 cells to a magnetic field pointing upward through the neuronal proliferation layer compared with the control group. On the other hand, proliferation rate would decrease in cells exposed to a magnetic field pointing downward through the neuronal growth layer compared with the control group. We confirmed results obtained from the Trypan-blue and automatic cell counting methods with those from the CyQuant and MTS cell viability assays. Our findings could have important implications for the preclinical development of TMS treatments of neurological disorders and represents a new method to control the proliferation rate of neuronal cells.

H1.00165 Accurate projected augmented wave (PAW) datasets for rare-earth elements (RE=La-Lu) , MEHMET TOPSAKAL, RENATA WENTZCOVITCH, Univ of Minn - Minneapolis — We provide accurate projected augmented wave (PAW) datasets for rare-earth (RE) elements with some suggested Hubbard $U$ values allowing efficient plane-wave calculations. Solid state tests of generated datasets were performed on rare-earth nitrides. Through density of state (DOS) and equation of state (EoS) comparisons, generated datasets were shown to yield excellent results comparable to highly accurate all-electron full-potential linearized augmented plane-wave plus local orbital (FLAPW+LO) calculations. Hubbard $U$ values for trivalent RE ions are determined according to hybrid functional calculations. We believe that these new and open-source PAW datasets will allow further studies on rare-earth materials.

H1.00166 Half-metallic magnetism and the search for better spin valves, KARIN EVERSCHOR-SITTE, MATTHIAS SITTE, ALLAN MACDONALD, Univ of Texas, Austin — We propose a simple formula for the temperature dependence of tunneling magnetoresistance to shed light on ongoing efforts to optimize spin valves. It captures a mechanism in which spin valve performance at finite temperatures is limited by uncorrelated thermal fluctuations of magnetization orientations on opposite sides of a tunnel junction. Furthermore, it directly reveals the advantages for spin-valve optimization by using materials with a high spin polarization of Fermi-level tunneling electrons, and by using materials with high ferromagnetic transition temperatures. We show that our theory is in good agreement with recent experimental studies of the temperature-dependent magnetoresistance of high-quality tunnel junctions with MgO barriers. We conclude that half-metallic ferromagnets can yield better spin-value performance than current elemental transition metal ferromagnet/MgO systems only if their ferromagnetic transition temperatures exceed $\sim$ 900 K.


H1.00167 Nonlinear damping effects in spin torque dynamics of magnetic tunnel junctions, IGOR BARSKOVUK, YU-JIN CHEN, HAN KYU LEE, University of California, Irvine, ALEXANDRE GONCALVES, CBPF, Rio de Janeiro, Brazil, JORDAN KATCHEV, HGST, San Jose, CA, RODRIGO ARIAS, Universidad de Chile, Santiago, Chile, BORIS IVANOV, Academy of Sciences, Kiev, Ukraine, ILYA KRIVOROTOV, University of California, Irvine — Performance of nanoscale spin torque devices such as memory (STT-MRAM) and auto-oscillators critically depends on magnetic relaxation. It is commonly assumed that magnetization dynamics in the presence of spin torque can be understood as simple competition between antidamping arising from spin torque and Gilbert damping of the free layer. However, our experiments reveal that the situation is more complex and that nonlinear damping processes in magnetic tunnel junctions (MIT-J) can strongly alter spin torque driven dynamics. Moreover, we observe MTJ nanopillars with in-plane magnetizations of the free layer and SAF layers by spin torque ferromagnetic resonance. We find an excitation spectrum associated with standing spin waves of the free layer. By varying the external field, the energy of a higher-order spin wave mode increases twice the energy of the main mode. This opens up a nonlinear, resonant relaxation channel, giving rise to a damping increase of approximately 20 percent. With increasing spin torque provided by a DC bias current, we find that this relaxation channel competes with antidamping in a nonlinear manner, increasingly contributing to and even dominating the relaxation at subcritical currents.

H1.00168 Generation of Spin and Orbital Current in Carbon Nanotubes by Spin-rotation Coupling , MASATO HAMADA, SHUICHI MURAKAMI, Tokyo Institute of Technology — Spin-rotation coupling represents a coupling between the electron spins and mechanical rotations, and may be used for generation of spin currents by mechanical rotation. In our presentation we consider carbon nanotubes, and use one of the phonon modes called a twist mode. This mode gives rise to a rotation around the tube axis and eventually an effective Zeeman field parallel to the axis is generated by spin-polarization rotation. We calculate a generated spin current by solving the spin diffusion equation. In addition to the effective Zeeman field along the axis, the rotation also generates an effective orbital magnetic field in the radial direction. We calculate diamagnetic susceptibility for the radial magnetic field, and discuss the generated orbital current.

H1.00169 Spin Trapped Driven Anti-vortex Dynamics in Patterned Nanomagnets, MUSTAFA METE, AHMET COSKUNER, ALI TAHM HABIBOGLU, VEDAT KARAKAS, YEMILHA BILAL KAYONCU, AISHA GORCE, OZMEN OZATAY, Bogazici University, ANNA GIORDANO, MARIO CARPENTIERI, University of Calabria, GIOVANNI FINOCCHIO, University of Messina, FEDERICA CELEGATO, CNR-Institute of Materials for Electronics and Magnetism , PAOLA TIBERTO, Istituto Nazionale di Ricerca Metrologica — Recent studies have shown that unconventional spin configurations in patterned nanomagnets like vortices are potentially applicable to ultrafast memory, rf oscillators and detectors utilizing the static and dynamic response of these structures under external magnetic field and current bias. Due to the difficulties of stabilizing an isolated anti-vortex, there is still much to be explored about its structure and dynamics. In this study, we report on our investigation of stable anti-vortex formation conditions and the subsequent magnetic field/dc current driven excitations. Permalloy based asteroid geometry devices exhibit anti-vortex nucleation at the center with the application of an in-plane AC demagnetizing field and an out of plane magnetic field. Changes in the stable localization of the spins immediately motivates the characterization of the dynamic response to the application of spin torque from a spin-polarized current as sensed using the anisotropic magnetoresistance effect (AMR). We will present the field and current dependence of the anti-vortex gyration frequency, the bandwidth and power in the asteroid devices. This work allows the evaluation of anti-vortex structures to be utilized in practical on-chip microwave oscillators.
H1.00170 Magnetic properties of layered III-VI Diluted Magnetic Semiconductors (DMS)\(^1\)
THOMAS PEKAREK, Physics, U. of N. Florida; I. MIOTKOWSKI, A.K. RAMDAS, Physics, Purdue U. — The new class of quasi-two-dimensional III-VI Diluted Magnetic Semiconductors (DMS) exhibits a rich collection of magnetic behavior. The Ga\(_{1-x}\)Mn\(_x\)S system exhibits a 3-D spin-glass transition, which was unexpected given its four atom thick two dimensional structure. The best scaling fit was found for critical exponents (\(\gamma = 4.0, \beta = 0.8, \text{and} \delta = 5.5\)) similar to the three dimensional Zn\(_{1-x}\)Mn\(_x\)Te system. Ga\(_{1-x}\)Fe\(_x\)Se exhibits a prominent magnetic anisotropy over the temperature range from 10 to 400 K. Theoretical models for In\(_{1-x}\)Mn\(_x\)Se, In\(_{1-x}\)Mn\(_x\)S, and Ga\(_{1-x}\)Mn\(_x\)S provide good agreement with experimental results over a wide range of temperatures and fields. The mechanism behind an unusually large thermal hysteresis (\(\Delta T \approx 200 \text{ K}\)) in In\(_{1-x}\)Mn\(_x\)Se, which extends up to room temperature, is not completely understood at this time. Typically, thermal hysteresis in most materials has a \(\Delta T \approx 20 \text{ K}\) occurring well below room temperature. The host III-V semiconductors themselves are among the best non-linear optical materials.

\[^1\]This research was supported by the UNF Terry Presidential Professorship, the Florida Space Grant Consortium, A Purdue U. Academic Reinvestment Program, and by NSF Grant Nos. DMR-07-06593 and DMR-14-29428.

H1.00171 Computational Aspects of Anisotropy Calculations \(^1\)
M. DAENNE, D. ABERG, L.X. BENEDICT, Lawrence Livermore National Laboratory, CRITICAL MATERIALS INSTITUTE TEAM — In order to predict magnetic properties from first principles, an accurate and reliable determination of the magnetic crystalline anisotropy is needed. We present results using multiple techniques and codes on the Fe\(_2\)B-Co\(_2\)B system. Furthermore, we investigate the influence of disorder in this system on the anisotropy.

H1.00172 Terbium-Aluminum (TbAl\(_2\)) Binary Alloy as High Magnetostrictive Material \(^1\)
MARY BOGOSIAN, CARLOS SANCHEZ, OSCAR BERNAL, ARMIN KOCHARIAN, California State University, Los Angeles, CA 90032, CAL STATE LA TEAM — Magnetic phase diagram for the cubic intermetallic terbium-aluminum (Tb-Al) binary alloy is being investigated for the purpose of developing material with high magnetostrictive properties that can be used for energy harvesting. Low temperature magnetizations, specific heat, combined with structural examinations, are few of the techniques that are being used for this purpose. Preliminary DC magnetization results on as-cast material show magnetic ordering of around 109 K in zero applied fields that varies in magnitude and direction with the increase in applied magnetic field. The preliminary results will be discussed.

\[^1\]Supported by grant # NS-DMR1105380.

H1.00173 Cold plasma cleaning of SmCo5 nano-flakes prepared by surfactant-assisted Ball-milling
GUANGBING HAN, Department of Physics, University of Texas at Arlington, Arlington, TX 76019, USA; College of Physics, Shandong University, Jinan, 250100, China; KE WANG, KEVIN E. ELKINS, ZHAOGUO QIU, Department of Physics, University of Texas at Arlington, Arlington, TX 76019, USA; RICHARD B. TIMMONS, CHARLES R. SAVAGE, Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX 76019, USA. JING WANG, Department of Physics, University of Texas at Arlington, Arlington, TX 76019, USA — Surfactant assisted high energy ball milling has recently been successfully utilized in producing nanostructured hard magnetic powders. However, it is challenging to remove the surfactant on the surface which deteriorates magnet’s properties during heat treatments. Cold plasma is suitable for removing organic surfactant on surface because of the high energetic ions etching at relatively low (room) temperature, while the surface of the powders will not be chemically altered by the physical method. In this work, SmCo5 nano-flakes were prepared by oleic acid (OA) assisted ball milling technique, and then Ar cold plasma was used to clean the OA from the SmCo5 flakes’ surface on a homemade facility. The results show that the remaining carbon atoms can be removed effectively by Ar plasma. Good magnetic properties can be retained in the SmCo5 flakes when the plasma power, Ar pressure, and cleaning time were properly chosen.

H1.00174 Magnetic and magneto-transport studies of MBE grown Cr\(_2\)Te\(_3\) thin films with perpendicular magnetic anisotropy \(^1\)
ANUPAM ROY, SAMARESH GUHHAIT, RIK DEY, TANMOY PRAMANIK, CHENG-CHIH HSIEH, AMRITESH RAI, SANJAY BANERJEE, Microelectronics Research Center, The University of Texas at Austin, TX — Cr\(_2\)Te\(_3\) is one of the very intriguing compounds in the layered chalcogenides family because of its unusual magnetic and magneto-transport properties. Here we have presented studies of magnetic layer epitaxy (MBE) grown (001)-oriented Cr\(_2\)Te\(_3\) thin films on Al\(_2\)O\(_3\)(0001) and Si(111)-(7\times7) surfaces. Reflection high energy electron diffraction (RHEED), scanning tunneling microscopy (STM), vibrating sample magnetometry (VSM) and other physical property measurements are used to investigate the structure, morphology, magnetic and magneto-transport properties of as-grown films. Sharp streaks in RHEED patterns imply smooth film growth on both the substrates. STM studies show hexagonal arrangements of surface atoms and measured lattice parameters agree well with the bulk crystal structures. Magnetic studies confirm the film to be ferromagnetic having a Curie temperature of about 180 K and a spin glass-like behavior is observed below 35 K. The grown substrates. STM studies show hexagonal arrangements of surface atoms and measured lattice parameters agree well with the bulk crystal structures. Magnetic properties during heat treatments. Cold plasma is suitable for removing organic surfactant on surface because of the high energetic ions etching at relatively low (room) temperature, while the surface of the powders will not be chemically altered by the physical method. In this work, SmCo5 nano-flakes were prepared by oleic acid (OA) assisted ball milling technique, and then Argon cold plasma was used to clean the OA from the SmCo5 flakes’ surface on a homemade facility. The results show that the remaining carbon atoms can be removed effectively by Ar plasma. Good magnetic properties can be retained in the SmCo5 flakes when the plasma power, Ar pressure, and cleaning time were properly chosen.

\[^1\]This work is funded by NRI-SWAN.

H1.00175 Influence of the magnetic properties and repetitions on the energy product in layered thin film hard soft magnetic nanocomposites
DAVID ZAGARDO, JAMILEH BEIK MOHAMMADI, ANDREW TUGGLE, CLAUDIA MEWES, TIM MEWES, TAKAO SÜZUKI, University of Alabama, MINT CENTER TEAM — Exchange spring composites (hard-soft magnetic composites) are interesting for many applications such as rare-earth free permanent magnets \([1]\) and information storage \([2]\). One key aspect is the figure of merit, the energy product, also called (BH)\(_\max\). The system of study is a magnetic nano composite where each bilayer consists of a soft and hard magnetic material of total height of 22 nm. Using micromagnetic simulations we have investigated the influence of different ratios of the volume of the hard and soft layers on the energy product and the number of bilayer repetitions. Our findings indicate that the maximum energy product depends strongly on the volume ratio as well as on the number of repetitions. In addition we have studied the influence of different anisotropy contributions of the hard and soft magnetic layer on the energy product. Finally we have studied the influence of the interlayer exchange coupling on the energy product, which show that strong interlayer exchange coupling is necessary to reach a high energy product.


\[^2\]J. Lee et al., Nanotechnology 25, 045604 (2014); T. Tanaka et al., IEEE Transactions on Magnetics 150, 3000503 (2014).
H1.00176 Hard magnetic phase evolution in nanocrystalline mechanically milled amorphous Pr$_2$Co$_3$B powder 1. CAJETAN NLEBEDIM, Ames Laboratory, U.S. Department of Energy, HUSEYIN UCAR, PARANS PARANANTHAMAN, Oak Ridge National Laboratory, U.S. Department of Energy, R.W. MCCALLUM, Ames Laboratory, U.S. Department of Energy — In this work, the evolution of the structural and magnetic properties of Pr$_2$Co$_3$B with mechanical milling and heat-treatment is presented. Understanding the phase evolution of magnetic properties in hard magnetic materials is crucial for developing high performance permanent magnets. Mechanical alloying/milling offers a traditional and easily deployable approach to synthesizing nanostructured materials. Nevertheless, such can result in amorphization due to high defect density leading to disorder in atomic arrangement. The crystalline phase can be thermally recovered but requires the understanding of how the properties evolve with temperature, in order to achieve useful hard magnetic properties desired for developing permanent magnets. This work shows how properties such as energy product, coercivity, remanent magnetization, saturation magnetization and Curie temperature evolve when PrCoB alloy transitions from amorphous to crystalline phase. The presentation will also include how different levels of amorphization affect the magnetic properties.

1This work was supported by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office.

H1.00177 Effect of 3d-metal doping on magnetic properties of Fe$_3$Se$_4$ , RENAT SABIRIANOV, NABIL AL-AQTASH, Univ of Nebraska - Omaha, DEBASISH SENGUPTA, CFDRC — Fe$_3$Se$_4$ exhibits large magnetocrystalline anisotropy (MAE) and coercivity up 40kOe. The large anisotropy of Fe$_3$Se$_4$ should be accompanied by large magnetization for permanent magnet applications. The magnetization of Fe$_3$Se$_4$ suffers from antiferromagnetic (AFM) superexchange coupling of Fe across the Se planes. We present density functional theory study of the magnetic properties of Fe$_3$Se$_4$ doped with TM (Co, Cr, Ni and Mn), TM ions doped in Fe sites, Fe$_3$-x(TM)$_x$Se$_4$ (x = 0.5), to examine a potential increase of the magnetization and Curie temperature of Fe$_3$Se$_4$. We performed screening of the exchange interactions and magnetization modifications upon the substitution of Fe by 3d-transition metals at various Fe sites in the Fe$_3$Se$_4$. We find that the performance of Fe$_3$Se$_4$ with 3d-elements does not remove AFM coupling across layers. The increase in the strength of exchange interactions on doping with Cr should increase the Curie temperature of the system. We compare the results of doped alloy with the ones for Fe$_3$Se$_4$ because Fe$_3$Se$_4$ has four d-electrons. We find that Cr$_3$Te$_4$ has ferromagnetic coupling and magnetization larger than one possible in Fe$_3$Se$_4$. Magnetization per unit cell is 18.24µJ/µm. MAE of this material is large (MAE =1.67 MJ/m$^3$).

H1.00178 Effects of TiN buffer layer on microstructure and magnetic anisotropy of FePt thin films, ZHAOGOU QIU, Department of Physics, University of Texas at Arlington; School of Materials Science and Engineering, South China University of Technology, GUANGBING HAN, Department of Physics, University of Texas at Arlington, DECHANG ZENG, School of Materials Science and Engineering, South China University of Technology, J. PING LIU, Department of Physics, University of Texas at Arlington, UNIVERSITY OF TEXAS AT ARLINGTON COLLABORATION, SOUTH CHINA UNIVERSITY OF TECHNOLOGY COLLABORATION — FePt films were deposited at room temperature on TiN buffer layer followed by annealing. The effects of thickness of the TiN layer on the microstructure and magnetic properties of FePt films were investigated. It was found that TiN layer has significant effects on the magnetic anisotropy of the FePt films. The L1$_0$ phase transformation of the FePt films with TiN layer was more completely than that without a TiN layer. The FePt film with TiN (111) layer of 30nm thickness exhibited out-of-plane anisotropy and enhanced ordering parameter. When the thickness of TiN (111) layer further increased, the coercivity tended to decrease. The anisotropy gradually switched from out-of-plane to in-plane when the annealing temperature was increased to 700 degree. The in-plane coercivity was increased to 0.96 kOe when the thickness of randomly oriented TiN layer was 80nm. The high in-plane coercivity may come from the smooth surface morphology of FePt films induced by the small relaxation of internal stress of the thick TiN layer.

H1.00179 Transient Reflectivity of a Low-Dimensional Quantum Magnet, MICHAEL BISHOP, Natl High Magnetic Field Lab, HAIDONG ZHOU, University of Tennessee Knoxville, STEPHEN MCGILL, Natl High Magnetic Field Lab — Frustrated, low-dimensional spin systems have drawn wide interest due to their ability to exhibit novel quantum phenomena such as superconductivity, spin-liquid phases, and gapped spin excitations (e.g. Haldane, Spin-Peierls, etc.). SrCu$_2$(BO$_2$)$_2$, or SCBO, a close experimental realization of the Shastry-Sutherland model, is one such quantum system in which the singlet ground state is separated from the excited triplet state by an energy gap (35 K) that can be closed by high magnetic fields (>20 T). Furthermore, high magnetic field magnetization measurements reveal an unusual series of plateaus which occur when the magnetic field-tuned density of triplets becomes commensurate with the lattice periodicity. We have investigated the coupling of singlet and triplet pairing in SCBO to changes in its electronic structure using transient near-infrared reflectivity measurements. We investigated the temperature and magnetic field dependences of the transient reflectivity, and we will discuss these behaviors and their correlation with dimer spin excitations.

H1.00180 Strong effect of low-dimensional Fe-doped cobalt niobate on a strongly ferrimagnetic system 1, CAJETAN NLEBEDIM, Ames Laboratory, U.S. Department of Energy, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — In this work, the first investigation of the effect of Fe-doped cobalt niobate (CoNb$_2$O$_6$) imbedded in the matrix of a strongly ferrimagnetic cobalt-iron oxide, is presented. The temperature dependence of the magnetic properties and how they change with variations in the concentration of CoNb$_2$O$_6$ is also presented. CoNb$_2$O$_6$ is a prototypical low-dimensional material belonging to the pyrochlore-type AB$_2$O$_6$ systems. Its low-dimensional magnetic characteristics can help in understanding the magnetic properties of higher order systems. It has been investigated for applications in resonators and capacitors. This work shows that the magnetization of the ferrimagnetic phase is strongly affected by the concentration of Co ions in the low-dimensional phase, below 15 K but changes in coercivity with temperature were predominantly due to the ferrimagnetic phase. The systematic variation in the concentration of both phases and the cation ratio in each phase, enable us to understand the variation of the magnetic properties with temperature. This work provides useful insights into tuning the magnetism in strongly magnetic materials with transition metal AB$_2$O$_6$ systems imbedded in their matrices.

1This work was supported by the USDoE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. The research was performed at Ames Laboratory, operated for the USDoE by Iowa State University (contract # DE-AC02-07CH11358)

H1.00181 Crystallization behavior and recoilless fraction determination of amorphous and nanocrystalline Fe$_{56}$Co$_{24}$Nb$_{14}$B$_{13}$Si$_2$Cu$_{1}$ system 1, MONICA SORESCU, JULIA LIMONGELLI, CHRISTOPHER STROH, Duquesne University, KEVIN BYERLY, Spang — Amorphous ferrimagnetic alloy with the composition Fe$_{56}$Co$_{24}$Nb$_{14}$B$_{13}$Si$_2$Cu$_{1}$ was obtained by rapid quenching from the melt. Samples cut from the ribbons were annealed at 450, 550, 650 and 750 C in a vacuum furnace. 57Fe Mossbauer spectroscopy was used to identify the phases formed based on the refined values of the hyperfine parameters. The as-quenched specimen was analyzed with a hyperfine magnetic field distribution and corresponded to an in-plane orientation of the magnetic moment directions. The sample annealed at 450 C was found to be in a nanocrystalline state due to observation of the (FeCo)-Si alloy with the DO3 structure. The balance of the composition was represented by a metalloid-enriched amorphous grain boundary phase. In contradistinction to this, the samples annealed at 550-750 C were totally crystallized, but the new phases formed were alpha-(FeCo), (FeCo)$_2$(BSi) and (FeCo)$_3$(BSi). The f factor value dropped from 0.6 to 0.37 for the sample annealed at 450 C, consistent with the onset of nanocrystallization in the system. For the completely crystallized specimens, the f factor maintained values close to 0.5. This indicates that the presence of quenched-in stresses may play a role in the ability of samples to undergo recoilless emission and absorption of gamma rays.

1NSF-DMR-0854794
H1.00182 Scaling and memory effects in the reentrant spin glass phase of nanostructured Mn$_x$TaS$_3$. PAUL SHAND, JOHN DANKER, XUN XIAO, TIM KIDD, LAURA STRAUSS, University of Northern Iowa — We have investigated the nature of the reentrant spin glass phase of nanostructured Mn-intercalated TaS$_3$. The sample consisted of bundles of nanoscale fibers with an average atomic concentration of intercalated Mn of 22%. The sample exhibits a ferromagnetic transition at 74 K and a transition to a cluster glass state at 40 K. The ac susceptibility measured in small dc bias fields near the cluster glass transition exhibited scaling behavior, indicating a magnetic-field dependent crossover to glassy dynamics. At temperatures below the cluster-glass transition, the nature of the dynamics was probed by ac susceptibility and zero-field cooled (ZFC) magnetization measurements. Aging and memory effects were observed, consistent with the non-equilibrium dynamics exhibited by glassy magnetic systems. In particular, we probed the ZFC magnetization memory effect as a function of cooling rate, aging time and magnetic field. The behavior is explained in terms of domain growth within the framework of droplet theory.

1Supported by National Science Foundation Grant No. DMR 1206530

H1.00183 Enhanced Tunneling Magnetoresistance in Voltage-controlled CoFeB/MgO Junctions. HAMID ALMASI, MENG XU, CHRISTIAN GENTRY, DI YU, TY NEWHOUSE-ILLIGE, Department of Physics, University of Arizona, Tucson, Arizona 85721, USA, Y. H. LIU, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, J. W. FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA, S. G. E. TE VELTHUIS, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, WEIGANG WANG, Department of Physics, University of Arizona, Tucson, Arizona 85721, USA — Perpendicular magnetic anisotropy (PMA) at the CoFeB/MgO interface originates from the hybridization of d orbitals of Fe and Co and the Pz orbital of Oxygen. Due to different electronic band structures, the hybridization of the d orbitals of Fe and Co is likely different, therefore contributing unequally to the total PMA. This difference has been probed by an X-ray magnetic circular dichroism (XMCD). The orbital moment of Fe was found to be much larger than that of Co by XMCD. These results demonstrated that Fe contributes most to the PMA at the interface. MTJs with Fe-rich electrodes were fabricated and a substantially larger PMA was achieved. With further optimization in post-growth thermal annealing, we have achieved over 150% TMR in these voltage-controllable CoFeB/MgO MTJs.

2This work was supported in part by NSF (ECCS-1310338) and by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA. Work at ANL was supported by the DOE-BES, MSE and SFU.

H1.00184 Fermi level tuning of highly spin-polarized complex Heusler alloys via materials genome. SUDIP PANDEY, ABDIEL QUETZ, ANIL ARYAL, MICHAEL FRAIAIDE, Southern IL Univ-Carbondale, TAPAS SAMANTA, Louisiana State University, Baton Rouge, KAMRAN MUNIRA, WILLIAM BUTLER, University of Alabama, Tuscaloosa, IGOR DUBENKO, Southern IL Univ-Carbondale, DIPANJAN MAZUMDAR, SHANE STADLER, Louisiana State University, Baton Rouge, NAUSHAAD ALI, Southern IL Univ-Carbondale — Heusler alloys are the largest family of half-metals (100% spin polarized at the Fermi level) and most promising for spintronic device applications. Many half-metallic full-Heusler alloys are predicted from ab-initio calculations, but may or may not be experimentally realizable. Here, we present a novel strategy to utilize these predicted materials to tune the Fermi level of well-known, highly spin-polarized Heusler alloys. We start with the test sample of [Co$_2$MnSi]$_{1-x}$[Co$_2$CrGe]$_x$ and, by controlling the ratio of these materials, we were able to shift the Fermi level of Co$_2$MnSi. Experimentally, we studied the structural and magnetic properties of such Heusler alloys by room temperature X-ray diffraction (XRD) and magnetization measurements. It was found that these complex combinations of materials are single phase even though some components (Co$_2$CrGe for example) might not be stable in bulk form alone.

3This work was supported by the Office of Basic Energy Sciences, Material Science Division of the U.S. Department of Energy (DOE Grant No. DE-FG02-06ER46291 and DE-FG02-13ER46946).

H1.00185 Phase Transitions and Magnetocaloric Effects in GdNi$_2$Mn$_x$. ANIL ARYAL, ABDIEL QUETZ, SUDIP PANDEY, Southern IL Univ-Carbondale, TAPAS SAMANTA, Louisiana State University, ICOR DUBENKO, Southern IL Univ-Carbondale, SHANE STADLER, Louisiana State University, NAUSHAD ALI, Southern IL Univ-Carbondale — The structural and magnetic properties of the GdNi$_2$Mn$_x$ system (for x = 0.5, 0.6, 0.8, 1.0, 1.2, 1.4, 1.5) have been studied by x-ray diffraction and magnetization measurements. A rhombohedral PuNi$_5$-type structure was observed in the XRD data. A second order magnetic phase transition from ferromagnetic (FM) to paramagnetic (PM) was found, characterized by a long-range exchange interaction as predicted by mean field theory. A magnetic entropy change of ∆S$_M$ = 3.1 J/kg K and 2.9 J/kg K for ∆H = 5 T was observed in the vicinity of the Curie temperature (T$_C$) for GdNi$_2$Mn$_{0.8}$ and GdNi$_2$Mn$_{1.4}$ respectively. In spite of the low values of ∆S$_M$, the relative cooling power (RCP) was found to be 176 J/kg for the GdNi$_2$Mn$_{0.8}$ compound.

4This work was supported by the Office of Basic Energy Sciences, Material Science and Engineering Division of the U.S. Department of Energy (USDOE-DE-FG02-06ER46291 and DE-FG02-13ER46946).

H1.00186 Influence of Ga content on structure and anomalous Hall effect of Fe$_{1-x}$Ga$_x$ thin films on GaSb(100). THI MINH HAI NGUYEN, ANH TUAN DUONG, YOOLEEMI SHIN, VAN QUANG NGUYEN, SUNGLAE CHO, Univ of Ulsan, Korea — The Fe-Ga alloys have recently attracted great interests because they exhibited ferromagnetic properties with high Curie temperature, high saturation magnetization and unique magnetostriiction properties which are promising to real applications such as actuators, acoustic sensors, torque sensors, and positioning devices in particular for micro and nano-electromechanical systems and the integrated magnetostrictive devices. Recently, electrical spin injection from Fe$_{0.7}$Ga$_{0.3}$ produces an electron spin polarization above 70% on GaAs(001). However, the out-of-plane saturation field and magnetization decrease rapidly with Ga content. The Fe$_{1-x}$Ga$_x$ thin films (x = 0.4, 0.5) have been grown on GaSb(100) substrate using MBE. An epitaxial film with bcc α-Fe crystal structure (A2) was observed in Fe$_{0.7}$Ga$_{0.3}$ film, while an impure Fe$_3$Ga phase with DO$_3$ structure appeared in Fe$_{0.5}$Ga$_{0.5}$ film. The saturated magnetizations are 570emu/cm$^3$ and 180emu/cm$^3$ and the coercivities are 170 and 364Oe at room temperature for Fe$_{0.7}$Ga$_{0.3}$ and Fe$_{0.5}$Ga$_{0.5}$, respectively. A hysteresis trend in Hall resistance vs. magnetic field was observed for Fe$_{0.7}$Ga$_{0.3}$ film. However, there is a weak hysteresis in Fe$_{0.5}$Ga$_{0.5}$ film.

5This work was supported by the Office of Basic Energy Sciences, Material Science and Engineering Division of the U.S. Department of Energy (USDOE-DE-FG02-06ER46291 and DE-FG02-13ER46946).
H1.00187 Magnetic Properties of MnFe$_2$Ga Heusler Alloys . AHMED A. ELGENDY, MOHAMMAD SALEHI-FASHAM, University of Delaware, DAVID SELLMYER, University of Nebraska, GEORGE HADJIIPANAYIS, University of Delaware — Recently, MnFe$_2$Ga Heusler alloys have attracted significant attention due to their interesting physical properties such as large magnetic-field-induced strain, giant magnetocalaric effects, large magneto-resistance, and exchange bias behavior [1-2]. These properties make them promising candidates for various practical applications in the field of smart materials, magnetic refrigeration and spintronics. In this work, we prepared MnFe$_2$Ga alloys by melt-spinning and sputtering and studied the structural and magnetic properties. The melt-spun ribbons were prepared with a wheel speed of 30 m/s. The ribbons were annealed at different temperatures for 1 hour and grinded to make fine powders. The grinded powders were also used to make the target that is used in the cluster gun for the fabrication of MnFe$_2$Ga nanoparticles. The structure of the as-made, annealed ribbons, and powders displayed a face-centered-cubic structure. The microstructure of the as-made ribbons showed equiaxed grains with an average size of 3-5 μm while the annealed ribbons showed bigger grains with small particles covering homogeneously their surface. The magnetic properties show an enhancement of magnetization while coercivity remains the same with values M(3T) and HC of 85 emu/g and 150 Oe, respectively. Transmission electron microscopy with elemental mapping is currently underway to determine the structure and composition of the surface nanoparticles. The work was supported by DOE-BES-DMSE (Grant No. DE-FG02-04ER4612).


H1.00188 Growth and Structural Study of Epitaxial NaMnF$_3$ Thin Films on SrTiO$_3$. AMIT KC, TRENT JOHNSON, PAVEL BORISOV, DAVID LEDERMAN, WWU — Perovskite fluorides (ABF$_3$) exhibit many interesting phenomena, e.g. dipolar and magnetic long-range order superconductivity, as well as magnetoelectric coupling. Recently, G. C. Garcia-Castro et al. predicted that orthorhombically distorted Pnma NaMnF$_3$ perovskite should have a particularly soft ferroelectric mode, and is expected to demonstrate ferroelectric order regardless of elastic strain, despite the competing antiferrodistortive instability. Thus, in combination with weak ferromagnetic order, this material is expected to be multiferroic. Here, we report the growth of epitaxial NaMnF$_3$ thin films on SrTiO$_3$(100) single crystal substrates via Molecular Beam Epitaxy (MBE). Structural qualities of the films were studied as a function of the substrate temperature and film thickness by the techniques of X-ray diffraction (XRD), in-situ reflection high-energy electron diffraction (RHEED), and atomic force microscopy (AFM). The best films were smooth single phase NaMnF$_3$, grown with four in-plane and two out-of-plane twin domains.

H1.00189 Developing Nuclear Magnetic Resonance Force Microscopy (NMRFM) as an Electronic Probe of Nanoscale Condensed Matter Systems . JEREMY W. PASTER, DANIEL M. TENNANT, SHIRIN MOZAF-FARI, JOHN T. MARKERT, Department of Physics, The University of Texas at Austin — The investigation of NMR via magnetic force coupling in a large field gradient has led to vast improvements in spatial resolution over the conventional inductive method. It has been demonstrated that nanoscale force sensors could be scaled to distinguish a single nuclear spin, assuming experimental noise can be minimized and other spurious force signatures stifled. Accordingly, there are many efforts aimed at repurposing NMR for 3D imaging on the atomic scale [1]. In addition to proof-of-concept experiments aimed at separately resolving some of the eventual experimental barriers to atomic resolution, some of us have directed our attention to using NMR to probe the electronic environment in larger condensed matter systems which are not well suited for other scanning probe microscopy techniques and which are prohibitively small for inductive NMR detection. Previously, we proposed using NMRFM to probe superconducting transitions in microcrystals. In parallel, we revamped our investigation of thin films [2] to explore two-dimensional conducting interfaces between oxide interfaces. Presented here is a survey of the technical impediments as well as current strategies for unlocking this exciting potential for NMRFM, as a tool to investigate sub-surface electronic transport in microscale and nanoscale condensed matter systems.


H1.00190 Competition between itinerant ferromagnetism and spin-density wave antiferro-magnetism in FeGa . YAN WU, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, 70803, HUIBO CAO, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, 37831, GREGORY MCCANDLES, JULIA CHAN, Department of Chemistry, The University of Texas at Dallas, Richardson, 75080, AMAR KARKI, RONGYING JIN, JOHN DITUSA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, 70803 — The metallic magnet FeGa displays a rich magnetic behavior that includes transitions between a FM ground state to an AFM intermediate state exhibit many interesting phenomena, e.g. dipolar and magnetic long-range order superconductivity, as well as magnetoelectric coupling. Recently, G. C. Garcia-Castro et al. predicted that orthorhombically distorted Pnma NaMnF$_3$ perovskite should have a particularly soft ferroelectric mode, and is expected to demonstrate ferroelectric order regardless of elastic strain, despite the competing antiferrodistortive instability. Thus, in combination with weak ferromagnetic order, this material is expected to be multiferroic. Here, we report the growth of epitaxial NaMnF$_3$ thin films on SrTiO$_3$(100) single crystal substrates via Molecular Beam Epitaxy (MBE). Structural qualities of the films were studied as a function of the substrate temperature and film thickness by the techniques of X-ray diffraction (XRD), in-situ reflection high-energy electron diffraction (RHEED), and atomic force microscopy (AFM). The best films were smooth single phase NaMnF$_3$, grown with four in-plane and two out-of-plane twin domains.

H1.00191 COMPLEX STRUCTURED MATERIALS INCLUDING GRAPHENE –

H1.00192 Thickness dependence of mechanical properties of free-standing graphene oxide papers . TAO GONG, Advanced Institute of Nano Technology (SAINT), Sungkyunkwan University, DO VAN LAM, Nano Mechatronics, Korea University of Science and Technology, SEJEONG WON, Korea Advanced Institute of Science & Technology, RENLONG LIU, School of Mechanical Engineering, SKKU, HWANGBO YUN, Korea Institute of Machinery & Materials, SANGHYUK KWON, JINSEONG KIM, School of Mechanical Engineering, SKKU, KE SUN, SAINT-SKKU, SEUNGMO LEE, Nano-Mechanical Systems Research Division, KIMM, CHANGGU LEE, Advanced Institute of Nano Technology, and School of Mechanical Engineering, Sungkyunkwan University, GRAPHENE ENGINEERING LAB TEAM, NANO-MECHANICS LAB COLLABORATION — We have characterized thickness dependence of mechanical properties, such as Young’s modulus, fracture strength, fracture strain and toughness, of graphene oxide papers using tensile and bulge test methods. The GO papers were made from Hummer’s method and the fabricated GO paper’s thickness varied from 0.1 ~ 100 μm. The measured Young’s modulus and fracture strength decreased with increasing thickness ranging from 44.6 ~ 8.5GPa and 170.2 ~ 40MPa respectively. Through TEM, SEM and AFM characterization, the inner structure and surface morphology such as crack formation and roughness change are the keys to the variation of mechanical properties in the GO papers by the thickness. The thicker GO papers are weaker because it has more manufacturing voids in it that cause it to fail easily and less stiff. Surface wrinkle and residual stress are the mechanism of terraced fracture strain.

H1.00193 ABSTRACT WITHDRAWN –
H1.00194 Transition metals-graphene interaction: the role of the screened van der Waals energy. ALBERTO AMBROSETTI, PIER LUIGI SILVESTRELLI, Università degli Studi di Padova — The interaction of graphene with transition metals is of particular interest for practical applications, which include for instance the efficient production of high-quality graphene. The accurate theoretical description of transition metals-graphene interfaces, however, is a particularly challenging problem due to the complex interplay between van der Waals (vdW) and hybridization effects. Here we apply the DFT/vdW-WF2s method [1], which allows to augment semi-local Density Functional Theory through the introduction of screened vdW interactions. Notably, we find that a reliable modeling of the van der Waals interaction should account for complex metal screening effects, that are due to the combined contributions of the p- and s-like quasi-free-electrons, and the more localized d-states. The resulting geometry and energetic properties are in good agreement with experimental data and sophisticated theoretical calculations. Moreover, the Maximally Localized Wannier Functions underlying the DFT/vdW-WF2s method allow for an intuitive understanding of the complex binding mechanism.


H1.00195 Synthesis of carbon nano-structures using organic-molecule intercalated taeniolite layered silicates. TAKAAKI MAEZUMI, NOBORU WADA, Toyo University, Japan — By calcinating organic-molecule intercalated taeniolite layered silicates, carbon nano-structures were made between the 2:1 layered silicate sheets. Raman scattering, XRD, TGA and SEM were used to characterize the samples. Large taeniolite crystals (NaLiMg2SiO(F) were first prepared by melting appropriate chemicals at high temperatures using a platinum crucible. Then, the taeniolite crystals made were cation-exchanged with Li+, K+, NH4+, Ca2+ and Mg2+ in salt solution. Finally, various organic molecules such as ethylene glycol, pyridine and so on were intercalated into the taeniolite crystals, and calcinated under a N2 atmosphere at about 1000K. The resulting crystals are usually gray or black. X-ray (00l) diffraction patterns suggested that the carbon structures may be monolayer thick (i.e., graphene-like). Raman scattering spectra which exhibited a sharp G-band peak with a high G-band/D-band ratio indicated that the carbon structures were relatively well crystallized. Cation-organic-molecule dependence on the carbon structures will be discussed. In addition, evidence for stage-2 taeniolite will be presented.

H1.00196 A first principles study on CVD graphene growth on copper surfaces: C-C bonding reactions at graphene edges. NOBUO TAJIMA, TOMOAKI KANEKO, JUN NARA, National Institute for Materials Science, Materials Research Consortium for Energy Efficient Electronic Devices (MARCEED), OHNO TAKAHISA, National Institute for Materials Science, Materials Research Consortium for Energy Efficient Electronic Devices (MARCEED).University of Tokyo — Graphene has attracted considerable research interest owing to its potential applications in electronics. First principles electronic structure calculations of graphene growth processes in the CVD reactions have been studied extensively as key steps that affect the graphene growth behavior. We have been studying the carbon atom reactions in these processes by theoretical approaches. In the present study, we have focused on the later stage of CVD reaction, that is, carbon atom reactions at graphene edges by which carbon clusters grow in the Cu-CVD. We have found that these reactions have energy barriers of ~1 eV. First principles simulation code PHASE http://www.ciss.iis.u-tokyo.ac.jp/riss/english/project/device/) was used in the theoretical calculations.

H1.00197 ABSTRACT WITHDRAWN

H1.00198 Ab-initio investigation of optical absorption spectra properties of doped Graphene. GIRIJA DUBEY, Department of Earth & Physical Sciences, York College, CUNY, NY, POOJA RANI, VIJAY JINDAL, Department of Physics, Panjab University Chandigarh-160014 — Ab-initio calculations based on density functional theory (DFT) have been performed to study the changes in the absorption spectrum of graphene substituted with B, N and BN. The dielectric function and hence the absorption spectrum of single layer graphene sheet have been calculated. The present study can be concluded as, the individual B and N doping does not significantly affect the imaginary dielectric function and hence the absorption spectrum. However, red shift in the absorption towards visible range of the radiation at high doping is found to occur in case of B/N co-doping at high doping concentration. It can be inferred the B/N co-doping of graphene can alter the optical properties of graphene to make it reflect in the visible region.

H1.00199 Molecular dynamics simulation of graphene friction: the interplay of tip, graphene and substrate. MINWOONG JOE, CHANGGU LEE, Sungkyunkwan Univ — Graphene is a promising future platform material that could be harnessed in wealth of new applications by virtue of its superior electronic and mechanical properties. Also, atomically thin graphene provides an ideal testbed for investigating fundamental aspects of nanoscale friction. Here, molecular dynamics simulations are performed to study frictional behaviors of atomic force microscope tip on graphene. The effects of tip crystallinity, scan direction (or graphene orientation), and graphene thickness are examined. Puckering hypothesis is revisited with comparison by rigid/supported/suspended graphene cases. Our studies provide broader perspectives into the friction mechanism on graphene.

H1.00200 Effect of Ar Overpressure Ratio on the Growth of Graphene on Cu(111) 1. HEIKE GEISLER, SEAMUS MURRAY, SUNY College at Oneonta, ENG WEN ONG, TYLER MOWLL, University at Albany-SUNY, PARUL TYAGI, Global Foundaries, CARL A. VENTRICE, JR., SUNY Polytechnic Institute — A graphene growth study was performed on Cu(111) in a UHV chamber by CVD using ethylene. The sample holder consisted of an oxygen series button heater with Ta heat shields to allow annealing the crystal to 900 °C at pressures as high as 100 mTorr. The crystal structure of the surface was determined using LEED. Growth attempts on the clean Cu(111) surface at ethylene pressures as high as 5 mTorr only resulted in trace amounts of graphene being grown on the surface. This is attributed to the low catalytic activity of the Cu(111) surface and the high vapor pressure of Cu at the growth temperature. To suppress the sublimation of Cu, an Ar overpressure was used. Ethylene partial pressures of 2, 5, 10, and 50 mTorr were used, keeping the total pressure at 50 mTorr. The films for 2 and 5 mTorr showed predominately single domain epitaxy. At 10 mTorr ethylene partial pressure, additional diffraction spots 30° out of phase with the Cu(111) substrate were observed. At 50 mTorr ethylene and no Ar overpressure, broad diffraction arcs were observed in LEED that were ±15° out of phase with the substrate. Therefore, the carbon deposition rate, which depends on the ethylene partial pressure, has a large effect on the quality of the graphene film.

1 This research was supported by the NSF (DMR-1006411).

H1.00201 Origin of the 2450 cm−1 peak (G* band) in the Raman spectrum of graphene, RA-MKRISHNA PODILA, Clemson University, RAHUL RAO, Honda Research Institute US, MEHMET KARAKAYA, JINGYI ZHU, APPARAO RAO, Clemson University, DEPARTMENT OF PHYSICS AND ASTRONOMY, CLEMSON NANOMATERIALS CENTER, CLEMSON UNIVERSITY TEAM, HONDA RESEARCH INSTITUTE US TEAM — Here, we report the Raman studies of mechanically exfoliated and chemical vapor deposited (CVD) pristine, ionirradiated, and Ndoped graphene (SLG, BLG, and FLG), which identify the origin of the so-called G*-band in graphene ~ 2450 cm−1. Our results show that the asymmetry of the G*-band clearly increases with interlayer stacking, with the high frequency peak exhibiting more sensitivity to intralayer defects compared to the lower component. The sub-peaks (i.e., low and high frequency components) in the G*-band were observed to merge with increasing excitation energy and could be understood in terms of the energy dependent scattering rates of photo-excited carriers.
H1.00202 Chemical Vapour Deposition of Graphene with Re-useable Pt and Cu substrates for Flexible Electronics

SHUMAILA KARIMAT, Department of Physics, Middle East Technical University, Ankara Turkey 06800, SELDA SONUSEN, Faculty of Engineering and Natural Sciences, Sabanci University, Istanbul, Turkey 34956, UMIT CELIK, NanoMagnetics Instruments Ltd., Ankara, Turkey, YIGIT UYSALLI, AHMET ORAL, Department of Physics, Middle East Technical University, Ankara Turkey 06800 — Graphene has gained the attention of scientific world due to its outstanding physical properties. The future demand of flexible electronics such as solar cells, light emitting diodes, photo-detectors and touch screen technology requires more exploration of graphene properties on flexible substrates. The most interesting application of graphene is in organic light emitting diodes (OLED) where efforts are in progress to replace brittle indium tin oxide (ITO) electrode with a flexible graphene electrode because ITO raw materials are becoming increasingly expensive, and its brittle nature makes it unsuitable for flexible devices. In this work, we grow graphene on Pt and Cu substrates using chemical vapour deposition (CVD) and transferred it to a polymer material (PVA) using lamination technique. We used hydrogen bubbling method for separating graphene from Pt and Cu catalyst to reuse the substrates many times. After successful transfer of graphene on polymer samples, we checked the resistivity values of the graphene sheet which varies with growth conditions. Furthermore, Raman, atomic force microscopy (AFM), I-V and Force-displacement measurements will be presented for these samples.

H1.00203 Non-covalent interactions in the colloidal graphene dispersions

DORSARA PARVIZ, Texas A&M Univ, ZINU YU, SRYA DAS, FAHMIDA IRIN, RONALD HEDDEN, Texas Tech Univ, MICAH GREEN, Texas A&M Univ — We have studied stabilization mechanisms in colloidal dispersions of pristine graphene. Electrostatic and steric stabilization in presence of pyrene derivative as dispersants depends on the dispersant concentration, functional groups and the solution pH. The graphene-dispersant yield obtained by pyrene derivaties was considerably higher compared to conventional dispersants. Pyrene-graphene π-π interactions were combined with a designer functional group (polydimethylsiloxane (PDMS)) to synthesize a polymer with dual functionality as dispersant and polymer matrix. The same strategy was applied to produce graphene/ PMMA and graphene/ PS films. Controllable crumpling of graphene nanosheets was induced through rapid evaporation of dispersion droplets within a spray dryer. Dimensional transition of 2D nanosheets to 3D crumpled particles was directly observed. Multi-faced dimpled morphology of pristine graphene was different than highly wrinkled morphology of crumpled graphene oxide. Changing the compressive forces during drying allowed for controllable folding of the nanosheets, while the unfolding of the redispersed crumpled particles was controlled by the solvent choice.

H1.00204 Surface plasmons in doped graphene excited by the Attenuated Total Reflection technique in the THz regime

F. RAMOS-MENDIETA, Departamento de Investigacion en Fisica, Universidad de Sonora, Hermosillo, Sonora, Mexico., J.A. HERNANDEZ-LOPEZ, M. PALOMINO-OVANDO, Facultad de Ciencias Fisico-Matematicas, Benemerita Universidad Autonoma de Puebla, Puebla, Mexico — Surface plasmons of transverse electric (TE) and transverse magnetic (TM) polarization in doped free-standing graphene are numerically investigated at THz frequencies. For detecting these modes sufficient sensitivity of the prism-based Otto configuration is demonstrated. Complete agreement with the THz dispersion relation is found in doped graphene of Fermi level μ = 0.8 eV, perfect absorption due to wave interference is also observed. On the other hand, TE surface plasmons are special surface vibrations without induced surface charge; they are self-sustained oscillations (unique of graphene) that arise in frequency ranges where the imaginary part of the graphene dynamical conductivity is negative. We found that TE plasmons are excited for angles of incidence very close to the critical angle between prism and air, as predicted from their dispersion relation. Reflection profiles and field intensities of these waves are presented for μ = 0.2, 0.3 eV.

1 This work was supported by SESIC Mexico, Promep Grant FOFM-2008 and by CONACyT, Mexico.

H1.00205 Hetero epitaxial graphene on various substrates

GARY HARRIS, HNF-Howard University, GURPREET KAUT, CRAWFORD TAYLOR, Howard University — Large-scale production of graphene is pivotal for the development of graphene-based electronics. These results focus on the synthesis and characterization of graphene layers. Two methods were used to grow graphene films. First, graphene films were epitaxially grown on silicon carbide substrates by thermal decomposition of SiC at high temperature and low pressure. In-house built reactor consisting of induction furnace was used to form epitaxial graphene for electronic applications. Second, chemical vapor deposition method was used for direct graphene synthesis on 3C-SiC with the use of copper as a catalyst. In thermal CVD process, hydrogen and methane gases were used as precursors. Methane acts as a carbon source and annealing and cooling were performed in hydrogen environment. Different polypyrroles of silicon carbide (6H-SiC and 3C-SiC) and their crystal orientations were exploited as substrates to form epitaxial graphene. Hetero epitaxial 3C-SiC epilayer was first deposited on Si substrate using chemical vapor deposition technique in cold wall, low pressure, and horizontal CVD reactor. The reactor temperature, argon pressure, flow rate and concentration of different gases (propane, silane, hydrogen and argon) was investigated to control the growth of 3C-SiC and silicon sublimation rate. The resulting graphene films were confirmed using Raman spectroscopy. Further, graphene films have been characterized with the tools of atomic force microscopy (AFM) and scanning electron microscopy (SEM). Mobility, electrical resistivity and carrier density measurements were taken using hall measurements.

1 NSF_PRDM

H1.00206 Graphene oxide membrane for liquid phase organic molecular separation

RENLONG LIU, GIRISH ARABALE, JINSUN KIM, KE SUN, YONGWOON LEE, CHANGKOOK RYU, CHANGGU LEE, Sungkyunkwan Univ — The selective permeation of organic solvents and water through graphene oxide (GO) membranes has been demonstrated. Water was found to permeate through GO membranes faster than various alcohols. The permeation rates of propanol are about 80 times lower than that of water. Taking advantage of the differences in the permeation rates, we separated water from the alcohols and obtained alcohols with high purity. For ethanol and 1-propanol, binary solutions of the alcohol and water were filtered efficiently to produce alcohols with concentration of about 97%. However, the selectivity of the filtration of methanol is significantly lower than that of the other alcohols. To understand the mechanism we followed the structural changes in the GO membranes by X-Ray diffraction analysis. From the X-ray diffraction results we speculate that the selectivity of the permeation of water and alcohols is closely related to the molecular sizes of the solvents and their polarity. In order to demonstrate the potential applications of this process for the selective removal of water from aqueous organic mixtures, we performed the separation of water from a bio-oil containing 73% of water. The majority of the water was filtered out resulting in a higher purity bio-oil.

H1.00207 Magneto-electronic and optical properties of transition metal dicalcogenide monolayers

YEN-HUNG HO, Physics, National Tsing Hua University, Taiwan, CHIH-WEI CHIU, MING-FA LIN, Physics, National Cheng Kung University, Taiwan, WU-PEI SU, Physics and Texas Center for Superconductivity, University of Houston, TX — A generalized tight-binding model is utilized to study the Landau level spectra of various transition metal dicalcogenide monolayers. The intrinsic spin-orbit coupling effectively gives rise to multiple splitting of Landau levels. With a close inspection of wavefunction characteristics, these levels can be classified into specific groups in terms of their orbital, spin and valley signatures. In the calculation of magneto-oscillation spectra, the physical origins of optical selection rules are clearly resolved. Compounds are different from one another in terms of transition energies and appearance of twin peaks. Our numerical results clearly demonstrate the magnetic control of spin and valley charge carriers and provide a basis for future experiments.

1 Robert A. Welch Foundation (E-1070); National Science Council of Taiwan (NSC 101-2112-M-003-005-MY3); NTHU Start-Up Grant (103H1114)
H1.00208 Understanding the optical and electronic properties of Ga-doped graphene\(^1\) . N.C. CREANGE, C. CONSTANTIN, Department of Physics and Astronomy, James Madison University; J.-X. ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, A.V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory, J.T. HARALDSEN, Department of Physics and Astronomy, James Madison University — We simulate the optical and electrical responses in gallium-doped graphene, using density functional theory with a local density approximation. We show the effects of impurity doping (0.3-9.1\%) in the graphene sheet and for each doping percentage the change in electron density, refractive index, and optical conductivity are reported. Here, gallium atoms are placed randomly (using a 5-point average) throughout a 12-atom sheet of graphene. These calculations demonstrate the effects of hole doping due to direct atomic substitution, where we find a disruption in the electron density for small doping levels, which is due to impurity scattering of the electrons. However, there seems to be a doping percentage, above which we have calculated, at which the system transitions to produce metallic or semi-metallic behavior. These calculations are compared to a purely theoretical 100\% graphene sheet for comparison of conductivity. Furthermore, we examine the change in the electronic band structure and density of states, where the introduction of gallium electronic bands produces a shift in the electron bands and dissolves the characteristic Dirac cone within graphene.

\(^1\)We acknowledge support from the Center for Integrated Nanotechnologies User Program and the Institute for Materials Science.

H1.00209 Van der Waals Epitaxy of Two-Dimensional α-MoO\(_3\) Nanosheets using Mica as Grown Templates\(^1\) . WANG DI, ZHOU YU, WANG MU, PENG RUWEN, XIONG XIANG, Nanjing University — The orthorhombic Molybdenum trioxide, α-MoO\(_3\), is one kind of graphene-like layered materials. Since the great promise for future electronic and optoelectronic application, this molybdenum-based two-dimensional (2D) layer material has recently attracted much attention. In this work, we report a Van der Waals epitaxy of α-MoO\(_3\) nanosheets on mica substrate under ambient pressure. This simple physical vapor-phase deposition process is proposed to mediate through the weak Van der Waals interaction between layered α-MoO\(_3\) and mica substrate. As a result, the grown α-MoO\(_3\) nanosheets, whose lateral dimension is up to 0.1mm and thickness less than 2.8 nm (about bilayer MoO\(_3\) octahedral structure), exhibit defined lattice orientation. From bulk to bilayer, Raman spectra of α-MoO\(_3\) nanosheets show independent wavenumber number, which unlike to MoO\(_3\) nanosheets. The measurement of electric resistances at room temperature shows the conductance of original α-MoO\(_3\) nanosheets is already high, moreover, which can be greatly improved by hydrogen doping. Our works indicate that VDWE with mica templates is a simple and feasible strategy to grow high-quality ultrathin α-MoO\(_3\) nanosheets, which have superiorities for investigating its novel physical properties and potential application in future.

\(^1\)National Natural Science Foundation of China (Grant Nos. 51302268); National Natural Science Foundation of China (Grant Nos. 51472123)

H1.00210 Photoluminescence Quenching in Single-Layer MoS\(_2\) via Oxygen Plasma Treatment . NARAE KANG, HARI P. PAUDEL, MICHAEL N. LEUENBERGER, LAURENE TETARD, SAIFUL I. KHONDAKER, NanoScience and Technology Center and Department of Physics, University of Central Florida — Ultrathin two-dimensional (2D) layered transition dichalcogenides (TMDs) families have emerged as a new class of semiconducting candidates due to its intrinsic bandgap. The ability to control the properties of 2D TMDs will become a key in the development of future electronic and optoelectronic applications; however, altering the properties via creating and manipulating defects through external control is not fully investigated yet. In this work, we studied tunable optical properties of single-layer (SL) MoS\(_2\) by applying time-dependent oxygen plasma exposure. As the exposure time increased, the strong photoluminescence (PL) of SL MoS\(_2\) changed to complete quenching accompanied by clear changes in Raman spectra with gradual reduction of MoS\(_2\) peaks as well as an appearance of oxidation-induced peak of Mo-O bonds formation. Using band structure calculations, we found that the creation of MoO\(_3\) disordered-domains led to plasma-induced direct-to-indirect bandgap transition in defective SL MoS\(_2\), resulting in PL quenching with lattice distortion. Our results suggest new opportunities of tailoring and understanding the properties of 2D TMDs.

H1.00211 Scanning Photocurrent Microscopy on Single-Layer CVD MoS\(_2\), MoSe\(_2\), and Alloys , EDWIN PRECIADO, VELVET KLEE, DAVID BARROSO, Univ of California - Riverside, KRISTÓFER ERICKSON, Sandia NL, MARK TRIPPLETT, Univ of California - Davis, ARIANA NGUYEN, CHRIS LEE, H-I SU, SARAH BOBEK, JOHN MANN, Univ of California - Riverside, ALEC TALIN, FRANCOIS LEONARD, Sandia NL, LUDWIG BARTELS, Univ of California - Riverside — We report scanning photocurrent measurements on CVD-grown single-layer films of MoS\(_2\), MoSe\(_2\), and layered MoS\(_2\)-MoSe\(_2\) alloys. Measurements of electric resistances at room temperature shows the conductance of original α-MoO\(_3\) nanosheets is already high, moreover, which can be greatly improved by hydrogen doping. Our works indicate that VDWE with mica templates is a simple and feasible strategy to grow high-quality ultrathin α-MoO\(_3\) nanosheets, which have superiorities for investigating its novel physical properties and potential application in future.

H1.00212 Lateral hydrogenated graphene/h-BN Tunneling Magnetoresistance Devices , SHAYAN HEMMATIYAN, CRISTIAN CERNOV, ARTEM ABANOV, Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA, MARCO POLINI, NEST, Istituto Nanoscienze - CNR and Scuola Normale Superiore, I-56126 Pisa, Italy, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin, Austin, Texas 78712-1081, USA, JAIRO SINOVA, Institut für Physik, Johannes Gutenberg Universitäten Mainz, D-55099 Mainz, Germany — Based upon first-principle calculations, we propose a practical heterostructure of hydrogenated graphene on the top of hexagonal-boron nitride, which exhibits ferromagnetic properties and relatively large spin orbit coupling. We propose to use this functional substrate for the lateral spin valve systems.

H1.00213 The Optical Properties of Germanane , PATRICK ODENTHAL, WALID AMAMOU, DANTE’ O’HARA, Univ of California - Riverside, LUYI YANG, W. D. RICE, SCOTT CROOKER, National Magnetic Field Labratory, Los Alamos National Labratory, ROLAND KAWAKAMI, Univ of California - Riverside, The Ohio State University — Hydrogenated 2D germanium, known as germanane (GeH), is predicted to be a direct bandgap semiconductor with high electron mobility (\(\sim 10^4\ cm^2/Vs\)) and circularly polarized optical selection rules. However, very little experimental work on the optical properties of germanane has been reported to date. Here, we present temperature-dependent photoluminescence (PL) and photoluminescence excitation spectroscopy (PLE) data on several-layer germanane grown by Molecular Beam Epitaxy (MBE). We observe a broad PL band that is Stokes-shifted by hundreds of meV below the predicted direct bandgap of 1.53 eV. The PL intensity increases by several orders of magnitude upon decreasing the temperature from room temperature to 4K.

H1.00214 Adsorption of Fluorine on Single layer MoS\(_2\): a first principles study\(^1\) . CONRAD TROHA, DUY LE, TALAT S. RAHMAN, Department of Physics, University of Central Florida — One of the effective methods for tuning properties of single layer MoS\(_2\) is to impose interactions with adsorbates. Using density functional theory, with the optB88-vdW exchange correlation functional, we have studied the adsorption of fluorine atoms on a single layer MoS\(_2\). We find that fluorine atoms prefer to adsorb on top of sulfur atoms (in \(2 \times 2\), \(3 \times 3\), and \(4 \times 4\) overlayer structures and that at 1/9 ML or smaller coverage, the interactions between fluorine atoms are small and can be ignored. The band structures of the considered overlayer structures suggest that the adsorption of fluorine atoms introduces defect state inside the band-gap of MoS\(_2\). This state disperses near the Fermi level in the \((2 \times 2)\) overlayer structure and is dispersionless in the \((3 \times 3)\) or larger overlayer structures.

\(^1\)Work supported in part by DOE Grant DE-FG02-07ER15842
H1.00215 Femtosecond Time Resolved Spectroscopic Measurements of Mono and Few-layers WS\textsubscript{2}, SHROUQ ALEITHAN, SUDIKSHA KHADKA, MAX LIVSHITS, JEFFERY RACK, ERIC STINAFF, Ohio University — Methods for producing samples of transition metal dichalcogenide monolayers, a new two-dimensional direct-band gap semiconductor potentially useful for applications in electronics and photonics, have dramatically improved from mechanical and chemical exfoliation, to current chemical vapor deposition (CVD) techniques. We present an experimental investigation carried out to study the exciton dynamics in mono-to-few layer sheets of WS\textsubscript{2}. The experiment was performed on commercially CVD grown WS\textsubscript{2} on a sapphire substrate employing femto-second transient absorption spectroscopy and microscopy. The sample was excited using a pump pulse of 405nm and then probed with differential absorption spectra over the spectral range of 350 nm - 800 nm, using white continuum. These results should help further the understanding of exciton dynamics in two dimensional sheets of WS\textsubscript{2}.

H1.00216 Raman Characterization of Graphene and 2D TMD Heterostructures, BENJAMIN DERBY, American University, National Institute of Standards and Technology, ANGELA HIGHT WALKER, National Institute of Standards and Technology — We report efforts to produce and characterize graphene and two-dimensional transition-metal dichalcogenides (TMD) heterostructures. Using PDMS stamps, exfoliation of graphene, Mo\textsubscript{5}S\textsubscript{3}, h-BN, and Ta\textsubscript{5}S\textsubscript{3} precedes the stacking of these mono- and few layers into heterostructures. The goal is to engineer mis-orientation to enhanced Raman signatures of various layers within the heterostructures. Previous studies have reported a Raman signal strength that is angle dependent between bi-layers \cite{1}. Using resonant Raman spectroscopy, we probe the quality of these constructed heterostructures. Ultimately, we plan to combine our optical measurements with an applied magnetic field to probe the complex magneto-Raman interaction. Previous studies \cite{2} show a magneto-phonon resonance at specific field strengths and laser excitations. Our results to date will be summarized.


H1.00217 Transport Properties of CVD Grown TMDs on Flat and Patterned Substrates, JOSEPH MARTINEZ, ARIANA NGUYEN, University of California Riverside, THOMAS SCOTT, University of Nebraska-Lincoln, EDMON PRECIADO, VELVETH KLEE, University of California Riverside, DEZHENG SUN, Columbia University, PANKAJ SHARMA, University of Nebraska-Lincoln, I-HSI LU, DAVID BARROSO, University of California Riverside, SUKHYN KIM, Columbia University, V. YA. SHUR, Ural Federal University, ALEXEI GRUVERMAN, PETER A. DOBWEB, University of Nebraska-Lincoln, LUDWIG BARTELS, University of California Riverside — Transition Metal Dichalcogenides (TMDs), MX\textsubscript{2} (M=Mo, W, etc., X=S, Se, Te), have shown great promise for applications as electronic, spintronic and photonic materials. We show growth of MX\textsubscript{2} materials under UHV (ultrahigh vacuum) and via CVD (chemical vapor deposition) on both flat and patterned substrates. Deposition on periodically-poled ferroelectric substrates reveals the impact of poling domains and the ability to reversibly invert the transport characteristics from n- to p-doped. 3D geometric patterning of substrates permits the growth across trenches and at angles to the substrate plane leading to modifications of the commonly-addressed in-plane transport properties.

H1.00218 Temporal evolution of Trion-Exciton coupling in transition metal dichalcogenide\textsuperscript{1}. KHA TRAN, AKSHAY SINGH, Univ of Texas, Austin, GALAN MOODY, National Institute of Standards and Technology, SANFENG WU, JASON ROSS, XIAODONG XU, University of Washington, XIAOQIN LI, Univ of Texas, Austin — Transition Metal Dichalcogenides (TMD’s), especially in the two-dimensional limit, show remarkable physical phenomena including large light absorption by single layers (up to 10\%) and coherent many-body effects. Increased interactions in these two-dimensional materials have been attributed to reduced screening and these are reasoned to cause large binding energies of quasiparticles including excitons (coulomb bound electron-hole pairs) and trions (charged excitons). The coupling amongst these quasiparticles is an interesting fundamental problem relating to strength of electronic interactions as well as having applications in photo-detectors working beyond diffusive transport. We use two-color pump-probe spectroscopy to measure these quasiparticle interactions as a function of time. We concentrate on the special condition of pumping at the trion transition, which is lower in energy than the exciton, and probing the exciton transition. We observe an optical response with distinct temporal response compared to other excitation conditions. The observations are well explained by a phenomenological model incorporating Optical Bloch Equations which suggests many-body effects, including excitation induced shifts, are involved.

\textsuperscript{1} We acknowledge NSF and AFOSR

H1.00219 Intrinsic transport of h-BN encapsulated few-layer black phosphorus, GHIDEWON AREFE, YOUNG DUCK KIM, DANIEL CHENET, XU CUI, DAMIEN CHANG, JAMES HONE, Columbia University — Few-layer black phosphorus (BP) is an exciting two-dimensional material with ambipolar behavior, large on/off ratio, and high mobility with a direct bandgap. The anisotropic atomic nature of black phosphorus exhibits unique angle dependent electronic and optical features. One of the primary difficulties in fabricating few-layer BP devices to study transport is the reactive nature of the material in ambient conditions as it degrades in the presence of air and moisture. In order to characterize the intrinsic physical properties of BP, we fabricated few-layer BP flakes that are fully encapsulated by hexagonal boron nitride (h-BN) with a clean stacking technique. We also characterized the electrical transport of h-BN encapsulated BP devices that show greatly improved environmental stability and high mobility at low temperature due to the suppression of extrinsic scattering effects such as charge impurities, surface polar optical phonons, and absorbents from air. H-BN encapsulated BP devices will be an essential platform for the observation of new physics from BP and realization of BP based advanced opto-electronic application devices body.

H1.00220 ABSTRACT WITHDRAWN

H1.00221 Ultrafast Dynamics in Bulk and Monolayer Mo\textsubscript{2} Measured with Femtosecond Pump-Probe Technique, XUANGHAI MEN, Department of Mechanical Engineering, The University of Texas at Austin, Austin, TX 78712, WENZHI Wu, Department of Electrical Engineering, Heilongjiang University, China, AVINASH NAYAK, Department of Electrical and Computer Engineering, The University of Texas at Austin, TX 78712, JUNG-FU LIN, Department of Geological Sciences, The University of Texas at Austin, Austin, TX 78712, DEJI AKINWANDE, Department of Electrical and Computer Engineering, The University of Texas at Austin, TX 78712, YAGUO WANG, Department of Mechanical Engineering, The University of Texas at Austin, TX 78712. Mo\textsubscript{2} is a typical material of transition-metal dichalcogenide family. It exhibits unique properties when thickness reduces to monolayer. Recent studies have shown strong photoluminescence (PL) and high carrier mobility on monolayer Mo\textsubscript{2}, which makes it a promising candidate for future photonic and field-effect transistor (FET) applications. Our ultrafast measurement utilizes optical 400nm-pump 800nm-probe spectroscopy to reveal the relaxation dynamics of photo-excited carriers in both bulk and monolayer Mo\textsubscript{2}. Measurement is carried out at ambient pressure for different pump fluences. Both a fast and a slow carrier lifetime are acquired in monolayer Mo\textsubscript{2} due to different carrier scattering mechanisms. Carrier lifetimes are measured at different pump fluences, from which we propose possible carrier relaxation mechanisms. In suspended bulk Mo\textsubscript{2}, coherent acoustic phonons with a peak frequency around 38GHz are observed. Phonon lifetime and amplitude at different pump fluences have also been investigated.

H1.00222 ABSTRACT WITHDRAWN
H1.00223 Hydrogen Molecule Adsorption on a Borophene-Titanium System. GREGORIO RUIZ-CHAVARRIA, Universidad Autonoma Chapingo — From the synthesis of graphene have developed a wide range of researches on their use, both theoretical and experimental. So there have been research on graphene-based electronics, but also on issues of energy, particularly hydrogen adsorption on graphene-based systems. Given the potential represented by these structures is very natural to wonder about similar structures, but based in elements near carbon. One of the lines developed very recently consider the boron as the element to build graphene-like structures. Different studies, both theoretical and experimental have been made where the studied structures are graphene type or fullerene, where boron is used in place of carbon. We will use as a starting point the proposed structures by Xiaobao[1] and Tang[2]. This structure is known as the borophene, which in first place will be decorated with titanium and then, this system interact with hydrogen molecule. In our calculation we use functional density theory, atomic pseudopotentials, Born approximation and molecular dynamic.


H1.00224 Transport Properties Across Misoriented Bilayer MoS2 using Ab-initio Calculations, KUAN ZHOU, SUPENG GE, DARSHANA WICKRAMARATNE, ROGER LAKE, Univ of California - Riverside — Fabrication of electrical and opto-electronic devices with vertically stacked transition metal dichalcogenides (TMDCs), leads to interfaces that are misoriented. Prior experimental and theoretical studies of misorientation in graphene bilayers demonstrated that a few degrees of misorientation is sufficient to decouple the low energy states of the individual layers. Experimental and ab-initio calculations have shown the bandgap of misoriented bilayer MoSremains indirect. The transport properties across the misoriented interface of the bilayer TMDCs is currently unknown. The coherent interlayer transmission across two stacks of MoSis calculated for unrotated and rotated MoSbilayers using ab-initio calculations. The energy dependence of the interlayer transmission is analyzed.

H1.00225 Fluorinated graphene as an efficient diffusion barrier in Ge semiconductor devices, WEI REN, HENG GAO, Shanghai University — We evaluate the efficient diffusion barrier effects of the fluorinated graphene from the first principles. By taking its advantage of impermeability, we discover such monoatomic layer can suppress the formation of the unstable interfacial oxide in Ge-based semiconductor devices. To elucidate the physical mechanism governing this shielding functionality, nudged elastic band method is adopted to calculate the barrier height of one oxygen or one germanium atom penetrating the pristine graphene and fluorinated graphene. The energy of the adsorbed O or Ge atom on different sites of the graphene is calculated, namely three positions on the honeycomb lattice, bridge, hollow, and top. Our results reveal that both the O and Ge atoms adsorbed on the graphene are most stable on the bridge site, followed by the top and hollow sites with higher energies. Different penetration paths of O and Ge atoms are considered, and the calculated values of the energy barriers for both graphene and fluorinated graphene exhibit superior impermeability and hence to hinder diffusion of O and Ge atoms across the graphene and fluorinated graphene. This latter insulating structure is expected to expedite the implementation of germanium as channel materials in next-generation nanoelectronic devices.

H1.00226 Fabrication of graphene field-effect transistor on top of ferroelectric single-crystal substrate, NAHEE PARK, HAEYONG KANG, YOURACK LEE, JEONG-CYUN KIM, JOONG-CYU KIM, YOOJU JUN, JEONGMIN PARK, TAEYOO KIM, JUNG HO KIM, YOUNG SEON SHIN, YOUNG HEE LEE, DONGSEOK SUH, Center for Integrated Nanostructure Physics (CINAP/IBS) and Dept. of Energy Science (DOES), Sungkyunkwan University — In the analysis of Graphene field-effect transistor, the substrate material which has the direct contact with Graphene layer plays an important in the device performance. In this presentation, we have tested PMN-PT(1-x)Pb(Mg1/3Nb2/3)O3-xPbTiO3) substrate as a gate dielectric of Graphene field-effect transistor. Unlike the case of previously used substrates such as silicon oxide or hexagonal Boron-Nitride(h-BN), the PMN-PT substrate can induce giant amount of surface charge that is directly injected to the attached Graphene layer due to its ferroelectric property. And the hysteresis of polarization versus electric field of PMN-PT can cause the device to show the ferroelectric nonvolatile memory operation. We had successfully fabricated Graphene field-effect transistor using the mechanically exfoliated Graphene layer transferred on the PMN-PT(001) substrate. Unlike the case of mechanical exfoliation on the surface of silicon-oxide or the Poly(methyl methacrylate) (PMMA), the weak adhesion properties between graphene and PMNPT required the pretreatment on PMMA before the exfoliation process. The device performance is analyzed in terms of the effect of ferro- and piezo-electric effect of PMNPT substrate.

H1.00227 Study of quantum capacitance in N doped few layer graphene, MEHMET KARAKAYA, JINGYI ZHU, RAMAKRISHNA PODILA, Clemson University, ANURAG SRIVASTAVA, IIITM- Gwalior, Madhya Pradesh, India, APPARAO RAO, Clemson University, DEPARTMENT OF PHYSICS AND ASTRONOMY, CLEMSON NANOMATERIALS CENTER, CLEMSON UNIVERSITY TEAM, IIITM- GWALIOR, MADHYA PRADESH, INDIA TEAM — The intrinsically small density of states at the Fermi level in graphene results in a small serial quantum capacitance CQ, which diminishes the total device capacitance value (Ctot) in supercapacitors. In this work, we studied CQ of N doped graphene in pyrolic(N1), graphitic (N2) and pyridinic (N3) configurations. The observed CQ value for sample N1 was significantly different from samples N2 and N3, as predicted by DFT calculations, thus implying that precisely engineered dopant configurations, rather than concentration, can enhance CQ. Such approaches are pivotal for alleviating the existing bottlenecks in both graphene-based device scaling and supercapacitor electrode limitations.

1NSF-1124733

H1.00228 Effect of adsorbed gases on the G and D’ peaks of the Raman spectrum of graphene, GINA GREENIDGE, JOSHUA HALPERN, Department of Chemistry, Howard University, Washington, DC 20059 — The ability of graphene to function as a gas sensor for polar molecules has been widely investigated by monitoring the conductivity of graphene near the Dirac point. Here we demonstrate that Raman spectroscopy can also monitor the interaction of these molecules with graphene. Using a Raman microscope we observe measurable changes in the width and position of the G peak, and the intensity of the D’ prime peak upon exposure to water vapor (H2O and D2O). The changes are reversible. Baking the material at 350 °C restores the graphene spectrum to its original state. We are investigating the effects of additional gases as well as the relationship of these shifts to the conductivity and the gas-graphene interaction.

1Funding for this research was provided by the Partnership for Reduced Dimensional Materials (PRDM), an NSF Partnership for Research and Education in Materials (PREM) (Award Number DMR-1205608).
H1.00220 Effect of Al2O3 deposition on electronic Transport in Graphene: DFT-NEGF study1
TOMOA KI KANEGO, TAKAHISA OHNO, National Institute for Materials Science, MATERIALS RESEARCH CONSORTIUM FOR EFFICIENT ELECTRONIC DEVICES TEAM, UNIVERSITY OF TOKYO TEAM — In order to screen the charged impurities and to prevent the adsorption of contaminant on graphene, the deposition of high-k materials such as Al2O3 on graphene surface is important issue for graphene device application. Since the interfacial structure of graphene and high-k materials are not identified, theoretical study on the interfacial structure dependence on electronic transport is highly demanded. In this paper, we performed the electronic transport simulation in graphene under Al2O3 based on the density functional theories (DFT) and nonequilibrium Green’s function method (NEGF). We investigated the effect of Al2O3 surface termination on the electronic transport properties. According to the calculation of stability of interfaces and electronic structures, the graphene’s linear band structure is preserved in O2 deficient condition. In O2 rich condition, on the other hand, the graphene’s unique electronic structure is disturbed. These properties are important for the electronic transport in graphene under Al2O3. Graphene shows relatively good transport properties in O2 deficient condition, but transport is considerably suppressed in O2 rich condition. Our results suggest O2 deficient condition is desirable for the device application.

1 A portion of this research was supported by the grant for “Strategic Programs for Innovative Research” Field No. 4: Industrial Innovations.

H1.00230 Asymmetric capacitance and ambipolar metal insulator transition in black phosphorus1
YUI SAITO, YOSHIHIRO IWASA, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo, Japan — Black phosphorus is a van der Waals type semiconducting layered material with a puckered honeycomb structure where each phosphorus atom is covalently bonded with three adjacent phosphorus atoms and has a direct band gap of 0.3 (bulk) - 2 (monolayer) depending on the number of layers [1], which can be promising material for optoelectronics such as photodetectors. In this presentation, by using ionic liquid gating method, we report the ambipolar transistor operation and the field effect controlled ambipolar metal-insulator transition in black phosphorus thin flake. We observed a large modulation of the sheet resistance by more than 4 orders of magnitude in both electron channel and hole channel. These results suggest black phosphorus will be a key material not only for understanding the physical properties of the conduction channel produced by ionic gating, but also potential functions including formation of p-n junction and therefore lateral tunnel diode utilizing intrinsic narrow band gap.


H1.00231 Graphene/GaN diodes for ultraviolet and visible photodetectors1
FANG LIN, SHAOWEN CHEN, JIE MENG, GEOFFREY TSE, XUEWEN FU, FUJIN XU, BO SHEN, ZHI MIN LIAO, DAPENG YU, Peking Univ, NANOLAB TEAM — The Schottky diodes based on graphene/GaAs interface are fabricated and demonstrated for the dual-wavelength photodetection of ultraviolet (UV) and green lights. The physical photoresponsive transient times of several ms. photocurrent response leading up to 0.5 A/W photoresponsivities and high external quantum efficiencies of up to ∼90% indicate the photo-electrical response is not from the area surrounding the electrical contacts. It was found that the three-layer WSe2 FETs display a strong electronic applications. Here, we investigate wavelength dependent absorption and transport properties of optically excited carriers via photoconductivity on the W-based monolayer; this finding agrees with recent ultrafast spectroscopy experiments. We discuss how the radiative lifetime tunability can be employed to manipulate excitons in 2D-TMDs.

H1.00232 Exciton Radiative Lifetimes in Layered Transition Metal Dichalcogenides
MAURIZIO PALUMMO, Department of Physics, University of California, Berkeley, CA 94720, USA, MARCO BENARDI, Department of Physics, University of Rome Tor Vergata, Italy, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, MA 02139, USA — Light emission in two-dimensional (2D) transition metal dichalcogenides (TMDs) changes significantly with number of layers and stacking sequence. While the electronic structure and optical absorption are well understood in 2D-TMDs, much less is known about exciton dynamics and radiative recombination. In this talk, we show first-principles calculations of intrinsic exciton radiative lifetimes at low temperature (4 K) and room temperature (300 K) in TMD monolayers with chemical formula MX2 (M=Mo,W and X=S,Se), in bilayer and bulk MoS2, and in two MX2 hetero-bilayers. Our results elucidate the time scale and microscopic origin of light emission in TMDs, which have been the subjects of recent intense investigation. We find radiative lifetimes of a few ps at low temperature and a few ns at room temperature in the monolayers, and slower radiative recombination in bulk and bilayer than in monolayer MoS2. The MoS2/WS2 and MoSe2/WS2 hetero-bilayers exhibit long-lived (∼30 ns at room temperature) inter-layer excitons constituted by electrons localized on the Mo-based and holes on the W-based monolayer; this finding agrees with recent ultrafast spectroscopy experiments. We discuss how the radiative lifetime tunability can be employed to manipulate excitons in 2D-TMDs.

H1.00233 ABSTRACT WITHDRAWN

H1.00234 Photoconductivity spectroscopy of epitaxial germanane devices1
ELIZABETH BUSHONG, YUNQIU KELLY LUO, The Ohio State University, JEREMIAH VAN BAREN, WALID AMAMOU, PATRICK O'DENTHAL, DANTE O'HARA, University of California, Riverside, IGOR PINCHUK, JYOTI KATOCH, ADAM AHMED, The Ohio State University, ROLAND KAWAKAMI, The Ohio State University; University of California, Riverside — Germanane, a 2D sheet of hydrogen terminated germanium atoms, has recently generated a great deal of interest. Unlike graphene, which has been the focus of 2D materials for almost a decade, germanane has a direct band gap (1.5 eV) and strong spin-orbit coupling. Additionally, it is predicted that changing the surface functionalization of germanane will allow tuning of the band gap, which makes it promising for electronic and optoelectronic applications. Here, we investigate wavelength dependent absorption and transport properties of optically excited carriers via photoconductivity on germanane. Samples with thicknesses ranging from several atomic layers up to 250 nm have been studied. We observe an absorption edge as a function of wavelength, as expected for a semiconducting material. There appears to be a small shift to shorter wavelengths for thinner samples. The dependence on intensity and temperature are also investigated, as well as the bias dependence. These results have implications for the use of germanane in future applications.

H1.00235 Planar Nanoscale Capacitors from Laterally Stacked Graphene - Boron Nitride Layers
V. ONGUN OZCELIK, ENGIN DURGUN, SALIM CIRACI, Bilkent University — We propose a nanoscale planar capacitor model consisting of laterally stacked two-dimensional insulating BN layers placed between two commensurate and metallic graphene layers. First-principles calculations of structure optimized total energy and self-consistent field potential performed on these nanoscale capacitors for different levels of charging and different number of BN layers mark the values of capacitance per unit mass, which are larger than those measured values for the supercapacitors made from other carbon based materials.

H1.00236 High Photoresponsivity and Extrinsic Quantum Efficiency in Tri-Layer Tungsten Diselenide Phototransistors
ZHENGGUANG LU, NIHAR PRADHAN, KOMALAVALLI THIRUNAVUKKARASU, JONATHAN LUDWIG, DANIEL RHODES, DMITRY SMIRNOV, LUIS BALICAS, National High Magnetic Field Lab, Florida State University, 1800 E. Paul Dirac Dr. Tallahassee, FL 32310 — We report on the photoresponse properties of three-layer tungsten diselenide field-effect transistors (FETs) fabricated by mechanical exfoliation of bulk crystals on SiO2/Si substrates connected with Au/Ti contacts. These devices exhibit two-terminal field-effect hole mobilities of about 350 cm2/Vs at 300K increasing up to 500 cm2/Vs at T<50 K. The photoresponse properties were carried out at room temperature using various excitation wavelengths (405nm, 532nm, 670nm). In addition, we mapped photocurrent of these device with a laser spot size considerably smaller than the area of the conducting channel which indicate the photo-electrical response is not from the area surrounding the electrical contacts. It was found that the three-layer WSe2 FETs display a strong photocurrent response leading up to 0.5 A/W photoresponsivities and high external quantum efficiencies of up to ∼ 90%. Also, these transistors display fast photoresponsive transient times of several ms.
H1.00237 Study of Charge Density Wave Modulations in the Extended Hubbard Model

SAUMYA BISWAS, ROGER LAKE, University of California Riverside — Charge density wave (CDW) modulations in a two-dimensional lattice are modeled in the mean field approximation using the extended Hubbard Hamiltonian. The electron phonon coupling is included with an on-site interaction term. The effect of coupling strength and Fermi level on the CDW wavelength and amplitude is examined. Periodic and closed boundary conditions are considered. The effect of potential modulation by electrostatic gating on the CDW phase and wavelength is calculated.

1 This work was supported in part by the NSF and SRC-NRI project 2204.001 (NSF-ECCS-1124733)

H1.00238 Magneto-photoconductivity of atomically thin transition metal dichalcogenides

M. EGILGIL, C. ZOU, N. PEIMYOU, B. CAO, X. SHEN, J. SHANG, C. CONG, T. YU, Nanyang Technological University — Photoinduced effects of two-dimensional (2D) transition metal dichalcogenides (TMDs) are of great interest since the bandgap of these materials corresponds to visible range of spectrum. For instance, in molybdenum disulphide (MoS$_2$) a 2D semiconductor TMD and a non-centrosymmetric crystal, inherent broken inversion symmetry in monolayers leads to a large spin-orbit interaction which splits the valence band (VB) by 160 meV and gives rise to strong excitonic transitions due to the direct band gap at low energy K and K valleys. The same broken inversion symmetry together with time reversal symmetry is responsible for spin-valley coupling in monolayer MoS$_2$ and similar TMDs (such as tungsten disulphide, WS$_2$). Spin-valley coupled band edges in TMDs result in different localization behaviors for different scattering mechanisms. In this work, we present our magneto-photoconductivity studies of mono- and bilayer field-effect transistor devices of MoS$_2$ and WS$_2$, and discuss our results in terms of localization effects.

1 Supported in part by the Singapore Ministry of Education under MOE2013-T1-2-235, MOE2012-T2-2-049, and MOE2013-T2-1-044

H1.00239 Lateral MoS$_2$ p-n junctions formed by chemical doping method

WON JONG YOO, MIN SUP CHO, DESHUN QU, DAeyeong Lee, XIAOCHI LIU, YOUNGDae JANG, CHANGSik KIM, JUNGJin RYU, Sungkyunkwan Univ — Interests on transition metal dichalcogenides, especially MoS$_2$, are growing immensely due to its semiconducting nature with visible light range bandgap and strong light absorption property, which can pave the way to replace Si-based electronics and realize flexible and transparent electronics. For more versatile applications and industrialization, however, a proper doping process is required because various devices such as photonics and tunneling devices are composed of p-n junctions. Here, we demonstrated the formation of lateral MoS$_2$ p-n junction by using partially stacked of hBN and p-doping with AuCl$_3$ solution. The fabricated devices showed an ideal rectifying behavior with ideality factor about 1. Under the exposure of monochromatic light, it revealed the properties of conventional p-n diode and also highly efficient photonic properties, showing feasibility to be applied for photovoltaic cells and photodetectors. Furthermore, we fabricated novel tunneling devices with similar device structure where local gates are located under MoS$_2$. Its Fermi level can be effectively controlled by local gate modulation, so that the tunneling current can flow by band-to-band tunneling. This study provides an effective way to realize the practical devices such as photonic and tun

H1.00240 ABSTRACT WITHDRAWN

H1.00241 Magneto-resistance of multilayer carbon nanotube Fermat yarn and coil yarn

KIEU TRUONG, HAEYONG KANG, YOURACK LEE, JOONG-GYU KIM, YOUNG HEE LEE, DONGSEOK SUH, Sungkyunkwan Univ, IBs CENTER FOR INTEGRATED NANOSTRUCTURE PHYSICS, INSTITUTE FOR BASIC SCIENCE (IBS), SKKU, KOREA COLLABORATION, DEPARTMENT OF ENERGY SCIENCE, SUNGKYUNKwan UNIVERSITY, SUwon 445-746, KOREA COLLABORATION, DEPARTMENT OF PHYSICS, SUNGKYUNKwan UNIVERSITY, SUwon 440-746, KOREA COLLABORATION — Multilayer carbon nanotube (MWCNT) based yarn has attracted a great attention for the development of multifunctional super-fiber due to its light weight, high flexibility, high conductivity, and strong mechanical properties. Recently the importance of coil yarn structure was demonstrated for practical applications (Haines et al. 2014, Science). In this study, we measured the electrical resistance of neat yarn and coiled yarns at different temperatures and magnetic fields. The coiled yarn was formed by twist-insertion into the neat yarn, and the transverse and longitudinal magnetoresistance (MR) measurements were carried out. The logarithmic temperature dependence of normalized resistance and the magnitude difference of MR between two configurations and the survival of such difference even at room temperature indicate that one-dimensional transport features are quite significant in this system. Developing Route for sub-micrometer-scale coil is discussed.

This work was supported by Project code (IBS - R011-D1).

H1.00242 ABSTRACT WITHDRAWN

H1.00243 Carbon nanotube networks grown on various carbon nanostructures: SWCNT, MWCNT and Graphene

YOUNGWOO KWON, ANVAR ZAKHIDOV, Univ of Texas, Dallas, ALAN G. MACDIARMID NANOTECH INSTITUTE TEAM — Secondary growth of carbon nanotubes (CNT) on the various nanoscale substrates has been performed by using chemical vapor deposition (CVD). Spinnable CNT yarns, single wall CNT sheets and graphene flakes, in NMP have been used as scaffolds for such secondary networks. The CNT yarn drawn from spinnable CNT forest is one of the promising applications of the CNT. However, orientation of the yarn and comparatively high sheet resistance make them harder for applications. Processing secondary CVD grows CNTs on the CNT yarn without any orientation of the secondary grown CNTs. Thus, this decreases the effect of the orientation of the CNT yarn and also decreases sheet resistance since the yarn have more contact each other. This after-treating will make more application possible. Furthermore, since CNT yarn does not make perfect surface and have gap between each bundle, arranging yarns to certain orientation decreases the effect of the orientation of the CNT yarn and also decreases sheet resistance since the yarn have more contact each other. This after-treating will make more application possible. Furthermore, since CNT yarn does not make perfect surface and have gap between each bundle, arranging yarns to certain orientation decreases the effect of the orientation of the CNT yarn and also decreases sheet resistance since the yarn have more contact each other. This after-treating will make more application possible. Furthermore, since CNT yarn does not make perfect surface and have gap between each bundle, arranging yarns to certain orientation decreases the effect of the orientation of the CNT yarn and also decreases sheet resistance since the yarn have more contact each other. This after-treating will make more application possible. Furthermore, since CNT yarn does not make perfect surface and have gap between each bundle, arranging yarns to certain orientation decreases the effect of the orientation of the CNT yarn and also decreases sheet resistance since the yarn have more contact each other. This after-treating will make more application possible. Furthermore, since CNT yarn does not make perfect surface and have gap between each bundle, arranging yarns to certain orientation decreases the effect of the orientation of the CNT yarn and also decreases sheet resistance since the yarn have more contact each other. This after-treating will make more application possible.

1 Supported in part by the Singapore Ministry of Education under MOE2013-T1-2-235, MOE2012-T2-2-049, and MOE2013-T2-1-044

H1.00244 Structural transition and mechanical properties of one dimensional boron ribbons and chains from first principles

MINGJIE LIU, VASILI I. ARTYUKHOV, BORIS I. YAKOBSON, Department of Materials Science and Engineering, Rice University, Houston, TX — The past decade has brought great progress in fabrication and characterization of single-atom chains of carbon (carbyne). Very recently novel atomic chain arrangements such as BN and Csl were reported. The extreme and unusual properties of such 1D material motivate the search for other possible compositions with interesting behaviors. We use first-principles calculations to uncover the rich structural and mechanical properties of 1D boron. While the ground state structure of linear boron is a two-atoms-wide ribbon, tension can unravel it into a single-atom string structure. We analyze the mechanical and electronic properties of these two “phases” and study the thermodynamics and kinetics of transition between them using static first-principles calculations and semiempirical (DFTB) molecular dynamics. The interesting properties of 1D boron nanostructures make them an attractive system for experimental investigations.

1 M. Liu et al., ACS Nano 7, 10075 (2013)
H1.00245 Non-covalent functionalization of single wall carbon nanotubes and graphene by a conjugated polymer, JILILI JIWUER, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia, AYJAMAL ABDURAHMAN, ÖĞÜZ GÜLSEREN, Department of Physics, Bilkent University, 06800 Ankara, Turkey, UDO SCHWINGENSCHÖGL, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia — We report first-principles calculations on the binding of polyn-(9,9-bis-(6-bromohexyl)fluorene-2,7-diyI)-co-(benzene-1,4-diyI)] to a (8,0) single wall carbon nanotube (SWCNT) and to graphene. Considering different relative orientations of the subsystems, we find for the generalized gradient approximation (GGA) a non-binding state, whereas the local density approximation (LDA) predicts reasonable binding energies. The results coincide after inclusion of van der Waals (vdW) corrections, which demonstrates a weak interaction between the polymer and SWCNT/graphene, mostly of van der Waals type. Accordingly, the density of states shows essentially no hybridization. The physosorption mechanism explains recent experimental observations and suggests that the conjugated polymer can be used for non-covalent functionalization. (Reference: Appl. Phys. Lett. 105, 013103, 2014)

H1.00246 Design of Inorganic Electrides, YUNWEI ZHANG, HUI WANG, YANCHAO WANG, YANMING MA, State Key Lab of Superhard Materials, Jilin University — Electrides, in which all or part of the valence electrons occupy interstitial regions in the crystal and behave as anions, have been synthesized at ambient or high-pressure conditions [1]. Their loosely bound anionic electrons make electrides good candidates for electroactive materials. Here, we report a developed methodology to systematically design electrides for given chemical systems. The new approach is based on the swarm-intelligence CALYSPO algorithm on structure prediction [2] and requires only the chemical compositions to predict the electrode phases. In contrast to the traditional ground state structure prediction method where the total energy was solely used as the fitness function, we adopted a new fitness function in combination with the first-principles calculation to select the optimal solutions for a description of given chemical systems. The experimentally known electrides have been successfully reproduced. The results suggested that our approach is reliable and can be widely applied into design of new electrides.


H1.00247 Monte Carlo(MC) simulation study on ammonia anchored TON zeolite for carbon dioxide capture, HANSOL WEE, WONBO LEE, Sogang Univ — If zeolites are modified by ammonia, the electronic effect in ammonia resulted in different surface basicity of the zeolite materials. So, ammonia anchored materials show better adsorption rate of CO2 than pure materials at low pressure. MC simulations for CO2 adsorption were performed at 298K. The results show that, at pressure 1000 kpa CO2 loading is 1.404 mol/kg at ammonia anchored TON, and 0.529 mol/kg at pure TON. However, at high pressure, the ammonia effect becomes marginal. Ammonia anchored TON structures may be used to adsorb CO2 more effective than normal TON structure.

H1.00248 Anisotropic mechanical properties of hexagonal SiC sheet: a molecular dynamics study, MING YU, Univ of Louisville, EMILY LIU, duPont Manual High School, CONGYAN ZHANG, Univ of Louisville — The anisotropic mechanical properties of hexagonal SiC sheet have been studied using an efficient quantum mechanics molecular dynamics scheme based on a robust semi-empirical Hamiltonian (referred as SCED-LCAO) [PRB 74, 15540; PHYSE 42, 1]. It was found that the SiC sheet could sustain the heavy load up to about 20 %. In particular, it was found that the SiC sheet also shows large difference in the strain direction. It will quickly crack after 20 % of strain in armchair direction, but it will be slowly destroyed after 30% in the zigzag direction, indicating the anisotropic nature of the mechanical properties of the SiC sheet. The nominal and 2D membrane stresses will be analyzed, from which we will obtain the 2D Young’s modulus at infinitesimal strain and the third-order (effective nonlinear) elastic modulus for the SiC sheet. The detail results and discussions will be reported in the presentation.

H1.00249 Towards first-principles based prediction of highly accurate electrochemical Pourbaix diagrams, ZHENHUA ZENG, Purdue University, MARIA CHAN, Argonne National Laboratory, JEFF GREELEY, Purdue University — Electrochemical Pourbaix diagrams lie at the heart of aqueous electrochemical processes and are central to the identification of stable phases of metals for processes ranging from electrocatalysis to corrosion. Even though standard DFT calculations are potentially powerful tools for the prediction of such Pourbaix diagrams, inherent errors in the description of strongly-correlated transition metal (hydr)oxides, together with neglect of weak van der Waals (vdW) interactions, has limited the reliability of the predictions for even the simplest bulk systems; corresponding predictions for more complex alloy or surface structures are even more challenging. Through introduction of a Hubbard U correction, employment of a state-of-the-art van der Waals functional, and use of pure water as a reference state for the calculations, errors in structure and property predictions are systematically reduced. The strong performance is illustrated on a series of bulk transition metal (Mn, Fe, Co and Ni) hydroxide, oxyhydroxide, binary and ternary oxides where the corresponding thermodynamics of oxidation and reduction can be accurately described with standard errors of less than 0.04 eV in comparison with experiment.

H1.00250 Preferential adsorption positions for an adsorbed Li atom on the layered black phosphorus structures, CONGYAN ZHANG, MING YU, University of Louisville — The preferential adsorption positions for an adsorbed Li atom on the layered black phosphorus were determined by mapping out the total energy as a function of its positions on the layered black phosphorus using the density functional theory based method (referred as VASP [Phys. Rev. B 48, 13115 (1993)])]. Various possible adsorption positions including the top of the bridge, the valley, and the interstitial positions of the puckered layers have been studied. It is found that the adsorption energy strongly depends on these positions with different environment. In particular, the most preferential adsorption positions for an adsorbed Li atom are found at the valleys and the interstitials of the puckered layers. The analysis of structural and electronic properties of the black phosphorus layer with the adsorbed Li atom will be discussed.

H1.00251 Ab initio NMR Confirmed Evolutionary Structure Prediction for Organic Molecular Crystals, CONG-HUY PHAM, International School for Advanced Studies (SISSA), Trieste (Italy), EMINE KUCUKBENLI, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne (Switzerland), STEFANO DE GIRONCOLI, International School for Advanced Studies (SISSA), Trieste (Italy) — Ab initio crystal structure prediction of organic molecular crystals is extremely challenging due to several factors: limited experimental knowledge, molecular flexibility and difficulties in addressing the dispersion interaction from first principles [1]. We recently implemented vdW-aware density functionals and demonstrated their success in energy ordering of aminocacid crystals [2]. In this work we combine this development with the evolutionary structure prediction method [1] to study cholesterol polymorphs. Cholesterol crystals have paramount importance in various diseases, from cancer to atherosclerosis. The structure of some polymorphs (e.g. ChM, ChAl, ChAh) have already been resolved while some others, which display distinct NMR spectra and are involved in disease formation [3], are yet to be determined. Here we thoroughly assess the applicability of evolutionary structure prediction to address such real world problems. We validate the newly predicted structures with ab initio NMR chemical shift data using secondary referencing for an improved comparison with experiments [4]. [1]Zhu et al. Acta Cryst B 68, 215 (2012), [2]Quantum ESPRESSO, Sabatini et al. J Phys Cond Matt 24, 424209 (2012), [3]Jayalakshmi et al. SS Nucl Magn Res 36, 60 (2009), [4]Kucukbenli et al. JCP A 116, 3765 (2012)
**H1.00252 Exceptional Optoelectronic Properties of Si-related compounds.** BING HUANG, HOULONG ZHUANG, MINA YOON, ORNL, SU-HUI AI WEI, NREL, BOBBY SUMPTER, ORNL — The search of new silicon-related functional compounds are of great interests but still very challenging. In the last few decades, researchers have heavily studied the structural and electronic properties of silicon in order to improve its optical absorption in the visible light range using analyses of metastable silicon phases, silicon-based alloys, and silicon-based superlattices. In this talk, I will present our recent theoretical efforts on searching and designing new silicon phases, from bulk to two-dimensional (2D) silicon, with exceptional optoelectronic properties. Especially, we find that chemically functionalized 2D silicon and silicon alloys could be the best candidates to create efficient thin-film solar absorbers and silicon-based, white-light-emitting diodes, paving the way for new “green” energy applications.

**H1.00253 Maximizing the bandgap of BCN nanoribbons.** RAISI BALDEZ, PAULO PIQUINI, ALEX SCHMIDT, Universidade Federal de Santa Maria, MARCELO KURODA, Auburn University — Carbon and boron-nitride based compounds share many electronic and structural features. This fact permits mixed carbon-boron-nitride compounds to be easily synthesized without significant structural changes. Further, the partially ionic character of the boron-nitrogen bonds allow to modify the electronics of carbon based materials, introducing a variability that can be used to tune the electronic properties according to the boron and nitrogen contents. Graphene and graphene nanoribbons have emerged as promising materials for electronic applications, due to the high mobility of its charge carriers. In this work we use the genetic algorithm approach to search for configurations with variable B, C and N contents that maximize the band gap of B_xC_yN_z nanoribbons. Different stoichiometries are analyzed and the structural patterns that lead to the maximal band gaps are presented.

**H1.00254 Pd/W(110) as a highly CO tolerant electrocatalyst for hydrogen oxidation: insight from first principles.** NAGENDRA DHAKAL, SERGEY STOLBOV, University of Central Florida — Platinum perfectly catalyzes hydrogen oxidation reaction on the hydrogen fuel cell anodes. However, it has at least two drawbacks: a) it is too expensive; b) it has a low tolerance to CO poisoning. Pt-Ru bi-functional catalysts are more tolerant to CO, but they are still very expensive. In this work, we performed first-principle studies of stability reactivity of M/W(110) structures, where M=Pd,Ru,Ar monolayers. All three systems are found to be stable: formation energy of MLs is significantly higher than cohesive energy of the M-elements. The calculated binding energies of H, H_2, OH, CO, and H_2O were used to obtain the reaction free energies. Analysis of the free energies suggests that Au-W bonding does not activate sufficiently Au monolayer, whereas Ru/W(110) is still too reactive for the CO removal. Meanwhile, Pd/W(110) is found to catalyze hydrogen oxidation and at the same time highly tolerant to the CO poisoning. The latter finding is explained by the fact that CO binds much weaker to Pd on W(110) than to Pt, while the OH binding energy is strong enough to ensure CO oxidation. The obtained results are traced to the electronic structure of the systems.

**H1.00255 Electronic and vibrational properties of monolayer and bilayer TaSe_2.** MACK ADRIAN DELA CRUZ, JIA-AN YAN, Department of Physics, Astronomy, Geosciences, Towson University — Distinct from MoS_2, two-dimensional atomic crystal of tantulum diselenide (TaSe_2) is metallic and exhibits charge-density wave (CDW) transitions. Using density-functional theory, we present a first-principles study of the electronic and vibrational properties of monolayer and bilayer TaSe_2 without including the CDW-induced structural distortions. For monolayer 1T-TaSe_2, the frequencies of the Raman active modes are 159 cm^{-1} (E'_g) and 226 cm^{-1} (A'_1g), while the Raman-active modes for monolayer 2H-TaSe_2 are at 138 cm^{-1} (E''_g), 214 cm^{-1} (E''_g), and 241 cm^{-1} (A'_1g). For bilayer TaSe_2, different stackings of monolayer 2H-TaSe_2 and 1T-TaSe_2 phases have been calculated. Electronic band structures and vibrational properties of four energetically favorable configurations will be presented. Finally, the spin-orbit coupling on the structural and electronic properties will also be discussed.

1 We thank the Towson University Faculty Development and Research Committee (grant OSPR # 140269), the Fisher College of Science and Mathematics Fisher General Endowment as well as the Undergraduate Research Committee for the support.

2 Undergraduate

**H1.00256 Density Functional Theory Studies of Li-ion interaction with defected group 14 heteronanotubes and nanosheets.** TICHAKUNDA PASIPANODYA, PRABATH WANAGURU, RAYMOND ATTA-FYNN, University of Texas at Arlington — Nanomaterials show significant promise in enhancing Lithium ion (Li-ion) battery properties. Using density functional theory, we study the binding and diffusion of Li on defected nanotubes and nanosheets of silicon carbide (SiC) and silicon germanium (SiGe). Point and extended defects are considered to fully evaluate the influence of defects on the adsorption and diffusion properties. The trends in the adsorption-induced changes in the geometric and electronic properties will be presented. Furthermore, room temperature ab initio molecular dynamics simulations will be carried out to investigate finite temperature effects on the binding mechanisms and electronic structures.

**H1.00257 Ferromagnetism in SrTiO_3 Single Crystals Induced by Laser irradiation.** SRINIVASA RAO SINGAMANENI, Y.F. LEE, J.T. PRATER, A.I. SMIRNOV, J. NARAYAN, North Carolina State University — SrTiO_3 (STO) is diamagnetic in pristine state, important in emerging field of complex oxide electronics. No attention has been paid to explore the magnetic properties of STO crystal upon laser irradiation/annealing. In this presentation, we demonstrate [1-2] that STO single crystals show ferromagnetic order up to 400 K upon KrF (248 nm) laser irradiation. The high resolution x-ray photo emission spectroscopy (XPS) measurements reveal a strong shift of Sr-, Ti- and O-related peaks. X-ray diffraction (XRD) of laser annealed STO does not reveal a signature of either secondary magnetic or amorphous phases. 300 K X-band (~ 9.543 GHz) angle-dependent electron paramagnetic resonance (EPR) measurements showed no evidence of additional magnetic peaks up on laser irradiation. XPS and EPR data did not provide a strong evidence of Ti_3^+ formation upon laser annealing. No differences in the visible 300 K Raman spectra of pristine and laser annealed STO are noticed. Interestingly, the magnetic moment is decreased by almost 10-fold upon oxygen annealing of laser annealed STO, inferring that oxygen vacancies play an important role in establishing the observed ferromagnetism.


**H1.00258 Cross-over from antiferromagnetic to ferromagnetic interface exchange coupling in epitaxial ferromagnetic oxides.** SRINIVASA RAO SINGAMANENI, North Carolina State University, JOHN T. PRATER, Army Research Office, JAY NARAYAN, North Carolina State University — Interface magnetism in La_{1-x}Sr_xMnO_3/SrRuO_3 (LSMO/SRO) bilayer (BL) has been the subject of great interest in the recent past owing to interesting physics and potential applications. Through a novel approach [1-3], LSMO (13nm)/SRO (45nm) and LSMO (33nm)/SRO (45nm) bilayers have been epitaxially integrated with Si (100). Notably, in the former sample, positive exchange bias is observed –indication of antiferromagnetic exchange coupling and is found to be absent in the later. Interestingly, in the former sample, the cross-over from antiferromagnetic to ferromagnetic interface coupling is noticed by varying the cooling field. We have verified that the coupling is of magnetic origin, not due to electrostatic interaction by inserting a thin (~10nm) SrTiO_3 layer between LSMO and SRO. We believe that the formation of interface domain walls and strong interplay among Zeeman, spin-orbit and exchange energies could play a dominant role. Our results would have important implications for the physics of magnetic exchange coupled systems.

1 S. S. Rao et al, J. Appl. Phys. (in print, 2014);
2 Nano Lett., (under review, 2014);
H1.00259 Exchange bias study of epitaxial LSMO/Cr2O3 thin film heterostructures integrated on Si(100)\(^1\). SANDHYARANI PUNUGUPATI, FRANK HUNTE, JAGDISH NARAYAN, North Carolina State University — FM/AFM exchange bias continues to be an interesting phenomenon from both a fundamental physics and an applications point of view. Recent studies of multiferroic materials have also seen a revival of interest in the magnetoelectric (ME) and antiferromagnetic (AFM) material Cr2O3. The study of exchange bias in heterostructures consisting of ferromagnet (FM) and ME thin films provides an additional mechanism of switching the magnetization of the FM by the application of an electric field. La0.75Sr0.3MnO3 (LSMO) is a FM material with TC above room temperature and shows colossal magnetoresistance. We have studied exchange bias in epitaxial thin film heterostructures of LSMO/Cr2O3 grown on C-YSZ/Si(100) by the PLD technique. We present a detailed structural characterization of the films by XRD (2O and Φ) and TEM which confirm that the films were grown epitaxially. The heterostructures exhibited exchange bias as measured by SQUID magnetometry. The effects of LSMO deposition conditions, crystal orientation, temperature, and cooling field on the exchange bias will be discussed.

\(^1\)Part of this research is supported by the National Science Foundation and the Army Research Office

H1.00260 Probing defect ordering in the Curie-Weiss metallic phase of NaxCoO2\(^2\). BEN-LI YOUNG, P.-Y. CHU, J.Y. JUANG, Dept. of Electrophysics, Natl Chiao Tung Univ., G.J. SHU, F.C. CHOU, Center for Condensed Matter Sciences, National Taiwan Univ. — Single crystals of Na2/3CoO2, Na2/3CoO1.98, and Na2/3CoO2, which are metallic Curie-Weiss paramagnets, have been investigated by nuclear magnetic resonance (NMR) techniques, in order to clarify the Na atomic ordering among these samples. By analyzing the \(^{23}\)Na and \(^{59}\)Co NMR spectra, we confirm that the Na vacancies arrange orderly in Na2/3CoO1.98 and Na2/3Co2, so that a superlattice structure is formed due to such Na ordering. In addition, the oxygen vacancies in Na2/3CoO1.98 can be located by the NMR spectra. As for the Na2/3CoO2 single crystal, a long-range Na order is not observed.

\(^2\)This work was supported by NSF 102-2112-M-009-008 and NSF 101-2112-M-009-015-MY2.

H1.00261 Extended X-ray Absorption Fine Structure (EXAFS) Analysis of Vitreous Rare Earth Sodium Phosphates. CHANGYHEON YOO, KANISHKA MARASINGHE, Department of Physics and Astrophysics, University of North Dakota, Grand Forks, ND 58202, CARLO SEGRE, TOMOHIRO SHIBATA, Department of Physics & Center for Synchrotron Radiation Research and Instrumentation, Illinois Institute of Technology, Chicago, IL 60616 — The local structure around rare-earth ions (RE\(^{3+}\) in rare-earth ultraphosphate (REUP) glasses has been studied using RE L\(_{3/2}\) edge (RE = Nd, Er, Dy, and Eu) and K edge (RE = Nd, Pr, Dy, and Eu) extended X-ray absorption fine structure (EXAFS) spectroscopy. (RE\(_2\)O\(_3\))\(_x\)Na\(_{2-x}\)O\(_2\)(P\(_2\)O\(_5\))\(_{1-x-y}\) glasses in the compositional range 0 < x < 0.14 and x + y = 0.3 and 0.4 were studied. RE-oxygen (RE-O) coordination number decreases from ~ 10 to ~ 7.5 with increasing RE-content for Nd, Pr, Eu, and Dy. For Er, RE-O coordination number increases from ~ 8.7 to 10 with increasing RE-content. For the first oxygen shell, the RE-O distance ranges between 2.41-2.43 Å, 2.44-2.46 Å, 2.24-2.26 Å, 2.28-2.32 Å, and 2.32-2.36 Å for Nd, Pr, Er, Dy, and EU glasses, respectively. Second shell around RE ions consists of phosphorus atoms, with RE-P distance about 3.0-3.5 Å and coordination number ranging from 1 to 3. The third shell primarily contains oxygen and is at a distance about 4.0-4.1 Å from RE ions.

H1.00262 Extended X-ray Absorption Fine Structure (EXAFS) Analysis of Zirconium-Doped Lithium Silicate / Borate Glass-Ceramics\(^1\). CHANGYHEON YOO, KANISHKA MARASINGHE, Department of Physics and Astrophysics, University of North Dakota, Grand Forks, ND 58202, CARLO SEGRE, Department of Physics & Center for Synchrotron Radiation Research and Instrumentation, Illinois Institute of Technology, Chicago, RICHARD K. BROWN, Materials Science & Engineering, Missouri University of Science & Technology, Rolla, MO 65409 — Results of Zr K-edge Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy analysis of a series of Zr-doped (~ 3-10 mol\% Zr and atomic ratio Li/Si ~ 0.8) lithium silicate glass ceramics (ZLS) and their parent glasses and a series of Zr-doped (~ 2-6 mol\% Zr and atomic ratio Li/B ~ 0.25-0.18) lithium borate (ZLB) glasses are presented. Immediate coordination environment of all ZLS samples, i.e., the parent glasses and glass ceramics prepared via two different techniques, are remarkably similar. This observation suggests that zirconium ions may remain in the glass phase during nucleation and crystallization process. In contrast, immediate coordination environment of ZLB glasses appear to change markedly with the Zr concentration. These results also suggest that the structural role of Zr ions in ZLS and ZLB glasses may be significantly different. Details of analysis and results will be presented.

\(^1\)Support was provided by NSF (UND) and DoE (argonne Natl. Lab)

H1.00263 Direct Calculation of Modal Contributions to Thermal Conductivity via Green-Kubo Modal Analysis. WEI LV, ASEUNG HENRY, Georgia Inst of Tech — In studying the physics of thermal conductivity, tremendous progress has been made over the last 20 years toward understanding lattice thermal conductivity in crystalline solids. However, most of the existing methods are based on “phonon gas model”, which is the dominant paradigm. It essentially treats vibrations as gas particles, which scatter with each other. This analogy works well for crystals, but it hinges on the assumption that particle velocity being well defined. Because amorphous materials and molecules lack periodicity, it is difficult to define the phonon velocity. We used molecular dynamics simulations and a new formalism for calculating the modal contributions to thermal conductivity to study the amorphous materials, a-Si and a-SiO2. It is the first method that is able to obtain the modal details of phonon transport in amorphous materials including full anharmonicity. This method offers a different perspective on phonon-phonon interactions and allows for direct calculation of phonon contributions to thermal conductivity, which will advance our understanding of the phonon transport mechanism and facilitate heat transfer applications in disordered solids and polymers.

H1.00264 Effect of electron-electron interaction on the conductance plateaus of a quantum wire. YONATAN ABRANYOS, GODFREY GUMBS, Hunter College of the City University of New York, MICHAEL PEPPER, Department of Electronic and Electrical Engineering, University College London, DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate, Kirtland Air Force Base — We present a model which is employed to explain recent experimental results for the conductance in a channel within GaAs/AlGaAs heterostructures. This method offers a different perspective on phonon-phonon interactions and allows for direct calculation of phonon contributions to thermal conductivity, which will advance our understanding of the phonon transport mechanism and facilitate heat transfer applications in disordered solids and polymers.
H1.00265 Study of optical properties of titania nanotube arrays by FDTD Method . OOMMAN VARGHESE, PAWANJIT KAUR. University of Houston — Finite Difference Time Domain (FDTD) method is a powerful tool for understanding the propagation of electromagnetic waves through materials. The idea behind FDTD technique is to discretize both in time and space, the Maxwell equations with central difference approximations. The study of interaction between the nanostructured semiconductor materials and light is of high relevance in recent years primarily due to the applications of these materials in solar energy conversion process such as solar photovoltaics and solar photocatalysis. Titania nanotube arrays fabricated by anodic oxidation have already attracted considerable attention due to their unique properties and applications. This material has already demonstrated high light scattering and antireflection properties. To obtain a better understanding of nanotube-light interaction we used opti-FDTD software to study the influence of nanotube growth conditions on the optical properties. Simulations were carried out by defining the material properties and using the Lorenz drude model in 380-700nm range. In this presentation we will detail our findings on the correlation between the nanotube array fabrication conditions and its optical properties.

H1.00266 The magneto-optical properties of non-uniform graphene nanoribbons . HSJEN-CHING CHUNG, MING-FA LIN, Natl Cheng Kung Univ — When synthesizing few-layer graphene nanoribbons (GNRs), non-uniform GNRs would be made simultaneously. Recently, the non-uniform GNRs, which is a stack of two GNRs with unequal widths, have been fabricated by mechanically exfoliated from bulk graphite. Some theoretical predictions have been reported, such as gap opening and transport properties. Under the influence of magnetic fields, magnetic quantization takes place and drastically changes the electronic properties. By tuning the geometric configuration, four categories of magneto-electronic spectra are exhibited. (1) The spectrum is mostly contributed by quasi-Landau levels (QLLs) of monolayer GNRs. (2) The spectrum displays two groups of QLLs, and the non-uniform GNR behaves like a bilayer one. (3) An intermediate category, the spectrum is composite disordered. (4) The spectrum presents the coexistence of monolayer and bilayer spectra. In this work, the magneto-electronic and optical properties for different geometric configurations are given, such as energy dispersions, density of states, wave functions, and magneto-absorption spectra are presented. Furthermore, the transformation between monolayer and bilayer spectra as well as the coexistence of monolayer and bilayer spectra are discussed in detail.

H1.00267 Resonance Raman Spectroscopy of Single-Wall Carbon Nanotubes Separated via Aqueous Two-Phase Extraction . J. R. SIMPSON, Towson University, J. A. FAGAN, A. R. HIGHT WALKER, National Institute of Standards & Technology (NIST) — We report resonance Raman Spectroscopy measurements of single-wall carbon nanotube (SWCNT) samples dispersed in aqueous solutions via surfactant wrapping and separated using aqueous two-phase extraction (ATPE) into chirality-enriched semiconducting and metallic SWCNT species. ATPE provides a rapid, robust, and remarkably tunable separation technique that allows isolation of high-purity, individual SWCNT chiralities via modification of the surfactant environment. We report RRS measurements of individual SWCNT species of various chiral index including, semiconductors, armchair and zigzag metals. Raman provides a powerful technique to quantify the metallic SWCNTs in ATPE fractions separated for metallicity. We measure Raman spectra over a wide range of excitation wavelengths from (457 to 850) nm using a series of discrete and continuously tunable laser sources coupled to a triple-grating spectrometer. The spectra reveal Raman-active vibrational modes, including the low-frequency radial breathing mode (RBM) and higher-order modes. SWCNT chiral vectors are determined from Raman spectra, specifically the RBM frequencies and corresponding energy excitation profiles, together with input from theoretical models.

H1.00268 Roles of Multi-Walled Structures in Thermal Transport Properties of Nanotubes . TOMOYUKI HATA, HIROKI KAWAI, RYOTA JONO, KOICHI YAMASHITA, Department of Chemical System Engineering, Graduate School of Engineering, the University of Tokyo — The molecular structures of carbon nanotubes are thought to be deeply related with various physical properties. Understanding the relationship is one of the challenges in designing potential materials. In the research, we theoretically investigated the thermal transport properties of carbon nanotubes, focusing the multi-walled structures. We investigated the thermal conductance of the double-walled carbon nanotubes (DWCNTs) by using the nonequilibrium Green’s function method. It is found that the inter-layer interaction causes the suppression of thermal conductance at low temperature. The analysis of the transmission coefficients revealed that this suppression was attributed to the energy shifts of the normal modes from the synchronized vibrations. The mechanism of such energy shifts is examined by the coupled vibration model with the parameters extracted from our simulations, and we grasp the multi-wall effects on the thermal transport properties of the nanotubes.

H1.00269 Coulomb excitations for Gapped Graphene in a perpendicular magnetic field . ANDRII IUROV, University of New Mexico and Hunter College, CUNY, GODFREY GUMBS, Hunter College, CUNY and Donostia International Physics Center (DIPC), DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate — We investigate numerically the Coulomb excitations for gapped graphene and other buckled honeycomb lattices (such as silicone and germanene) in the present of a perpendicular magnetic field. The plasmons are calculated within the random phase approximation. The collective excitations in the presence of a perpendicular magnetic field for such gapped systems are shown to be different from those for both intrinsic gapless graphene as well as a standard two-dimensional electron gas. We present a theoretical description of Bernstein modes that appear due to the coupling between inter-Landau-level excitations and plasmons.

H1.00270 Calculating Observable Quantities for the Hofstadter-Type Spectrum of Graphene . LIUBOV ZHEMCHUZHNA, Hunter College, CUNY, DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate, GODFREY GUMBS, Hunter College, CUNY and Donostia International Physics Center (DIPC), ANDRII IUROV, CHTM, University of New Mexico and Hunter College CUNY, SANJAY KRISHNA, CHTM, University of New Mexico — We numerically obtain density of states and the conductivity of the periodically modulated graphene in the present of a perpendicular magnetic field. These quantities play most important role since they could be measured directly in experiment, so we compare our results with those from the existing experimental papers. The density of states has been calculated and shows a remarkable self-similarity like the energy bands. We estimate that for modulation period of 10 nm, the region where the Hofstadter butterfly is revealed at B ≤ 2 T. Both single layer and bilayer graphene have been considered.

H1.00271 Dielectric function for doped graphene layer with barium titanate. Manuel Martínez Ramos, Eric Garces Garcia, Fernando Magana, Gerardo Jorge Vázquez Fonseca. Univer Autonoma de Mexico — The aim of our study is to calculate the dielectric function for a system formed with a graphene layer doped with barium titanate. Density functional theory, within the local density approximation, plane-waves and pseudopotentials scheme as implemented in Quantum Espresso suite of programs was used. We considered 128 carbon atoms with a barium titanate cluster of 11 molecules as unit cell with periodic conditions. The geometry optimization is achieved. Optimization of structural configuration is performed by relaxation of all atomic positions to minimize their total energies. Band structure, density of states and linear optical response (the imaginary part of dielectric tensor) were calculated.

1We thank Dirección General de Asuntos del Personal Académico of the Universidad Nacional Autónoma de México, partial financial support by Grant IN-106514 and we also thank Mictl Super-Computing center the technical assistance.

H1.00272 Direct exfoliation of graphene in ionic liquids with aromatic groups. Rozana Barí, George Tamas, Fahtima Iríñ, Adelia Aquino, Edward Quitevis, Micah Green. Texas Tech University — The imidazolium cation of the designed and synthesized novel ionic liquids (ILs) having aromatic groups interact non-covalently with graphene. The graphene stabilized by the IL is neither covalently functionalized nor requires the presence of additive stabilizer and such process results in dispersion of pristine graphene. This graphene dispersion is stable against centrifugation and the concentration of the resulting graphene is high as well. It was observed that the ILs are less effective in dispersing graphene if the cation does not have these aromatic groups. The interaction between the cation and the graphene surface plays an important role in the final yield of graphene. The graphene dispersion was characterized by Raman spectroscopy, X-ray Diffraction, and X-ray photoelectron spectroscopy. The experimental observations were compared with the density functional theory (DFT-D3) calculations and the comparison indicated that the experimental observations and the theoretical calculations were in good agreement. These validated theoretical calculations can further be used in future to design and synthesize the ILs in order to optimize the graphene yield without the need for additional experimentation.

1National Science Foundation under CRIF-MU instrumentation grant CHE-0840493, National Science Foundation under CAREER award CMMI-1253085, Air Force Office of Scientific Research Young Investigator Program (AFOSR FA9550-11-1-0027).

H1.00273 Physical Adsorption of noble gases on a monolayer graphene sheet using Grand Canonical Monte Carlo Simulation. Siddi Maiga, Student, Silvina Gatica. Howard University — Adsorption is defined as the attachment of atoms, or molecules of a gas, liquid or dissolved solid onto a surface. Using the method of Grand Canonical Monte Carlo simulation we computed the adsorption of Ar, Kr, and Xe on a monolayer graphene sheet, at various temperatures for each gas. For each temperature, we compute the adsorption isotherm, Energy gas-surface and Energy gas-gas, radial distribution function and structure function. We constructed the phase diagrams for 2D Ar and Kr on graphene.

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H1.00274 Probing weak localization in chemical vapor deposition graphene with wide constriction by scanning gate microscopy. Chia-Shain Chuang, National Taiwan University, Matsunaga, Chiba University, Fan-Hung Liu, Tak-Pong Wóo, National Taiwan University, Nobuyuki Aoki, Chiba University, Li-Hung Lin, National Chiai University. Y. Ochial, Chiba University, Chi-Ti Liang, National Taiwan University, National Taiwan University COLLABORATION, CHIBA UNIVERSITY COLLABORATION, NATIONAL CHIAI UNIVERSITY COLLABORATION — We observe weak localization effect in different wide channels on this disordered CVD graphene device. We also perform the low temperature-scanning gate microscopy experiments under weak localization regime on CVD graphene with wide constriction. The movable local gate can sensitively perturb the total conductance in the wide constriction CVD graphene under magnetic field, suggestive the advantages in the local electric perturbation for the interference behaviors of transport carriers rather than that in fully covered and high consumption magnetic field, a great step for applications in graphene-based spintronics.

1The Aim for the Top University Project by National Taiwan University and Chiba University

H1.00275 Micron scale ballistic Josephson junctions in edge-contacted graphene. Sruiit Goswami, Víctor Calado, Gaurav Nanda. Delft University of Technology, Mathias Diez, Leiden University, Anton Akhmerov, Delft University of Technology, Kenji Watanabe, Takaaki Taniguchi, National Institute of Materials Science, Lieven Vandersypen, Delft University of Technology — Despite recent improvements in the electronic quality of graphene, it has remained challenging to make superconducting contacts to it while preserving its high quality. Here, we integrate monolayer graphene encapsulated in hexagonal Boron Nitride with a type-II superconductor (Molybdenum Rhenium - MoRe) via one-dimensional contacts along the edge of the graphene. We observe gate-tunable supercurrents over distances as long as 1.5 μm. Ballistic, phase coherent transport in these devices causes the switching current to oscillate periodically with the Fermi wave number, thus providing clear evidence of a ballistic Josephson junction. Furthermore, the large critical field of MoRe allows us to resolve several broken symmetry states in the quantum Hall regime, while the MoRe remains superconducting.

H1.00276 Tunable dichroism and optical absorption of graphene by strain engineering. Mauricio Oliva-Levy, Gerardo G. Naumis. Univer Autonoma de Mexico — Recently, the concept of strain engineering has been experimentally extended to the optical domain. However, strain-induced modifications of optical absorption in graphene have been only quantified in the case of a uniaxial strain. In this sense, our work opens a more rich scenario to explore strained-graphene transparency because it is applicable to an arbitrary uniform strain (e.g., uniaxial, biaxial, and so forth). From the corresponding Dirac-like equation [1], we compute the optical conductivity of graphene under a uniform strain [2,3]. This result allowed us to study the transmittance of linearly polarized light between two media separated by a strained graphene sheet [4]. We analytically characterize the degree of dichroism and the transparency of graphene as a function of an arbitrary uniform strain and the incident polarization. Also, we discuss how measurements of dichroism and transparency for two different polarization directions can be used to determine the magnitude and direction of strain. Ours findings result in very useful tools to tune the graphene absorption by mechanical strain [4]. [1] J. Phys. Rev. B 88, 085436 (2013). [2] J. Phys.: Condens. Matter 26, 125302 (2014). [3] J. Phys.: Condens. Matter 26, 279501 (2014). [4] arXiv: 1411.1376.
H1.00277 Enhanced hot-carrier luminescence in multilayer reduced graphene oxide nanospheres 1. QI CHEN, CHUNFENG ZHANG, MIN XIAO, Nanjing Univ. — We report a method to promote photoluminescence emission in graphene materials by enhancing carrier scattering instead of directly modifying band structure in multilayer reduced graphene oxide (rGO) nanospheres. We intentionally curl graphene layers to form nanospheres by reducing graphene oxide with spherical polymer templates to manipulate the carrier scattering. These nanospheres produce hot-carrier luminescence with more than ten-fold improvement of emission efficiency as compared to planar nanosheets. With increasing excitation power, hot-carrier luminescence from nanospheres exhibits abnormal spectral redshift with dynamic feature associated to the strengthened electron-phonon coupling. These experimental results can be well understood by considering the screened Coulomb interactions. With increasing carrier density, the reduced screening effect promotes carrier scattering which enhances hot-carrier emission from such multilayer rGO nanospheres. This carrier-scattering scenario is further confirmed by pump-probe measurements.

1This work is supported by the National Basic Research Program of China (2012CB921801 and 2013CB932903), the National Science Foundation of China (91233103, 61108001, 11227406 and 11021403), and the Program of International S&T Cooperation (2011DFA01400).

H1.00278 Momentum resolved optical pump-probe spectroscopy in monolayer graphene: An analytical model and measurements, MAXIM TRUSHIN, ALEXANDER GRUPP, GIANCARLO SOAVI, ARNE BUDWEG, University of Konstanz, Germany, DOMENICO DE FAZIO, ANTONIO LOMBARDO, UGO SASSI, ANDREA C. FERRARI, Cambridge Graphene Centre, University of Cambridge, UK, WOLFGANG BELZIG, ALFRED LEITENSTÖRFER, DANIELE BRIDA, University of Konstanz, Germany — Further development in graphene based photonics and optoelectronics requires fundamental information on the evolution of the strongly non-equilibrium charge carrier distribution created by the light-carrier interaction. Here, we report polarization and fluence dependent ultrafast optical pump-probe spectroscopy of high quality CVD-grown monolayer graphene. An analytical model has been developed and employed to describe the experiments. Graphene offers a unique opportunity to probe the photocarrier occupation, not only at different energies using a two-color setup, but also in different directions in momentum space applying linearly polarized beams. The latter approach is possible due to the pseudospin-momentum coupling which results in an optical pseudospin-selection rule. Our method allows us to quantify and control the relative contributions of both the strongly non-equilibrium anisotropic occupation and the hot Fermi-Dirac photocarrier distribution to the total differential transmission measured. We provide a conclusive and quantitative evidence for an anisotropic photocarrier occupation with a life-time of about 100 fs and claim that its relaxation towards the isotropic distribution occurs mostly due to optical phonon emission.

H1.00279 Probing the Doping level in Graphene Using Surface Plasmon Resonance, KAMRUL ALAM, YANG LI, JIMING BAO, University of Houston — The present work describes an investigation of the electrochemically doped large area CVD grown graphene by using surface plasmon resonance (SPR). As graphene was doped electrochemically its conductance changes based on electron and hole concentration, that have an effect on its permitivity which has influence on the refractive index. We have used SPR angle interrogation scheme, generally known as Kretschmann configuration, to detect this change in refractive index of graphene as a shift in the angle of the SPR curve. To verify our results we have use Raman spectroscopy of the graphene-Au hybrid sample that was used for SPR measurement. Shift in the G peak signifies that graphene is doped electrochemically which is also in agreement with the shift in the angle of the SPR curve.

H1.00280 Strain-Engineering of Graphene Based Topological Quantum Devices 1, GINETOM S. DINIZ, MARCOS R. GUASSI, FANYAO QU, Institute of Physics, University of Brasilia, Campus Darcy Ribeiro, DF, 70910-900, Brazil — We have investigated the spin-carrier transport in quantum devices based on graphene nanoribbons (GNR). Our calculation is based on the surface Green’s function technique, considering the presence of an uniform uniaxial strain, spin-orbit interactions (SOIs), exchange field and a smooth staggered potential. We propose the use of uniaxial strain as an efficient mechanism to tune the conductance profiles of GNR with different edge terminations. Our results show that distinct behaviors can be achieved: for armchair GNR there is a complete suppression of the conductance close to the Fermi level with the formation of a band gap that depends on the direction and strength of the strain deformation, while for zigzag GNR there is only a small conductance suppression. We also discuss the effects of SOIs and the appearance of spin-resolved conductance oscillations, and the local density of states of these GNR devices in the quantum anomalous Hall regime. Furthermore, we demonstrate that the local density of states show that depending on the smoothness of the staggered potential, the edge states of AGNR can either emerge or be suppressed. These emerging states can be probed by scanning tunneling microscope. Our findings can be potentially used in novel GNR based topological quantum devices.

H1.00281 Physisorption of Fullerenes in Graphene layers and carbon Nanoribbons 1, MONICA PACHECO, PEDRO ORELLANA, Universidad Tecnica Federico Santa Maria, JULIAN CORREA, Universidad de Medellin — The study of nanostructures based on carbon allotropes has captured the interest of the scientific community in the last two decades, due to its great versatility. In such structures a simple change of geometry leads to important changes in their physicochemical properties. In this paper we show a study of opto-electronic properties of fullerenes physisorbed on graphene nanoribbons. Our calculations are carried out within the framework of density functional theory (DFT) using the SIESTA package. Our results show that effectively the fullerenes bind both to the layer of graphene as well as to the nanoribbons, with binding energies of about 0.5eV. We find that when the complex is formed, the physical properties of fullerenes, graphene and nanoribbons are preserved and when graphene is functionalized with various fullerenes the electronic spectrum is composed of bands of energy which increases the intensity of the optical absorption spectrum of the complex.

Conicyt ACT 1204, USM 11.14.68

H1.00282 Thermoelectric properties of a trilayer graphene nanoribbon, PEDRO ORELLANA, NATALIA CORTES, LUIS ROSALES, MONICA PACHECO, Universidad Tecnica Federico Santa Maria, LEONOR CHICO, CSIC. — In this work the electronic and thermoelectric properties of a three-layer graphene with AAA stacking type are studied. By using a tight-binding model analytical expressions for the transmission and density of states are obtained. Thermoelectric properties are analyzed by numerical integration and results for thermopower and figure of merit, electronic conductance and thermal conductance are obtained. The results show that the interference effects present in this system, like Fano effect, directly affect the behavior of these thermoelectric properties 1 and as well as the Wiedemann-Franz law 2. There is an enhancement of the thermopower of the system and a violation of the Wiedemann-Franz law in the region of energies close the Fano antiresonances and this has as a consequence an enhancement of the figure of merit of the system.


Conicyt ACT 1204, USM 11.14.68
H1.00283 Polarized spin and valley transport across ferromagnetic silicene junctions. V. VAR-GIAMIDIS, P. VASILPOULOS, Concordia University, V. FESSATIDIS, Fordham University — We study ballistic transport of Dirac fermions through silicene barriers, of width $d$, with an exchange field $M$ and metallic gates above them that provide tunable potentials of height $U$. Away from the Dirac point (DP) the spin- and valley-resolved conductances, as functions of $U$, exhibit resonances and close to it a pronounced dip that becomes a transport gap when an appropriate electric field $E_z$ is applied. The charge conductance $g_c$ of such a junction changes from oscillatory to a monotonically decreasing function of $d$ beyond a critical $E_z$. This tuning of $g_c$ can be used to realize electric-field-controlled switching. Further, the field $M$ splits each resonance of $g_s$ into two spurious resonances. The spin polarization $p_s$ of the current near the DP increases with $E_z$ or $M$ and becomes nearly perfect above certain of their values. We also show that $p_s$ can be inverted either by varying $U$ or by reversing the direction of $M$. For two barriers there is no splitting in $g_c$ when the fields $M$ are in opposite directions. Most of these phenomena have no analogs in graphene.

H1.00284 Graphene optical-to-thermal converter1, ALEJANDRO MANJAVacas, Rice University, SUKOSIN THONGRAT-TANASIRI, Kasetart University, JEAN-JACQUES GREFFET, Institut d’Optique, Univ. Paris Sud, JAVIER GARCÍA DE ABAJO, ICF-TO-The Institute of Photonic Sciences — Infrared plasmons in doped graphene nanostructures produce large optical absorption that can be used for narrow-band thermal light emission at tunable frequencies that strongly depend on the doping charge. By virtue of Kirchhoff’s law, thermal light emission is proportional to the absorption, thus resulting in narrow emission lines associated with the electrically controlled plasmons of heated graphene. Here [1] we show that realistic designs of graphene plasmonic structures can release over 90% of the emission through individual infrared lines with 1% bandwidth. We examine anisotropic graphene structures in which efficient heating can be produced upon optical pumping tuned to a plasmonic absorption resonance situated in the blue region relative to the thermal emission. An incoherent thermal light converter is thus achieved. Our results open a new approach for designing tunable nanoscale infrared light sources.


1A.M. acknowledges financial support from the Welch foundation through the J. Evans Attwell-Welch Postdoctoral Fellowship Program of the Smalley Institute of Rice University (Grant L-C-004).

H1.00285 Evanescent field coupled graphene plasmon waveguide, WON JONG YOO, JAEHWAN KWEON, EUYHEON HWANG, Sungkyunkwan Univ — Surface plasmon polaritons (SPPs) is propagating electron-light coupled oscillation. There had been various methods to excite graphene plasmon such as fabricating graphene nano-ribbon and NSOM micro-tip assisted methods. These methods are used for reducing wavelengths of incident light and finally matching wavelength to propagating wave. However, when graphene sheet is inserted between two different media, evanescent field coupling and excited graphene plasmon properties are still unclear. There are several advantages in using this coupling method. We can control the direction of propagating plasmon and effectively find plasmon modes. Interestingly, propagating wavelength is scaled to 50 – 100 times depending on its modes and light is confined into extremely small mode size. Also its optical properties can be easily controlled by biasing voltage on its surface. To analyze graphene plasmon, we use random phase analysis (RPA) so as to figure out optical permittivity of graphene, and then we use the FDTD (finite difference time domain) and FDFD (finite difference frequency domain) computational methods so as to theoretically figure out the propagation of graphene plasmon waveguide. Also we will report various plasmon properties of graphene plasmon propagation such

H1.00286 All-Metallic Vertical Transistors Based on Stacked Dirac Materials. YANGYANG WANG1, ZEYUAN NI, School of Physics, Peking University, QIHANG LIU, University of Colorado, RUGE QUHE, School of Physics, Peking University, JIAXIN ZHENG, School of Advanced Materials, Peking University, CHENWEI WANG, Peking University, Shenzhen Graduate School, MENG YE, DAPENG YU, JUNJI SHI, JINBO YANG, School of Physics, Peking University, JU LI, Massachusetts Institute of Technology, JING LU, School of Physics, Peking University, COLLABORATIVE INNOVATION CENTER OF QUANTUM MATTER, BEIJING COLLABORATION — All metallic transistor can be fabricated from pristine semimetallic Dirac materials (such as graphene, silicene, and germanene), but the on/off current ratio is very low. In a vertical heterostructure composed by two Dirac materials, the Dirac cones of the two materials survive the weak interlayer van der Waals interaction based on density functional theory method, and electron transport from the Dirac cone of one material to the one of the other material is therefore forbidden without assistance of phonon because of momentum mismatch. First-principles quantum transport simulations of the all-metallic vertical Dirac material heterostructure devices confirm the existence of a transport gap of over 0.4 eV, accompanied by a switching ratio of over 10. Such a striking behavior is robust against the relative rotation between the two Dirac materials and can be extended to twisted bilayer graphene. Therefore, all-metallic junction can be a semiconductor and novel avenue is opened up for Dirac material vertical structures in high-performance FET by the addition of extra electrode for the clear identification of the quantum Hall state formation at given temperature and magnetic field. We suggest a simple model to explain the difference and similarity between two-terminal and multi-terminal configurations, including the discussion about the QHE devices without opening their band gaps.

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H1.00287 Identification of the existence of quantum Hall edge-state in graphene field-effect transistor at high temperatures, JOONG GYU KIM, HAEYONG KANG, JEONGMIN PARK, YOOJOO YUN, THUY KIEU TRUONG, JONG-GYUN KIM, NAHEE PARK, YOURACK LEE, CINAP, IBS, Department of Energy Science, Sungkyunkwan University, HOYEOL YUN, SANG WOOK LEE, School of Physics, Konkuk University, YOUNG HEE LEE, DONGSEOK SUH, CINAP, IBS, Department of Energy Science, Sungkyunkwan University — Quantum Hall effect (QHE) is one of the unique properties of two-dimensional electronic systems providing the universal standard of electrical resistance. Due to edge-state transport features in quantum Hall regime, the two-terminal graphene field-effect transistor (FET) is frequently examined for the study of the integer as well as the fractional QHEs of graphene. In this work, we present a simple method to identify the existence of quantum Hall state in the graphene FET especially at high temperatures. Using the monolayer graphene FET sample with fully broken degeneracy, we modified the equipotential line inside graphene FET by the addition of extra electrode for the clear identification of the quantum Hall state formation at given temperature and magnetic field. We suggest a simple model to explain the difference and similarity between two-terminal and multi-terminal configurations, including the discussion about the QHE devices connected in series.

H1.00288 SUPERLATTICES, NANOSTRUCTURES AND OTHER ARTIFICIALLY STRUCTURED MATERIALS

H1.00289 Three-Dimensional Lattice Matching for Epitaxially Embedded Nanoparticles, BRELON MAY, PETER ANDERSON, ROBERTO MYERS, Ohio State Univ - Columbus — Since Mathews-Blakeslee developed a theory of atomic lattice matched thin films, epitaxy has been modeled using only 2D lattice matching conditions between arbitrary films. For a given degree of in-plane lattice mismatch, the theory predicts a critical film thickness above which interface defects form to relax the film strain. Here we present a three-dimensional model to predict the conditions for epitaxially encased nanoparticles, which includes not only the in-plane lattice matching, but also the out-of-plane mismatch. We find that the consideration of the out-of-plane strain, due to the Poisson effect and particle shape change, can greatly alter the critical volume compared to what the Mathews-Blakeslee model predicts. Our results provide new insight to nanoepitaxy of low dimensional structures especially quantum dots and nanoparticles.
H1.00290 A DFT analysis of structure and energetics of Mg/Nb multilayers , ANIL KUMAR, IRENE BEYERLEIN, JIAN WANG, Los Alamos National Laboratory — Magnesium and its alloys, the lightest structural materials, have attracted the attention of the automotive industry for reducing the vehicle’s weight to increase its fuel efficiency. The magnesium phase characterized within Mg/Nb multilayers can adopt either body-centered cubic (bcc-Mg) or hexagonal close packed (hcp-Mg) structure depending on the Mg layer thickness. The bcc-Mg has a similar weight density as the hcp-Mg, but low Young’s modulus, high shear modulus and conventional slip systems of bcc structure. In this work, using first-principles density functional theory, we studied both structural and mechanical properties of bcc-Mg and hcp-Mg in Mg/Nb multilayers as a function of Mg layer thickness and developed a simple theoretical model to predict the structural stability of the bcc-Mg/Nb and hcp-Mg/Nb multilayers. We show that the bcc-Mg/Nb multilayer is energetically favorable when the bcc-Mg layer is less than 4.2 nm. We also studied the mechanism such as inter-mixing of Mg and Nb atoms, creation of vacancies and doping of solute atoms at Mg/Nb interface to minimize the Mg/Nb interface energy. We found that solute atoms such as Zr, Cd and Zn, whose metallic radius are smaller than Mg, can easily segregate at Mg/Nb interface and lower the interface energy.

H1.00291 Layer by Layer Fabrication of 3D Photonic Crystals by Substrate Conformal Imprint Lithography (SCIL) from Titania Nanoparticle Solutions , IRENE HOWELL, University of Massachusetts-Amherst, MARC VERSCHUUREN, Philips Research, ROHIT KOTHARI, JAMES WATKINS, University of Massachusetts-Amherst — We demonstrate a method for fabricating well-aligned, large-area, log-pile 3D photonic crystals. Using 15 nm titania (anatase) nanoparticles dispersed in a mixture of propanediol and methanol, we show that these nanoparticles can be patterned to produce robust, reproducible, 1 µm pitch, 500 nm line-width gratings. By planarizing the grating with an organic UV-curable resin (Norland Optical Adhesive 60), subsequent titania layers can be patterned in the proper orientation, ending with a calcination step to remove the organic resin and create a 3D photonic crystal. This method allows for a photonic stop band in the infrared region, but the limitations in feature size and alignment capability prevent fabrications of a photonic crystal with a band gap at shorter wavelengths. By applying Substrate Conformal Imprint Lithography (SCIL) technology to this method, we can produce 3D photonic crystals with features suitable for a band gap in the visible region. SCIL utilizes a higher modulus PDMS (X-PDMS) to easily achieve sub-500 nm features. Additionally, the alignment method, involving box-in-box and Moire patterns, enables reproducible, precise alignment of sequential layers within 5 nm.

H1.00292 Phonon Scattering at Nanoparticles in LuAs:InGaAs Nanocomposites , FENG HE1, RODOLFO SALAS2, SETH ROBERT BANK3, YAGUO WANG4, University of Texas System — Nanocomposites of III-V semiconductors embedded with semi-metallic rare earth nanoparticles grown with molecular beam epitaxy (MBE) have been widely used in optoelectronics and thermoelectrics. Manipulating the growth parameters, e.g. growth rate, particle concentration and surfactant, will allow precise control of electronic and thermal transport properties for specific applications. Fundamental understanding of phonon scattering at nanoparticles in these nanocomposites under various growth conditions is not only scientifically important, but also will facilitate the material growth and device design. We have investigated the ultrafast dynamics of coherent acoustic phonons (CAP) in LuAs:InGaAs nanocomposites with standard two-color femtosecond pump-probe technique. Phonon frequency and lifetime have been measured in samples grown under different conditions. Our results show that CAP lifetime increases with increasing LuAs deposition, as well as pump fluences. We have also studied the influences of growth rate and surfactant on phonon lifetime.

H1.00293 Study of plasmon-polariton in 1-D photonic crystals of dielectric and magneto optical layers under the effects of external magnetic field in the polar configuration , JAIME ANDRES GIRON SEDAS, EDWIN MONCADA VILLA, Solid State Group, NELSON PORRAS MONTENEGRO, Solid State Group, Universidad del valle, Cali, Colombia — Photonic crystals (PCs) are artificial microstructures with a periodic spatial distribution of the dielectric constant, which enables us to manipulate and control the photons. In particular, the existence of photonic bands in the energy spectrum as well as photonic band gaps, forbidden frequency regions for light propagation have permitted quite a number of analogies with physical properties of semiconductor, this provides a perfect base for the construction of great varieties of photonic devices. In this case the superlattice is composed of alternating slabs of two materials, one is a dielectric, and the other is magneto-optical material. The interaction between plasma excitations and the electromagnetic radiation in the frequency region around null electric and magnetic responses in these arrangements, it gives a requisite for the existence of longitudinal waves, results in the excitation of modes that couple plasmons and optical fields. Those are known as Plasmon- Polaritons. We analyze the magneto-optic response of this PCs and the Plasmon-Polaritons behavior when an external magnetic field is placed in the growth direction of the structure using the scattering matrix approach for anisotropic layer stacks.

H1.00294 Electronic structure of palladium and gold-palladium nano clusters, both free and supported on MgO(100) , CARLOS QUINTANAR, REYNA CABALLERO, RAUL ESPEJEL, ELIZABETH CHAVIRA, Universidad Nacional Autónoma de México, MAGALI UGALDE, FRANCISCO ESPINOZA, Centro de Investigación en Materiales Avanzados, SAMUEL TRICKEY, University of Florida — Ideal (or model) metal nano-clusters, both free and supported on MgO(100), have been the subject of numerous experimental studies. This work probes the characteristics of non-system ideals. For that, palladium nano clusters first were synthesized using a sol-gel-microwave method. A mono-phase of metallic Pd was obtained as corroborated by thermo gravimetric analysis, x-ray powder diffraction, scanning electron microscopy, and high resolution transmission electron microscopy studies (HRTEM). Among the HRTEM micro-graphs we found an almost planar nano-surface (facet) with only forty six atoms (Pd(46)). From that micro-graph we obtained the coordinates of the atoms in the Pd(46) nano-surface. With those coordinates, we did a DFT study of the Pd(46) nano-surface electronic structure. From the Pd(46) nano-surface, nine and eighteen Pd atoms were chosen to build A8 and A98 nano-surface clusters respectively. Starting from a near-planar Au8 cluster, the Au8 geometry was optimized over the fixed Pd8 and Pd18 nano-surfaces, charge transfer was determined with charge density difference analysis (CDDA) and Fukui analysis was done and. The Au8Pd8 cluster was positioned on an MgO(100) surface with an vertex and charge transfer was determined with CDDA.

H1.00295 Formation of finite layer MoS2 using ultrasonic agitation , TIM KIDD, RUI HE, ERIC CLAUSEN, University of Northern Iowa — We have developed a process in which finite layer MoS2 can be produced using ultrasonic agitation. The material shows optical properties consistent with an average layer thickness of less than five layers. The process uses ultrasonic agitation of MoS2 in an suspension using isopropanol. Interestingly, side products involving carbon nanoparticles are also produced. These side products are quite small, and become the dominant material when using a centrifuge to separate out the smallest particles. These carbon nanoparticle side products appear to include nanometer scale particles as well as materials with sizes consistent with fullerenes and graphene with nanoscale lateral dimensions. This process appears to represent a novel method for producing finite layer MoS2 and some forms of carbon nanoparticles using a relatively simple method.
H1.00296 Gyroid photonic crystal with Weyl points, SIYING PENG, HONGJIE CHEN, HARRY ATWATER, Thomas J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, California 91125, United States — Weyl points are degenerate energy states resulting from band crossing of linear dispersions in three dimensional momentum space. Unlike Dirac points in the two dimensional systems, Weyl points have been shown to be stable and the associated surface states are predicted to be topological surface states. These topologically protected surface states may potentially lead to various interesting phenomena such as backscattering immune transport. We fabricate and characterize photonic crystals in the infrared regime with Weyl points present in their band structures. Full wave FDTD simulations were utilized to optimize the unit cell size and material index of the gyroid structures. Three dimensional two-photon lithography method was used to fabricate optimized geometry from simulations in to polymers. We used sputtering process to coat the polymer structure with high index materials such as amorphous silicon at low temperature conformally. Optical properties of these gyroid geometries with high effective refractive index are characterized with angled resolved FTIR in order to map out the bulk and surface band structures in the momentum space. Initial FTIR measurement at normal incidence has shown strong absorption related to both structured polymer and a-Si structures.

H1.00297 Bimodal Distribution of Cadmium Selenide Quantum Dots Prepared by UV-Photolithography 1, AJITH DESILVA, University of West Georgia, M. KAVEH, University of Cincinnati, RAGHUVEER R. GADIPalli, SARAH G. MARTINO, University of West Georgia, H.P. WAGNER, University of Cincinnati — We employed wet chemical and UV photolithography methods to synthesize CdSe quantum dots (QDs). The dynamics of excitons in the QDs were studied using temperature-dependent photoluminescence (PL) ranging from 17 to 300 K. The inhomogeneous shape and size of the QDs led to an asymmetric PL spectrum at 17 K, which was approximately decomposed into two Gaussian emission bands, with peak energies at 2.182 and 2.299 eV and widths of 40 and 30 meV, respectively. These bands are attributed to the existence of two CdSe QDs ensembles with differently sized QDs. With increasing temperature the PL intensities of both bands weakly change; the PL yield of the larger QDs being higher at low temperatures while the smaller QDs show the stronger emission at higher temperatures. The stronger PL quenching of the larger QDs with increasing temperature is tentatively assigned to higher density of defects at the grain boundary compared with small QDs. TEM images of the sample revealed a distribution of nano-particles with average sizes around 10 and 15 nm supporting the existence of a bimodal QD distribution.

1This work is supported by UWise and SRAP programs at UWG.

H1.00298 SANS and SAXS Investigations of Selective Distribution of Single-Walled Carbon Nanotubes in a Polymeric System, JAE-MIN HA, HYUNG-SIK JANG, SUNG-HWAN LIM, SUNG-MIN CHOI, KAIST — Single-walled carbon nanotubes (SWNTs) have remarkable electrical, thermal, and mechanical properties which provide new possibilities for various applications, such as transparent conductive films, bio-sensor, composite and energy storage. For those applications, the fabrication of the self-assembly or guided assembly of SWNTs into highly ordered superstructures with well-defined morphology, density, and structure is demanded to enhance their physical properties and is the key to the realization of various potential applications of SWNTs. Block copolymers exhibit rich phase behaviors and have been extensively used as excellent templates for various nanostructured materials. Many efforts have been made to incorporate various nanoparticles into self-assembling block copolymers as an efficient way to organize nanoparticles in functionalized nanocomposites. The fabrication of block copolymer systems using small-angle neutron and x-ray scattering.

H1.00299 AlN nanowire growth using InN crystalline powders by physical vapor deposition, NAO TO KENOMOCHI, HIRAKU OTA, MIKKA NISHITANI-GAMO, NOBORU WADA, Toyo University, Japan — AlN nanowires were grown by heating an evacuated quartz ampule which contained InN crystalline powders and an Al substrate at 1300−1500 K. The nanowire samples were examined by SEM, TEM, EDX, XRD and Raman spectroscopy. Both EDX and Raman spectroscopy yielded that the nanowires should be crystalline InN. Almost all the nanowires exhibited a spherical head at the end, implying that the growth mechanism might be the vapor-liquid-solid (VLS) growth. The diameter typically varied from 30 nm to 500 nm, while the length could be several micron meters long. The nanowire growth was quite significant on the Al substrate close to the InN powder source. When the samples were kept at high temperatures for a longer time, both the spherical heads and nanowires were found to be thicker. The detailed mechanism for the growth and the growth conditions will be discussed. 

H1.00300 Metallic Nanoparticles Confined in Silica Matrices, SHIN HYUN KANG, MIN-JAE LEE, JEEUN LEE, JUN-KI LEE, SUNG-MIN CHOI, KAIST — Metallic nanoparticles are widely studied due to their noble properties based on the high surface area. In order to increase the practical applications, the nanoparticles should be protected from thermal damage which can cause agglomeration. A facile way of protecting metallic nanoparticles with a silica matrix is presented. Metal nanoparticles are synthesized and functionalized in aqueous solution, and are collectively confined in a silica matrix which is thermally stable enough to protect the embedded nanoparticles. The structure and morphology are investigated by small angle x-ray scattering measurements, transmission electron microscopy and scanning electron microscopy measurements. Physical and chemical properties of the heterogeneous system would be presented, too.

H1.00301 Synthesis, Structural and Electrical Properties of Mg$_x$Pb$_{(1-x)}$Ti$_3$O$_7$ produced by mecanosynthesis1, JALDAIR NOBREGA, ARIANO DE GIOVANNI RODRIGUES, MICHEL VENET ZAMBRANO, PAULO SERGIO SILVA JUNIOR, JULIO CESAR CAMILO ALBORNOZ DIAZ, PAULO SERGIO PIZANI, Univ Fed de Sao Carlos, ESPECTROSCOPIA RAMAN EM MATERIAIS NANOESTRUTURADOS COLABORATION, METALURGIA FISICA E DE ESPECTROSCOPIA MECANICA COLABORATION — Over last decades scientific studies about ceramic materials based in metallic oxides have pointed to an increasing wide range of applications. Among them, PbTiO$_3$ has been significantly applied to electronic components and optoelectronics devices. Another example can be found in the microwave dielectric MgTiO$_3$, which has been used on the production of devices. The development of a compound that combines the physical properties of these well-known materials aims the achievement of a new type of ceramics presenting distinctive applications. We report the production of Mg$_x$Pb$_{(1-x)}$Ti$_3$O$_7$ by means of mecanosynthesis techniques. Electric measurements were carried out in order to verify the dielectric behavior of the system. By analyzing the signatures of characteristic phases of Mg$_x$Pb$_{(1-x)}$Ti$_3$O$_7$ in X-Ray diffractograms, we could confirm that the stoichiometry of our solid solutions could be controlled by properly adjusting the amounts of the oxides used as precursors. The Raman spectroscopy allowed us to study the behavior of the soft mode, typical of ferroelectric, which is present in all composition. By determining the dependence of its energy with temperature variation, we could estimate the temperatures of phase transition for each composition.

1Supported by CAPES-Brazil and CNPQ-Brazil.

H1.00302 Synthesis and Characterization of Magnetic Nanoparticle Assemblies, MIN-JAE LEE, HO-HYUN KIM, SHIN-HYUN KANG, SUNG-MIN CHOI1, KAIST — The superstructure of magnetic nanoparticles, which may provide new properties, are of great interests for various potential applications as well as its own scientific merits. Despite recent advances in the fabrication and characterization of magnetic nanoparticle structures, it remains challenges to exploit for controllable organization of magnetic nanoparticles at the nanoscale. Here, we will report the synthesis and functionalization of monodisperse magnetic nanoparticles and their self-assembled structures.
H1.00303 Microwave metal-dielectric metamaterials with magnetic inclusions, BRITTANY BATES, BRANDON ALLISON, Norfolk State Univ, NICOLE GREENE, Cornell Univ, NATALIA NOGINOVA, Norfolk State Univ — Use of natural magnetic materials as a constituent part of metamaterials is attractive as they provide a possibility to tune material parameters at microwave range and THz frequency with external magnetic fields. Metal-dielectric multilayers and wire arrays structures were fabricated using both ferromagnetic and nonmagnetic metals. These structures were studied in free space microwave propagation experiment. We show that a cube of such a metamaterial operates as a focusing lens and a polarizer with a possibility of tuning with external magnetic field.

H1.00304 Magnetic, structural and adsorption properties for methylene blue of PAA/MnFe2O4 nanocomposite, WEI WANG, ZUI DING, School of Science, Beijing University of Chemical Technology, Beijing 100029, China, J. PING LIU, Department of Physics, University of Texas at Arlington, Arlington, TX 76019, USA — PAA/MnFe2O4 nanocomposite was fabricated by a hydrothermal procedure and ultrasonic wave-assisted method. The morphology of the synthesized MnFe2O4 ferrite nanocrystals reached 74.6nm/g. FTIR spectrum confirms the coating of PAA on the surface of MnFe2O4 ferrite nanoparticles. Here, the PAA coating does not lead to a deterioration in magnetic performance. Moreover, the PAA/MnFe2O4 nanocomposites were applied to remove Methylene Blue (MB) from wastewater. Compared with the nanoparticles without coating, the PAA coating significantly enhanced the adsorption capacity of MB onto MnFe2O4 magnetic nanoparticles, where a rapid and efficient removal of MB was observed. The research suggests that as-synthesized PAA/ MnFe2O4 nanocomposites have promising and potential applications in water treatment for removal of dyes.

H1.00305 Synthesis and Characterization of Au@Pd@Au core-shell nanostructures, ALEJANDRA LONDONO-CALDERON, J. JESUS VELAZQUEZ-SALAZAR, MIGUEL JOSE YACAMAN, Univ of Texas, San Antonio — In this work we present a systematic study on the synthesis of (Au@Pd@Au) nanostructures by a seed mediated method in aqueous solution. In the first step, single crystal Au octahedra nanoparticles are used as seeds to grow metallic Au particles to core-shell nanocubes of 40 nm in size. The growth mechanism of successive Au layers on the Au@Pd nanocubes and the crystallinity on the Au/Pd and Pd/Au interfaces are studied by the use of Scanning Electron Microscopy (SEM), High Resolution Transmission Electron Microscopy (HREM) and Scanning Transmission Electron Microscopy (STEM). A transformation from cubes to truncated polyhedrons is observed by Electron Tomography in the reconstruction of the surface.

H1.00306 Real-space and nanoscopic observation of phase transition behaviors of VO2 thin films using Kelvin probe force microscopy, DONG-WOOK KIM, AHRUM SOHN, Department of Physics, Ewha Womans University, TERUO KANKI, KOUTARO SAKAI, HIDEKAZU TANAKA, The Institute of Scientific and Industrial Research, Osaka University — VO2 undergoes a metal-insulator transition (MIT) and a tetragonal-monoclinic structural phase transition (SPT) near room temperature. We carry out transport and KPFM (Kelvin probe force microscopy) measurements on epitaxial VO2/TiO2 thin films simultaneously in the temperature range of 285-330 K. The samples have large grains due to very small lattice mismatch, which allows us to study in native nature of the phase transition in quasi-2D VO2 system. The sample’s work function decreases from 5.1 eV to 4.9 eV, while spanning the transition temperature. The work function maps can clearly reveal coexistence of the two distinct states at the intermediate temperature range, well explained by the 2D percolation theory.

H1.00307 Plasmon Excitations for a Coulomb-coupled Graphene Layer and a Thick Conductor, GODFREY GUMBS, Hunter College, CUNY and Donostia International Physics Center (DIPC), ANDRUIU IROV, University of New Mexico and Hunter college, CUNY, NORMAN HORING, Stevens Institute of Technology — Self-consistent field theory is used to obtain the plasmon dispersion relation of monolayer graphene which is Coulomb coupled to a thick conductor. We calculate numerically the undamped plasmon excitation spectrum for arbitrary wave number. For gapped graphene, both the low-frequency (acoustic) and high frequency (surface) plasmons may lie within the opening within the particle-hole region. Additionally, we obtain plasmon excitations in a region of the frequency-wave vector space which does not exist for free standing gapped graphene.

H1.00308 One and two dimensional shock waves of light, RICARDO FERRO, HASANUZZAMAN RAHMAN, GERMAN KOLMAKOV, MANAS KULKARNI, New York City College of Technology, City University of New York — By using numerical simulations for the dynamics of an exciton polariton condensate in an optical microcavity, we demonstrate that strongly nonlinear, spatially localized waves can be formed during the propagation of the condensate perturbations. We show that at the terminal stage of their evolution, the condensate density waves acquire the universal shape of a shock wave, which is similar to that known from a classical rarefied interacting gas dynamics. Since the exciton-polaritons in the condensate include photons as their constituents, we studied the shock front structure and then, investigate the propagation of light shock waves in a two-dimensional geometry in an unrestricted microcavity as well as in quasi-one-dimensional polariton channels. We also discuss the effects of the scattering of the polariton shock waves on the structural defects in the cavity, and the effects of the phase coherence during mutual scattering of two and more shock waves.

H1.00309 A quantum interferometer for studies of the exciton and polariton drag effects, ANDY HE, ROMAN YA. KEZERASHVILI, GERMAN V. KOLMAKOV New York City College of Technology CUNY — Recently, the drag effects of excitons and cavity polariton condensates by an electric current running in a quantum well embedded in a cavity were theoretically predicted. In our report, we propose a setup suitable for the studies of the exciton and polariton condensate drag effects based on self-interference of a split condensate in the presence of the driving current. By numerically simulating an output signal of a ring-shaped interferometer, we determine the range of parameters, at which the exciton and polariton drag effects in a microcavity can be observed and utilized in optical nanodevices.

H1.00310 Dynamics of self-trapped excitons in layered Pb1-xCd1xI2 semiconductors, YURIY GNATENKO, ANATOLII BUKIVSKIY, YURIY PIRYATINSKI, Institute of Physics of National Academy of Science of Ukraine — The dynamics of self-trapped excitons, localized on stretched Pb-I chemical bonds which are formed on PbI2 nanocluster surface was investigated. It should be noted that these nanoclusters are naturally formed in Pb1-xCd1xI2 (X = 0.5 and X = 0.7) layered semiconductor solid solutions. They have different sizes (from several nm to several tens of nm). The measurements of photoluminescence (PL) spectra and kinetics of PL intensity decay for those materials were performed at T=300 K. The kinetic dependencies were obtained for the maximum of PL band (600 nm) and for its short-wave shoulder (550 nm). It was shown that PL decay kinetics is approximated by Kohlrausch-Williams-Watts (KWW) function, i.e. by stretched exponential function \( I(t) = I_0 \exp(-(t/\tau_\beta)^\beta) \). Obtained values of \( \tau_\beta \) and \( \beta \) for X = 0.5 are equal about 800 ns and 0.76 at 600 nm. At 550 nm these values are 700 ns and 0.74, respectively. Similarly for X = 0.7 these values correspond about 800 ns and 0.80 at 600 nm. At 550 nm they are 800 ns and 0.92. Application of the Inverse Laplace Transformation (ILT) to our experimental data gave us an opportunity to estimate the probability density function of self-trapped exciton state lifetimes for Pb1-xCd1xI2 (X = 0.3, 0.5 and 0.7). The position of the maximum of \( F(\tau) \) gives us the average decay time \( \tau_{ave} \) which is about 1250 ns which significantly differs from \( \tau_\beta \) which is about 800 ns (for X = 550 nm). This complex dynamics of excitons is associated with strong heterogeneity of the investigated system.
H1.00311 Half-metallicity in a BiFeO$_3$/La$_2$Sr$_3$MnO$_6$ heterostructure: A first-principles study

JILILI JIWUER, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia, ULRICH ECKERN, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany, UDO SCHWINGENSCHLOGL, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia — We present first principles results for the electronic, magnetic, and optical properties of the BiFeO$_3$/La$_2$Sr$_3$MnO$_6$ heterostructure as obtained by spin polarized calculations using density functional theory. The electronic states of the heterostructure are compared to those of the bulk compounds. Structural relaxation turns out to have only a minor impact on the chemical bonding, even though the oxygen octahedra in La$_2$Sr$_3$MnO$_6$ develop some distortions due to the interface strain. While a small charge transfer affects the heterointerfaces, our results demonstrate that the half-metallic character of La$_2$Sr$_3$MnO$_6$ is fully maintained. (Reference: EPL, 102, 67009, 2013)

\textsuperscript{a}Research reported in this publication was supported by the King Abdullah University of Science and Technology (KAUST).

H1.00312 Magnetoresistance Anomalies in LaAlO$_3$/SrTiO$_3$(110): Fingerprints of Flat $d_{yz}/d_{xz}$ Band along [1-10] zigzag chain

HAIJIAO MA, NUS-Nanocore and Physics Department, NUS, QIFANG ZHANG, Yancheng Institute of Technology, YANG LIU, Laboratoire SPMS, Ecole Centrale Paris, ANIL ANNADI, NUS-Nanocore, NUS, WENXIONG ZHOU, NUS-Nanocore and Physics Department, NUS, SHENGWEI ZENG, NUS-Nanocore, NUS, THIRUMALAI VENKY VENKATESAN, ARIANDO ARIANDO, NUS-Nanocore and Physics Department, NUS, ARIANDO RESEARCH GROUP COLLABORATION\textsuperscript{b}, Q. F. ZHANG TEAM, Y. LIU TEAM — We report novel features in the in-plane magnetoresistance (MR) of anisotropic two-dimensional electron gas (2DEG) at LaAlO$_3$/SrTiO$_3$(110) heterostructures, which unveil the existence of a flat band in this system. One of the striking features is an anisotropy of the MR with a \textit{d}$_{yz}/\textit{d}$_{xz}-\textit{wave} like symmetry upon rotating the magnetic field $H$ within (110) plane at low temperature, which is caused by the existence of flat $d_{yz}/d_{xz}$ band. Combining with theoretical and experimental results, we confirm that a flat $d_{yz}/d_{xz}$ band formed along [1-10] Ti-O-Ti zigzag chain direction which might be very interesting for searching for topological state such as in superconducting regime.

\textsuperscript{b}Ariando Research Group is part of Department of Physics and of NUS-NanoCore, the inter-faculty and multidisciplinary Nano-Institute at the National University of Singapore.

H1.00313 Double perovskites nanoparticles: synthesis and magnetic properties (La$_2$NiMnO$_{6}$ vs La$_2$CoMnO$_{6}$)

YUANBING MAO, University of Texas-Pan American — Nanoparticles of double perovskite La$_2$MnO$_6$ (B = Ni and Co) with average particle size of about 50 nm were successfully prepared using a facile, environmentally friendly, scalable molten-salt synthesis method at 700 $^\circ$C in air. Their structural and morphological properties were characterized by X-ray diffraction and transmission electron microscopy. Their magnetic properties were evaluated using dc magnetic $M$–$T$ and $M$–$H$, and ac magnetic susceptibility versus frequency, temperature, and field for the first time. The magnetic properties of these double perovskite nanoparticles indicate that they possess very different magnetic behaviors. The following results will be discussed: (i) field-cooled and zero-field-cooled magnetization curves become divergent at their Curie temperature, i.e. 275 K and 210 K for La$_2$NiMnO$_6$ (LNMO) and La$_2$CoMnO$_6$ (LCMO) nanoparticles, respectively, which are almost unchanged from their bulk and thin film counterparts. (ii) ac susceptibility indicates that the LNMO particles are much more complex structurally and may have anti-site defects or a second-phase with a different transition temperature. For a better understanding of the nature of the magnetic state and dynamic characteristics observed here for these LNMO and LCMO nanoparticles, further detailed studies are needed.

H1.00314 Possible Mechanisms in Atomic Force Microscope-Induced Nano-Oxidation Lithography (negativity AFM tip case) in La$_{0.67}$Ba$_{0.33}$MnO$_{3−δ}$ Thin Films on SrTiO$_3$(001)

GRACE YONG, Towson University, WILLIAM VANDERLINDE, Laboratory for Physical Sciences, E. KEVIN TANYI, Norfolk University, DAVID SCHAEFER, CHRISTOPHER STUMPF, RAJESWARI M. KOLAGANI, Towson University — In this paper, we present possible microscopic mechanisms for La$_{0.67}$Ba$_{0.33}$MnO$_{3−δ}$ films that have been nano-oxidized by an AFM tip that is negatively biased with respect to the sample. Further analysis of comparative EDS elemental profile for an unmodified film versus AFM (negative tip) modified films yield fresh insights. We can qualitatively explain many of the observations with electrochemical half reactions, electrochemical migration and electromigration.

H1.00315 Heat flow and $\delta$-layers in Si nanowires

MEHMET B. BEBEK, T. MICHAEL GIBBONS, STEFAN K. ESTREICHER, Texas Tech — Modern semiconductor growth techniques allow the use of heterostructures in semiconductor devices such as $\delta$-layers or superlattices, and their behavior regarding heat flow is generating considerable interest. However, there is no fully ‘first-principles’ theoretical description of the interactions between heat flow and the interface between two dissimilar materials. In this contribution, we present the result of ongoing ab-initio, microcanonical, non-equilibrium MD simulations on Si/Ge or Si/C interfaces in a Si nanowire. We show that the ‘spatially-localized vibrational modes’ (SLMs) associated with the interface trap heat flow and the interface between two dissimilar materials. In this contribution, we present the result of ongoing ab-initio, microcanonical, non-equilibrium MD simulations on Si/Ge or Si/C interfaces in a Si nanowire. We show that the ‘spatially-localized vibrational modes’ (SLMs) associated with the interface trap

H1.00316 Local electrical imaging of tetragonal domains and field-induced ferroelectric domains in conducting SrTiO$_3$

HAIJIAO MA, Nanocore and Physics D., NUS, S. SCHARINGER, U. Tuebingen, S.W. ZENG, Nanocore, M. LANGE, A. STRR, U. TUEBINGEN, Z. HUANG, T. VENKATESAN, Nanocore, R. KLEINER, U. TUEBINGEN, M. COYE, Nanocore, D. KOTELLE, U. TUEBINGEN, A. ARIANDO, Nanocore and Physics D., NUS, NANOCORE TEAM, DIETER TEAM — We report intrinsic electric mapping of local conductivity due to tetragonal domains and twin boundaries in conducting SrTiO$_3$. Multidomains and stripe monodomains were observed in different samples at low temperatures. The distribution of these domains changes on thermal cycling above the STO cubic-to-tetragonal structural transition temperature and on electric field gating. The domains split into narrower domains when we applied side gating and we attributed this to field-induced ferroelectric domain. Twin boundaries with different orientations were observed. Angles of these domain boundaries in (110) plane are 0.55, 125 and 145 degrees. These angles were calculated from the intersection of twin planes and substrate cutting orientation. The domains split into narrower domain segments when $T$ decreases below 30 K.

\textsuperscript{1}We acknowledge support from the NSF grant ECCS 1128586 at Towson University.
H1.00317 Probing the mechanical properties and microstructure of WSi$_2$/Si$_x$Ge$_{1-x}$ multiphase thermoelectric material by nanoindentation, electron and focused ion beam microscopy methods. FRANCISCO SOLA, FREDERICK DYNYS, NASA Glenn Res Ctr — Silicon germanium (SiGe) thermoelectric (TE) alloys have been traditionally used in radioisotope thermoelectric generators (RTG) NASA applications. While RTG applications is the main driver of our current research, we are exploring other applications in the energy harvesting arena. There is still a need to improve the TE figure of merit (ZT) of SiGe based TE alloys and we have been working on ways to improve it by incorporating tungsten di-silicide (WSi$_2$) phases in to the matrix by directional solidification process. Considerable efforts have been focused until now in microstructural engineering methods that can lead to ZT improvement by microstructure optimization. Although critical for the previous mentioned applications, work pertinent to the mechanical integrity of WSi$_2$/SiGe based TE materials is lacking. In this presentation, we report local mechanical properties (hardness, modulus and fracture toughness) and microstructure of WSi$_2$/SiGe multiphase thermoelectric material by nanoindentation, scanning electron microscopy, focused ion beam and transmission electron microscopy methods.

H1.00318 Nanophononic metamaterial: Thermal conductivity reduction by dispersion-resonance hybridization. MAHMOUD I. HUSSEIN, HOSSEIN HONARVAR, LINA YANG, University of Colorado Boulder — Engineered manipulation of phonons can yield beneficial thermal properties in semiconducting materials. One pivotal application relates to thermoelectric materials, or the concept of converting energy in the form of heat into electricity and vice-versa. The ability to use nanostructuring to reduce the thermal conductivity without negatively impacting the power factor provides a promising avenue for achieving high values of the thermoelectric energy conversion figure-of-merit, ZT. In this work, we propose a novel nanostructured material configuration that seeks to achieve this goal. Termed “nanophononic metamaterial,” the configuration is based on a silicon thin-film with a periodic array of pillars erected on one or two of the free surfaces. The pillars qualitatively alter the base thin-film phonon spectrum due to a hybridization mechanism between their local resonances and the underlying atomic lattice dispersion. Using lattice dynamics calculations and molecular dynamics simulations, we predict a drop in the thermal conductivity to as low as 50% of the corresponding uniform thin-film value despite the fact that the pillars add more phonon modes to the spectrum.

H1.00319 Magneto-thermoelectric effects in the two-dimensional electron gas of a HgTe quantum well due to THz laser heating by cyclotron resonance absorption. MEHDI PAKMEHR, University at Buffalo, the State University of New York, CHRISTOPH BRUENNE, HARTMUT BUH曼NN, LAURENS MOLENKAMP, University of Wuerzburg, BRUCE MCCOMBE, University at Buffalo, the State University of New York — HgTe quantum wells (QWs) have shown a number of interesting phenomena over the past 20 years, most recently the first two-dimensional topological insulating state. We have studied thermoelectric photovoltages of 2D electrons in a 6.1 nm wide HgTe quantum well induced by cyclotron resonance absorption (B ≈ 2 - 5 T) of a focused THz laser beam. We have estimated thermo-power coefficients by detailed analysis of the beam profile at the sample surface and the photovoltage signals developed across various contacts of a large Hall bar structure at a bath temperature of 1.6 K. We obtain reasonable values of the magneto-thermopower coefficients.

H1.00320 The concept of position-dependent mass and its consideration in the study of a particle subjected to different types of potential. MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comision Nacional del Agua, LAMBERTO CASTRO-ARCE, CARLOS FIGUEROA-NAVARRO, Departamento de Fisica e Ingenieria, Universidad Regional Sur, Universidad de Sonora, JULIO CAMPOS-GARCIA, Departamento de Ciencias de la Salud, Universidad de Sonora, MATEO CASTRO-RODRIGUEZ, Departamento de Ciencias de la Salud, Universidad de Sonora — We present a study where is used the concept of position-dependent mass for a particle subjected to three kind of potential: infinite quantum potential well, harmonic oscillator potential and step potential. We solve the time-independent Schrödinger equation for each potential, considering different forms for the functional dependence of the mass respect the position. We obtain the ground state energy, the energies of some excited states and the corresponding probability densities. We make a comparison of the results with those that we would obtain if we consider an average mass for the particle.

H1.00321 Investigation of insulator-sandwich MCBJ device for single molecule detection. AKIHIDE ARIMA, MAKUSU TSUTSUI, MASATERU TANIGUCHI, The Institute of Scientific and Industrial Research, Osaka University — Mechanically controllable break junction (MCBJ) is one of the most excellent methods for accurate measurements of electron transport through single molecules because of its stability and repeatability of nanometer-scale gap distance. This method has been recently used to investigate electric conductivity of individual nucleotides in an aqueous solution. However, traditional bare electrodes of MCBJ substrate generates unexpected ionic current, which deteriorates S/N ratio and disturbs accurate control of the gap distance. To solve this problem, we report the novel MCBJ device architecture. Briefly, we covered whole junctions with insulating material. This insulator-sandwich architecture enables us to suppress such ionic current and flesh electrode surface can be used in measurement because the 100% of the ionic current is blocked.

H1.00322 Sheared graphene: Electronic properties shaped by a mechanical instability. ANDRES CONCHA, School of Engineering and Sciences, Adolfo Ibáñez University, Santiago, Chile., SHENGFENG CHENG, Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, USA, LUCIAN GYOLYI, Department Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium, L. MAHADEVAN, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA. — We explore the effects of shearing graphene ribbons on its geometry, and electronic properties. Inspired by macroscopic experiments, we show that spontaneous patterns appear when a wide ribbon is subject to shear. We compared this pattern and different regimes obtained via MD simulations with macroscopic experiments, and find good agreement between them. Beyond the low shear regime a second generation of wrinkles emerge when the system relaxes trying to keep the bond lengths as close to the relaxed length as possible. Remarkably, for all shear ratios the induced superlattice generates a momentum kick when electronic excitations enter the deformed region, an effective pseudo-magnetic superlattice, and a strong Fermi velocity renormalization. These effects modify electronic properties and suggest a simple route to engineer electronic waveguides and switches at the nanoscale. Our proposal is a concrete realization of a quantum device that takes full advantage of an elastic instability that spans from the nano to macro--scales.

1 Work at UB was supported by NSF DMR 1008138 and the Office of the Provost, and at the University of Wuerzburg by DARPA MESO contract N6601-11-1-4105, by DFG grant HA5893/4-1 within SPP 1666 and the Leibnitz Program, and the EU ERC-AG Program (Project 3-TOP.

2 AC was partially supported by Conicyt grant 79112004, and Fondecyt under grant 11130075. LC acknowledges individual support from FWO-Vlaanderen.
H1.00323 Ultrafast optical measurements of surface waves on a patterned layered nanostructure, BRIAN DALY, MATTEO BJORNSSON, AINE CONNOLLY, SUSHANT MAHAT, BRYAN RACHMILONWITZ, Vassar College, GEORGE ANTONELLI, Antonelli Research & Technology LLC, ALAN MYERS, HUI-JAE YOO, KANWAL SINGH, SEAN KING, Intel Corporation — We report ultrafast optical pump-probe measurements of 12 – 54 GHz surface acoustic waves (SAWs) on patterned layered nanostructures. These very high frequency SAWs were generated and detected on the following patterned film stack: 25 nm physically vapor deposited TiN / 180 nm porous PECVD-grown a-SiO:C:H dielectric / 12 nm non-porous PECVD-grown a-SiO:C:H etch-stop / 100 nm CVD-grown a-SiO2 / Si (100) substrate. The TiN layer was dry plasma etched to form lines of rectangular cross section with pitches of 420 nm, 250 nm, 180 nm, and 168 nm and the lines were oriented parallel to the [110] direction on the wafer surface. The absorption of ultrafast pulses from a Ti:sapphire oscillator operating at 800 nm generated SAWs that were detected by time-delayed probe pulses from the same oscillator via a reflectivity change (ΔR). In each of the four cases the SAW frequency increased with decreasing pitch, but not in a linear way as had been seen in previous experiments of this sort. By comparing the results with mechanical simulations, we present evidence for the detection of different types of SAWs in each case, including Rayleigh-like waves, Sezawa waves, and leaky or radiative waves.

This work was supported by NSF Award DMR1206681.

H1.00324 Molecular Dynamics Simulations of Surface Acoustic Waves on Patterned Layered Nanostructures, MATTEO BJORNSSON, AINE CONNOLLY, SUSHANT MAHAT, BRYAN RACHMILONWITZ, BRIAN DALY, Vassar College, GEORGE ANTONELLI, Antonelli Research & Technology LLC, ALAN MYERS, KANWAL SINGH, HUI-JAE YOO, SEAN KING, Intel Corporation — We report coarse-grained molecular dynamics (MD) simulations of surface acoustic waves on patterned layered nanostructures. The simulations were designed for comparison with samples consisting of the following patterned film stack: 25 nm physically vapor deposited TiN / 180 nm porous PECVD-grown a-SiO:C:H / 12 nm non-porous PECVD-grown a-SiO:C:H etch-stop / 100 nm CVD-grown a-SiO2 / Si (100) substrate. The TiN film was etched with lines of rectangular cross-section with pitch = 168 to 420 nm. Ultrafast optical experiments on these samples have detected high frequency surface waves in the range of 10's of GHz. The MD simulation demonstrates the presence of strongly excited modes at frequencies that closely match those found in the experiments. Moreover, the simulation predicts that the type of surface wave mode detected should change depending on the pitch. For larger pitch, Rayleigh-like waves are predicted, but for smaller pitch, Sezawa waves (surface waves with properties similar to free plate modes of the thin films) are predicted. The MD simulation also demonstrates the cutoff wavelength for the Sezawa modes, as is reflected in the experimental results and as is also predicted by isotropic elastic calculations of the surface modes of a thin film on an infinite substrate.

This work was supported by NSF Award DMR1206681.

H1.00325 Evolution of interface and surface structures of ZnO/Al2O3 multilayers upon rapid thermal annealing, H.H. LIU, Q.Y. CHEN, C.F. CHANG, W.C. HSIEH, National Sun Yat-Sen University, Taiwan, P.V. WADEKAR, University of Liverpool, UK, H.C. HUANG, National Sun Yat-Sen University, Taiwan, H.H. LIAO, Enli Technology Inc., Taiwan, H.W. SEO, University of Arkansas, USA, W.K. CHU, University of Houston, USA — ZnO/Al2O3 multilayers were deposited on sapphires by atomic layer deposition at 85°C. This low substrate temperature ensures good interface smoothness useful for study of interfacial reaction or interdiffusion. Our study aimed at the effects of rapid thermal annealing at different substrates are presented and their interpretations are compared with surface imaging techniques (SEM, STM) to evidence the usefulness of the technique.

In situ Reflection High-Energy Electron Diffraction, is a powerful characterization tool for predictability of the ability to introduce partial pressures of gases into the experimental chamber for growth of complex materials without interfering with the energy source (laser). Pulsed Laser Deposition is a state-of-the-art technique that allows for the fine tunability of the deposition rate, highly uniform and epitaxial sample growth, the Nanotechnology Association (STA) of the thin film as a whole.

H1.00326 Pulsed Laser Deposition and Reflection High-Energy Electron Diffraction studies of epitaxial long range order, nano- and microstructured Ag thin films grown on MgO, Al2O3, STO and Si, DANIEL VEILAZQUEZ, RACHEL SEIBERT, HAMDI MAN, LINDA SPENTZOURIS, JEFF TERRY, Illinois Institute of Technology — We study the evolution of the interface between the Ag thin films and the substrate material. We observe that the interface structure is strongly influenced by the deposition parameters. The MD simulation also demonstrates that the cutoff wavelength for the Sezawa modes, as is reflected in the experimental results and as is also predicted by isotropic elastic calculations of the surface modes of a thin film on an infinite substrate.

H1.00327 Indeterminate form 0/0 and tunneling in double quantum wells, IGOR FILIHKIN, BRANISLAV VLACHOVIC, North Carolina Central University — We study single electron tunneling between localized and delocalized states in double InAs/GaAs quantum wells (DQWs). Spectral distribution of localized (or delocalized) states demonstrates high sensitivity on inter-dot distance. The tunneling goes consecutively from the higher energy levels to the ground state when the inter-dot distance decreases. The spectrum is presented by set of quasi-doublet and may be described by three parts: localized states, delocalized states, and states with different probability for localization in each QW of DQW. For the last states, the ratio W/ ΔE of the wave functions overlapping integral W and the electron energy difference ΔE of isolated left and right QWs is a weight coefficient in the expansion of wave function on the basis of the wave functions of isolated QWs. In case of weakly coupled QWs in DQW the indeterminate form 0/0 takes a place for the electron wave function. It is found that a small violation of the DQW shape symmetry drastically affects tunneling. This effect also appears as a numerical instability calculations for small variations of input parameters of numerical procedure.

This work is supported by the NSF (HRD-1345219) and NASA (NNX09AV07A).

H1.00328 Emission energy control of semiconductor quantum dots using phase change material, SHOHEI KANAZAWA, YU SATO, ARIOYOSHI YAMAMURA, TOSHIHARU SAIKI, Keio Univ — Semiconductor quantum dots have paid much attention as it is a promising candidate for quantum, optical devices, such as quantum computer and quantum dot laser. We propose a local emission energy control method of semiconductor quantum dots using applying strain by volume expansion of phase change material. Phase change material can change its phase crystalline to amorphous, and the volume expand by its phase change. This method can control energy shift direction and amount by amorphous religion and depth. Using this method, we matched emission energy of two InAs/InP quantum dots. This achievement can connect to observing superradiance phenomenon and quantum dot coupling effect.
H1.00320 Magnetic field effects and nodal ground states in InP nanowire, TIA GO DE CAMPOS, PAULO EDUARDO DE FARI A JUNIOR, Universidade de S a o Paulo, State University of New York at Buffalo, IGOR ZUTIC, University of New York at Buffalo, GUILHERME SIPAHI, Universidade de S a o Paulo, State University of New York at Buffalo — Semiconductor nanowires (NWs) have attracted great interest in the last decade because oftheir unique optical, electronic, and spin-dependent properties. They are among the leading candidates to observe exotic states, such as Majorana Fermions [1]. In an assemblage of crystals of a single particle confined in a quantum dot, it was predicted that the valence band ground state with a node is possible and was attributed to the formation of orbital textures [2]. This peculiar behavior, may also be present in wurziteFP NWs with a diameter less than 10 nm [3]. The presence of a nodal state modifies its basic optical properties, such as the degree of off-axis polarization. Here we study the change in these states when an external magnetic field is applied along nanowire axis. We studied wurzite [001] and zincblende [111] InP nanowires calculated within a k.p method formulation that describes both crystal phases in a single-particle Hamiltonian [4] and account for the applied magnetic field.


H1.00330 Polarization dependent Optical Reflectance and Electroreflectance measurements of GaAs/AlGaAs multiple quantum well Bragg structure, MIM NAKARMILI, Department of Physics, Brooklyn College-CUNY, NAAREH SHAKAYA, Department of Applied Physics, NYU-Polytechnic School of Engineering, VLADIMIR CHALDYSHEV, Ioffe Physico-Technical Institute, Russia. — Electrorreflectionspectroscopy measurement provides sharp and derivative-like spectral features in the energy region of excitonic transitions, while suppressing uninteresting background effects due to electro-modulation. We employed both electroreflectance and optical reflectance spectroscopies to probe excitonic transitions in a GaAs/AlGaAs multiple quantum well (MQW) Bragg structure. The sample used in this experiment consists of 60 periods of quantum well structures with GaAs well layer (13 nm) and AlGaAs barrier layer (94 nm), grown by molecular beam epitaxy on a semi-insulating GaAs substrate. We observed a significant enhancement of excitonic features at the e2(hh2) exciton transitions due to double resonance along with sharp features of heavy-hole and light-hole ground state e1(h-h1) and e1(l-h1) exciton transitions around incident angle of 23 degree. We will present results on polarization dependent optical reflectance and electroreflectance measurements of this structure and discuss the effect of polarization in the first and second energy states.

1This work was partially supported by PSC-CUNY research grant.

H1.00331 Effective masses of Quasi-2D electrons in InGaAs/GaAsSb modulation-doped heterostructures, IMTIAZ TANVEER, BRUCE MCCOMBE, University at Buffalo, The State University of New York, HERMANN DETZ, GOTTFRIED STRASSER, Vienna University of Technology, Vienna, Austria — The electronic properties of In0.53Ga0.47As/GaAs/Ga0.51Sb0.49 2D electron gas (2DEG) systems, in spite of their use in high power electronics, have not been extensively investigated. Recently, they have been suggested as potential materials for IR quantum devices such as quantum cascade lasers (QCL), and they also show a strong Rashba effect [1,2]. Here accurate values of the effective masses are important. Two remotely donor (Si)-doped samples grown by MBE with a 2DEG at the single heterostructure interface were studied by FIR magneto-transmission spectroscopy with a BOMEM FTIR spectrometer. The maximum mobilities (near 70 K) are 43,000 cm²/Vs and 36,000 cm²/Vs with corresponding carrier densities of 1.07 × 10¹² cm⁻² and 2.13 × 10¹² cm⁻², respectively. Cyclotron resonance measurements between 4T and 9T yielded m* = 0.0495m₀ for the more heavily doped sample. Individual transmission profiles in this case showed broadening toward high energy, which may be due to contributions to the overall absorption profile from higher occupied subbands. The lower density sample shows an energy vs B dependence that does not extrapolate to zero at B = 0: The origin of this behavior will be discussed.

3Work at UB supported in part by NSF DMR #1305770 and the Office of the Provost and at the TU Wien by the Austrian Science Fund (FWF): P26100-N27 (H2N) and F4999-N23 (NextLite)

H1.00332 Carrier thermalization dynamics in single Zincblende and Wurtzite InP nanowires, YUDA WANG, HOWARD JACKSON, LEIGH SMITH, Dept. of Physics, Univ. of Cincinnati, TIM BURGESS, SURIATI PAIMAN, PHILIPPE CAROFF, HOE TAN, CHENNUPATI JAGADISH, Dept. of Electronic and Materials Engineering — Using transient Rayleigh scattering (TRS) measurements, we obtain photocarrier carrier thermalization dynamics for both zincblende (ZB) and wurzite (WZ) InP single nanowires (NW) with picosecond resolution. A phenomenological fitting model based on direct band to band transition theory is developed to extract the electron-hole plasma density and temperature as a function of time from TRS measurements of single nanowires which have complex valence band structures. We find that the thermalization dynamics of hot carriers depends strongly on material (GaAs NW vs. InP NW) and less strongly on crystal structure (ZB vs. WZ). The thermalization dynamics of ZB and WZ InP NWs are similar. But a comparison of the thermalization dynamics in ZB and WZ InP NWs with ZB GaAs NW reveals more than an order of magnitude slower relaxation for the InP NWs. We interpret these results as reflecting their distinctive phonon band structures which lead to different hot phonon effects. Knowledge of hot carrier thermalization dynamics is an essential component for effective incorporation of nanowire materials into electronic devices. We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the Australian Research Council.

H1.00333 Fluorescent DNA-templated silver nanoclusters, DMY TRO NYKYPANCHUK, Brookhaven National Laboratory, RUOQIAN LIN, YOLANDA SMALL, CUNY — Silver nanoclusters synthesized in the presence of templating DNA molecules show tunable optical properties that depend on cluster size and structure as well as on templating DNA sequence. In this paper we study the effect of DNA sequence and temperature on the cluster photoluminescence and discuss the results in the context of thermodynamics of DNA bases binding to the silver atoms in the clusters.

H1.00334 Plasmon Enhanced Ultrathin Film Broad-Band Nanoporous Absorber, JIN-YOU LU, Masdar Institute of Science and Technology, LONG LIOU, Tsinghua University, KYLE WILKE, MIT, SUMAYA NOORULLA, Masdar Institute of Science and Technology, NICHOLAS FANG, MIT, TIE-JUN ZHANG, Masdar Institute of Science and Technology — Ultrathin absorbing films have attracted much attention due to their strong interference persisted inside the lossy dielectric film, which has much smaller thickness compared with conventional resonators. The absorber was realized by coating a lossy dielectric film with tens of nanometers in thickness on a metallic substrate. The ultrathin absorber was further developed to obtain perfect absorption at a given wavelength by inserting a spacer TiO2 between the dielectric and metallic substrate. However, this interference mode just contributes to the narrow band absorption. Here, we propose to combine the strong interference inside the ultrathin film absorber with localized surface plasmons (LSPs) to achieve broad-band absorption. This concept is realized by coating ultrathin absorbing Ge/Au films on nanoporous substrate, where the LSP mode is supported by pore-shape cavities. The near-field optical properties of ultrathin film on nanoporous substrate are analyzed by using the finite difference time domain method to study the spectroscopy and energy flow patterns. Simulation shows the absorption increases with the pore radius until the pore is too large to sustain LSP. Light is trapped in nanopores and penetrate into the lossy dielectric film around the pore entrance.

1Supported by cooperative agreement between Masdar Inst and MIT.
H1.00335 Optical Properties of CdSe Nanocrystalline Photoanodes AMANDA LESAR, ROHANA GARITHARA, Hofstra University — Cadmium selenide (CdSe) nanocrystalline photoanodes were prepared by chemical solution deposition, with deposition time varied from 24 hours to 120 hours. Photoluminescence (PL) spectroscopy, reflectance and transmittance spectra, and photoelectric current were measured to optically characterize each sample. Photoelectric current was measured in a liquid junction configuration, with sodium sulfide as the electrolyte and platinum foil as the electrode. The PL, reflectance, and transmittance spectra were measured for each sample from 79 K to room temperature. Chemical solution deposition should lead to quantum size effects, as longer deposition times form larger size nanocrystals. Quantum size effects were observed, as longer depositions times led to a shift towards lower energy in the peak of the PL spectra. The temperature dependence of the PL peak energy position was also analyzed; as the temperature increased, the peak shifted towards higher energy. Using the reflectance and transmittance spectra, the absorption coefficient $\alpha$ was calculated, and the Tauc's plot of $(\alpha h\nu)^2$ versus $(h\nu)$ was graphed. A correlation between the observed absorption edge and the PL spectra was seen, as the absorption edge energy was approximately equal to the PL energy peak.

H1.00336 Plasmon excitations of multi-layer graphene interacting with a conducting substrate , PAULA FEKETE, US Military Academy at West Point, NY, GODFREY GUMBS, Hunter College, City University of New York — We generalize the procedure for calculating the plasmon excitations of a 2D layer that is Coulomb-coupled to a thick conducting substrate to the case when there is an arbitrary number of layers. In this work, we will present results for the plasmon excitations for up to five layers with arbitrary separation, energy gap between the valence and conduction bands for graphene and doping concentrations. Our procedure involves determining the inverse dielectric function for the composite hybrid system in the random-phase approximation (RPA). Effects due to nonlocality will be investigated.

H1.00337 Invisibility’s Flicker: Detecting Thermal Cloaks via Transient Effects1, SOPHIA SKLAN, Massachusetts Inst of Tech-MIT, XUE BAI, BAOWEN LI, National University of Singapore, XIANG ZHANG, University of California, Berkeley — Recent research on the development of a thermal cloak has concentrated on engineering an inhomogeneous thermal conductivity and homogeneous volumetric heat capacity. While the perfect cloak of inhomogeneous $\kappa$ and $\rho_c$ is known to be exact (no signals scattering or penetrating to the cloak’s interior), no such analysis has been considered for this case. Using analytic, computational, and experimental techniques, we demonstrate that these approximate cloaks are detectable. Although they work as perfect cloaks in the steady-state, their transient (time-dependent) response is imperfect and a detectable amount of heat is scattered. This is sufficient to determine the presence of a cloak and any heat source it contains, but the material composition hidden within the cloak is not detectable in practice.

H1.00338 Generating Steep Phase Anisotropy With Zero-Backscattering By Arrays of Coupled High Permittivity Dielectric Nanoresonators , FENG WANG, CINT, Los Alamos National Lab, QI-HUO WEI, Liquid Crystal Institute, Kent State University, HAN HTOON, CINT, Los Alamos National Lab — Simultaneous excitation of electric and magnetic dipolar modes in high-permittivity dielectric nano-resonators can lead to zero-backscattering, i.e. full transmission. Here, we numerically demonstrate that stable or unstable zero-backscattering by 2-dimensional (2D) arrays of Si nano-resonators can be realized. We also show that this Si nano-resonator array with anisotropic periodicity can generate approximate $2\pi$ optical phase anisotropy for the transmitted light at the wavelength of zero-backscattering. By introducing strong Fano-type coupling into unit cells of the array, ultra-steep phase anisotropy can be achieved. These special optical properties promise applications in various transmissive photonic devices, and we show their potential applications in transmissive polarization conversion and sensing.

H1.00339 Calculus of bands and profiles of study the system mirror - resonance of the Fibonacci Pt/Zn , LAMBERTO CASTRO-ARCE, Departamento de Fisica e Ingenieria, Unidad Regional Sur, Universidad de Sonora, CARLOS FIGUEROA-NAVARRO, Departamento de Ingenieria Industrial, Unidad Regional Centro, Universidad de Sonora, JULIO CAMPOS-GARCIA, Departamento de Ciencias de la Salud, Unidad Cajeme, Universidad de Sonora, MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comision Nacional del Agua, FELIPE RAMOS-MENDIETA, Departamento de Investigacion en Fisica, Unidad Regional Centro, Universidad de Sonora, BETZABE MANZANARES-MARTINEZ, Departamento de Fisica, Universidad Regional Centro, Universidad de Sonora — In order to analyze the behavior of a mirror - located resonance of 2pi, in a given system and with a given filling factor equal to 0.4 a study has been realized in an arrangement fibonacci, also in periodic slabs jobs. It is observed how in a study of profile that some waves are annulled giving birth to the mirror placed in 2pi. With regard to the resonance in a profile study the maxima are in certain structure Pt Pt Zn Pt Pt. Even if we increase the number of repetitions these are preserved, that means that they are related to effects of segments isolated inside the multilayer.

H1.00340 Atomic structure prediction of metal clusters using the evolutionary algorithm . NABIL AL-AQTASH, University of Nebraska- Omaha, KHALDOUN TARAWNEH, Princess Sumaya University for Technology, RENAT SABIRIANOV, University of Nebraska- Omaha — The evolutionary algorithm coupled with density functional (DFT) method is used to identify the global energy minimum atomic structure of metal clusters. Using evolutionary crystal structure optimization algorithm, as implemented in USPEX, we studied the atomic structure, binding energies, and magnetic properties of 13-atom Cu, Co and Cr clusters. A set of metastable and global minimum atomic structures are identified. Several new lower energy configurations were identified for 13-atom Cu, Co and Cr clusters and previous known atomic structures were confirmed by our calculations. We found that the Cu13 cluster has a distorted hexagonal bilayer (HBL) –like structure, which is composed by two layers as in the ideal HBL structure. The distorted HBL Cu13 is 1.17 eV lower in total energy compared to close-packed icosahedral (ICO) configuration, which reported as the lowest-energy structure for Cu13 in previous studies. Our calculations show that Cu13 has an ideal HBL structure and Cr13 cluster has distorted ICO structure, which are consistent with the previous studies. Moreover, our calculations show that Cr13 has another lower energy atomic configuration with 0.003 eV difference form ICO. Cr13 has ferrimagnetic (FIM) interaction which plays an important role in finding the lowest energy structure. We discuss the predictive capabilities of evolutionary algorithms for nanoclusters.

H1.00341 Electron with position-dependent mass confined in a two-dimensional infinite square well , MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comision Nacional del Agua, CARLOS RUVALCABA-CORNEJO, Departamento de Matematicas, Unidad Regional Centro, Universidad de Sonora — In order to have a case of study for introduce the concept of position-dependent mass, we propose to analyze the following case. Creating a rectangular crystal structure from the two-dimensional deposit of GaAs and Al0.35Ga0.65As on a substrate, we study the confinement of an electron with position-dependent effective mass. Knowing how the electron mass of the electron and its potential energy varies with the concentration of the semiconductor, we solve the time-independent Schrödinger equation using a linear combination of wave functions of a particle enclosed inside a two-dimensional square well with infinite potential walls. The ground state energy and the energies of some excited states with the probability density of these states are found. Making a two-dimensional growth of the structure we analyze if appears sub-bands energy and if the Bloch theorem manifests. We compare our results with those that we would obtain if we consider and constant effective mass inside the crystal.
H1.00342 Conformational electroresistance and hysteresis in nanoclusters. XUANG-GUO LI, XIAO-GUANG ZHANG, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — Abstract: Existence of multiple thermodynamically stable isomer states is one of the most fundamental properties of small clusters. We show that the conformational dependence of the Coulomb charging energy of a nanocluster leads to a giant electroresistance, where charging induced conformational distortion changes the blockade voltage. The intricate interplay between charging and conformation change is demonstrated in a nanocluster Zn$_2$O$_4$ by combining a first-principles calculation with a temperature-dependent transport model. The predicted hysteretic Coulomb blockade staircase in the current-voltage curve adds another dimension to the rich phenomena of tunneling electroresistance. The new mechanism provides a better controlled and repeatable platform to study conformational electroresistance.

Acknowledgement: DOE/BER-DE-FG02-02ER45995; NERSC

H1.00343 Finite-size scaling study of the one-dimensional Bose-Hubbard model via matrix product state representations. SUNG-BEEN PARK, MIN-CHUL CHA, Hanyang University — The Bose-Hubbard model is a prototypical simple model showing quantum phase transition with a continuous symmetry. In one dimension, the quantum critical properties of the model has been studied via various methods, but still some basic properties remain unknown, such as the exact location of the critical point. It is a computational challenge to study this model with more elaborated numerical methods. The matrix product state (MPS) representations are new variational solutions to one-dimensional quantum systems. By using this method to find the ground state, we study the critical properties of the one-dimensional Bose-Hubbard model with a periodic boundary condition. Finite-size scaling analysis provides the phase diagram and the critical exponents.

H1.00344 Solution of the homogeneous electromagnetic wave equation with velocity time depending on the discrete space-time. JULIO CAMPOS-GARCIA, Departamento de Ciencias de la Salud, Unidad CajaM, Universidad de Sonora, MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comisión Nacional del Agua, LAMBERTO CASTRO-ARCE, Departamento de Fisica e Ingeniería, Universidad de Sonora, CARLOS FIGUEROA-NAVARRO, Departamento de Ingeniería Industrial, Universidad Regional Centro, Universidad de Sonora, RODRIGO ROSAS-BURGOS, Departamento de Física, Universidad Regional Centro, Universidad de Sonora — We present in this meeting the solution of the homogeneous electromagnetic wave equation with a speed of light time depending on the discrete space-time. The solutions are compared with those that are obtained for a standard case, where the speed of light is constant. In addition, the limiting cases of the discrete and continuum space-time are analyzed.

H1.00345 POSTDEADLINE ABSTRACTS –

H1.00346 Fabrication and In-situ TEM Characterization of Freestanding Graphene Nanoribbons Devices. QING WANG, RYO KITAURA, SHOJI SUZUKI, HISANORI SHINOHARA, Department of Chemistry, Nagoya University, SHINOHARA TEAM — Edge-dependent electronic properties of graphene nanoribbons (GNRs) have attracted intensive interests. To fully understand the electronic properties of GNRs, the combination of precise structural characterization and electronic property measurement is essential. For this purpose, a new experimental technique using freestanding GNR devices has been developed, leading to the simultaneous characterization of electronic properties and edge structure of GNRs. To prepare freestanding GNR devices, graphene is first transferred on a Si substrate with an open slit covered by a silicon dioxide layer, and then silicon dioxide membrane underneath the graphene is etched away by buffered hydrogen fluoride acid. The so-prepared freestanding graphene device was assembled to a home-made TEM holder for in-situ characterization. The freestanding graphene was sculpted by a focused electron beam in TEM, purified and narrowed by Joule heating down to several nanometers width. Structure-dependent electronic properties were performed in TEM. We have observed significant increase in resistance and semiconductive behavior became more dominant with decreasing width of GNR.

H1.00347 Surface Premelting Coupled with Bulk Phase Transitions in Colloidal Crystals. BO LI, FENG WANG, DI ZHOU, XIN CAO, YI PENG, The Hong Kong University of Science and Technology, RAN NI, Universiteit van Amsterdam, MALIJA LIAO, YI LONG HAN, The Hong Kong University of Science and Technology — Colloids have been used as outstanding model systems for the studies of various phase transitions in bulk, but not at interface yet. Here we obtained equilibrium crystal-vapor interfaces using tunable attractive colloidal spheres and studied the surface premelting at the single-particle level by video microscopy. We found that monolayer crystals exhibit a bulk isostructural solid-solid transition which triggers the surface premelting. The premelting is incomplete due to the interruption of a mechanical-instability-induced bulk melting. By contrast, two- or multilayer crystals do not have the solid-solid transition and the mechanical instability, hence they exhibit complete premelting with divergent surface-liquid thickness. These novel interplays between bulk and surface phase transitions cast new lights for both types of transitions.

H1.00348 Entrance Pressure Fluctuation of LLDPE in Capillary Flow. HAIQING HU, SHUAI LI, LUYAO YAN, TONGJIE SUN, LINLIN LIU, Ministry of Education/Shandong Provincial Key Laboratory of Rubber-plastics; Qingdao University of Science and Technology, HE CHENG, Dongguan Institute of Neutron Physics, China; China Spallation Neutron Source, Institute of High Energy Physics CAS, Dongguan — Oscillating flow, which usually refers to the whole capillary pressure oscillation under constant piston speed, has been widely studied as an important instability phenomenon in capillary flow. The coil-stretch transition of entangled polymer molecules can be considered as a critical factor resulting in oscillating flow, which is only observed under controlled piston speed. It has been theorized by Weill since 1980 that the appearance of surface distortions may originate from a high-frequency oscillatory flow created at the die entry, but no experimental evidence has been found to prove it over 30 years. Wall slipage plays an important role in capillary extrusion flow instability for LLDPE melt. Local slip to stick transition leads to perturbations on the exit stress and sharkskin distortion, while global slip to stick transition leads to oscillatory flow and pressure perturbation. This article has revealed the correspondence relationship between entrance pressure fluctuation and exit stress perturbation experimentally and illuminated it by Uhlman model. We have further confirmed the idea that local wall slip-stick transition can induce the entrance pressure fluctuation. In brief, the molecular disentanglement in die exit determines the critical shear stress of entrance pressure fluctuation.

This work was supported by NSFC (61373884)

H1.00349 Superconductivity and Magnetism from First Principles. ANDREAS LINSCHIEID, ANTONIO SANNA, FRANK ESSENBERGER, E.K.U. GROSS, Max Planck Institute of Microstructure Physics — Magnetism has intriguing effects in superconductors. On the one hand static magnetic fields are known to suppress the superconducting state while dynamic spin-fluctuations are the probable candidate to explain the pairing in the Fe-based Superconductors. Achieving an ab-initio description is important. First, because this allows to compute the critical field and whether a local coexistence of magnetic and superconducting phases exist. Second, the critical temperature of a material is among the predicted properties which allows to search yet unknown superconductors on a computer. The Density Functional Theory for Superconductors (SCDFT) has been very successful in predicting Tc of phonon mediated superconductors. We include the magnetic density into SCDFT so that the electronic Kohn-Sham system now reproduces the electronic density μ(r), the order parameter of superconductivity Ψ(r, y), and the magnetic density μ(r). We derive the xc-potential and discuss some first results. Furthermore, we discuss an effective electron interaction mediated by spin-flip processes based on the exact spin-susceptibility. We drive a xc-functional for SCDFT that includes this effective interaction and present some results.
H1.00350 Iterative backflow renormalization procedure for many-body ground state wave functions of strongly interacting normal Fermi liquids. MICHELE RUGGERI, DEMOCRITOS National Simulation Center, Istituto Officina dei Materiali del CNR and SISSA, Via Bonomea 265, I-34136 Trieste, Italy. MICHELE TADDEI, Dipartimento di Fisica, Sapienza Universitá di Roma Piazzale A. Moro 2, I-00185, Roma, Italy. SAVERIO MORONI, DEMOCRITOS National Simulation Center, Istituto Officina dei Materiali del CNR and SISSA, Via Bonomea 265, I-34136 Trieste, Italy. MARKUS HOLZMANN, LPMC, UMR 5493 de CNRS, Université’ Grenoble Alpes, F-38100 Grenoble, France. We propose a new trial wavefunction for the ground state of a normal Fermi liquid. We apply iterative backflow transformations to obtain a sequence of renormalized coordinates. At each iteration two and three body correlations between quasiparticles are taken into account. We use these wavefunctions to compute the ground state energy of liquid $^3$He at freezing density in two dimensions with Variational and Diffusion - Fixed Node Monte Carlo simulations. Comparing with exact transient estimate results for systems with small number of particles, we find that variance extrapolations provide accurate results for the true ground state together with stringent lower bounds. For larger systems these bounds can in turn be used to quantify the systematic bias of fixed-node calculations. These wave functions are size consistent and the scaling of their computational complexity with the number of particles is the same as for standard backflow wave functions.

H1.00351 Comparative Study Between GGA and LDA Approximation Using First-Principles Calculations of Structural, Electronic, Optical and Vibrational Properties of CaTiO$_3$ Crystal. SUBENIA MEDEIROS, MAEVA ARAUJO, Universidade Federal do Semi-Árido — The structural, electronic, vibrational, and optical properties of perovskite CaTiO$_3$ in the cubic, orthorhombic, and tetragonal phase are calculated in the framework of density functional theory (DFT) with different exchange-correlation potentials by CASTEP package. The calculated band structure shows an indirect band gap of 1.88 eV at the Γ–H points in the Brillouin zone in the cubic structure, a direct band gap of 2.41 eV at the Γ–I points to the orthorhombic structure, and an indirect band gap of 2.31 eV at the M – I' points to the tetragonal phase. It is still known that the CaTiO$_3$ has a static dielectric constant that extrapolates to a value greater than 300 at zero temperature, and the dielectric response is dominated by low frequency ($\nu \approx 90$ cm$^{-1}$) polar optical modes in which cation motion opposes oxygen motion. Our calculated lattice parameters, elastic constants, optical properties, and vibrational frequencies are found to be in good agreement with the available theoretical and experimental values. The results for the effective mass in the electron and hole carriers are also presented in this work.

H1.00352 Electron relaxation of DNP free radicals BDPA and DPPH at W-band. ARMIN KHAMOSHI, UT Dallas; PAVANJEET KAUR, LIKAI SONG, NHHML, LLOYD LUMATA, UT Dallas — The stable, spin-$1/2$ organic free radicals BDPA and DPPH are efficient polarizing agents for dissolution dynamic nuclear polarization (DNP). Despite the hydrophobic nature of these two free radicals, BDPA and DPPH can be dissolved in specialized solvents such as sulfolane or dimethyl sulfoxide. In this work, we have investigated the temperature dependence of the spin-lattice relaxation rate $1/T_2$ of these two DNP free radicals at W-band from 250 K down to 4 K. We have found that at high temperature above 40 K the relaxation rates of these free radicals (at optimum DNP concentration) behave closely according to the Raman process prediction. At lower temperature below 40 K, the relaxation rate slows down according to the direct process behavior. The results obtained here may elucidate the correlation between the relaxation of electrons and the efficiency of these free radicals in DNP.

H1.00353 Power laws and extreme values in antibody repertoires. SEBASTIEN BOYER, DIPANWITA BISWAS, NATALE SCARAMOZZINO, ANANDA SOSHEE KUMAR, Laboratoire Interdisciplinaire de Physique - CNRS & Université Grenoble Alpes, CLÉMENT NIZAK, ESPCI ParisTech/CNRS, OLIVIER RIVOIRE, Laboratoire Interdisciplinaire de Physique - CNRS & Université Grenoble Alpes — Evolution by natural selection involves the succession of three steps: mutations, selection and proliferation. We are interested in describing and characterizing the result of selection over a population of many variants. After selection, this population will be dominated by the few best variants, with highest propensity to be selected, or highest "selectivity." We ask the following question: how is the selectivity of the best variants distributed in the population? Extreme value theory, which characterizes the extreme tail of probability distributions in terms of a few universality class, has been proposed to describe it. To test this proposition and identify the relevant universality class, we performed quantitative in vitro experimental selections of libraries of $>10^9$ antibodies using the technique of phage display. Data obtained by high-throughput sequencing allows us to fit the selectivity distribution over more than two decades. In most experiments, the results show a striking power law for the selectivity distribution of the top antibodies, consistent with extreme value theory.

H1.00354 Single Crystal Diffuse X-ray Scattering Using Continuous Rotation. MATTHEW KROGSTAD, OMAR CHMAISSEM, KEITH TADDEI, Northern Illinois University, Argonne National Laboratory, JARED ALLRED, RAYMOND OSBORN, STEPHAN ROSENKRANZ, JUSTIN WOZNIAK, Argonne National Laboratory — Single crystal diffuse scattering provides a measure of the 3D pair distribution function and is thus useful for investigating short-range order in materials. Using very bright synchrotron x-ray sources and fast area detectors, large volumes of reciprocal space can be mapped quickly with a dynamic range large enough to measure both Bragg peaks and the much weaker diffuse scattering. With the appropriate tools for processing and analyzing large data sets (10 to 30GB), this technique can be used to track changes in the defect structures of a material as a function of different parameters, providing a sensitive and efficient method for investigating phenomena associated with disorder. We have been developing methods of measuring diffuse scattering using continuous sample rotations (shutterless mode) at the Advanced Photon Source, and will show data from several systems, including iron nitrdates, for a range of temperatures and doping levels.

H1.00355 Chemical Bonding Forces and Metallization of Hydrogen. IVAN NAUMOV, RUSSELL HEMLEY, Carnegie Inst of Washington, CARNEGIE INST OF WASHINGTON COLLABORATION — Recent theoretical and experimental studies reveal that compressed molecular hydrogen at 200-350 GPA transforms to layered structures consisting of distorted graphene sheets. The new phases of dense solid hydrogen contrast with the long-held view that symmetric close-packed, ambient alkali-metal-like structures form at these high pressures –this raises the question about the nature and fate of molecular bonding in hydrogen on compression. The realization of such unexpected structures can be explained by consideration of simple low-dimensional model systems – H$_6$ rings and graphene-like monolayers. Both molecular quantum chemistry and well-tested solid state approaches show that these model systems like aromatic hydrocarbons exhibit a special stability, associated with the cation that is the completely filled set of bonding orbitals or valence bands. The latter nevertheless can occur upon further compression via destroying the closed shell electronic structure which is mainly determined by the s orbitals. The most likely scenario is the lowering of the bonding bands (their bottoms) stemming from the unoccupied atomic $2s$ and $2p$ orbitals. [1] This research was supported by EFree, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DESC0001057. [1] I. I. Naumov and R. J. Hemley, Acc. Chem. Res. 47, 3551-3559 (2014).
H1.00356 Generation of internal gravity waves by tidal flow over random oceanic topography. 
JIA JUN ZHAO, Natl Univ of Singapore, LIKUN ZHANG, HARRY SWINNEY, University of Texas at Austin — Internal waves (IW) are gravity waves that propagate within density-stratified fluids such as the ocean, atmosphere, and protoplanetary disks. IWs generated by tidal flow over oceanic topography provide much of the energy needed to sustain vertical mixing, which plays a critical role in ocean circulation and global climate. Therefore, it is important to determine the amount of energy that is extracted from tidal flow over topography and radiated into IWs. We conduct 2D numerical simulations to determine the IW power generated by tidal flow over random topographies that have the seafloor spectrum. The power is found to saturate with increasing topographic roughness, and to scale linearly with the characteristic height of the topography. The linear dependence on the topographic height is, surprisingly, nearly independent of the value of the exponent characterizing the topographic spectrum. Our results should lead to improved predictions of the IW power generated by tidal flow over global ocean topography.

1Research supported by the Office of Naval Research and the Texas Advanced Computing Center. JZ is supported also by the Presidents Graduate Fellowship from the National University of Singapore.

H1.00357 Photoresponse of Single Mn doped ZnO nanowires in UV application. 
MON-SHU HO, Department of Physics, National Chung Hsing University — This paper reports the fabrication of Mn doped ZnO nanowires(NWs) using a low temperature hydrothermal method. The resulting nanowires were characterized using field emission scanning electron microscopy, energy dispersive spectroscopy, X-ray diffraction analysis, transmission electron microscopy and photoluminescence spectroscopy. A single Mn doped ZnO NW sensor with high performance sensing capabilities was then assembled using a focused ion beam technique. The photoresponse of the ZnO NW sensors was investigated under irradiation from 365 nm and 400 nm ultra-violet lamps. The proposed sensor exhibited rapid photoresponse speeds and short recovery times with a photocurrent ratio \( \Delta I / I_{dark} \) superior to that of pure ZnO NW sensor. A possible mechanism to account for adsorption-desorption of oxygen and water molecules on Mn/ZnO NW surfaces was finally proposed to give the expression.

H1.00358 Power-law-like correlation between condensation energy and superconducting transition temperatures in iron pnictide/chalcogenide superconductors: Beyond the BCS understanding. 
JIE XING, SHENG LI, Center for Superconducting Physics and Materials, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, BIN ZENG, GANG MU, BING SHEN, National Laboratory for Superconductivity, Institute of Physics and National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, J. SCHNEELOCH, R.D. ZHONG, T.S. LIU, G.D. GU, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, HAI-HU WEN, Center for Superconducting Physics and Materials, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University — Superconducting condensation energy \( U_{BCS} \) has been determined by integrating the electronic entropy in various iron pnictide/chalcogenide superconducting systems. It is found that \( U_{BCS} \propto T_c^{n} \) with \( n \approx 3 \) to 4, which is in sharp contrast to the simple BCS prediction \( U_{BCS} \propto T_c^{3} \). A similar correlation holds if we compute the condensation energy through \( U_{cal} \propto 3\gamma_{eff}^{N} \Delta^2_{F} / 4\pi k_B^2 \), with \( \gamma_{eff}^{N} \) the effective normal state electronic specific heat coefficient. This indicates a general relationship \( \gamma_{eff}^{N} \propto T_c^{m} \) with \( m \approx 1 \) to 2, which is not predicted by the BCS scheme. A picture based on quantum criticality is proposed to explain this phenomenon.

H1.00359 ABSTRACT WITHDRAWN

Tuesday, March 3, 2015 12:30PM - 2:00PM –
Session H2 APS: Graduate Student Lunch With The Experts Ballroom A -
12:30PM H2.00001 Lunch With the Experts –

Tuesday, March 3, 2015 5:30PM - 6:30PM –
Session K20 APS: Student Reception, Awards Ceremony, and Dance Party Ballroom A -
5:30PM K20.00001 Student Receiption, Awards Ceremony, and Dance Party –

Wednesday, March 4, 2015 8:00AM - 9:30AM –
Session L4 APS: Tutorial for Authors and Referees Mayor Cockrell Room 004 -
8:00AM L4.00001 Tutorial for Authors and Referees –

11:00AM - 11:00AM –
Session P1 APS DPOLY/DBIO GSNP/GSOFT: Poster Session II (11:00 am - 2:00 pm) Exhibit Hall C -
P1.00001 SOFT CONDENSED MATTER –
P1.00002 Slow Relaxations of Supercooled Water Determined by Energy Landscape Sampling, NATHAN WALTER, YANG ZHANG, Univ of Illinois - Urbana — Molecular Dynamics simulations have been widely used to provide insight into atomistic scale materials behavior and to compare with neutron scattering experiments. However, such simulations are inhibited by temporal scale and spatial scale constraints. As a consequence, it is only possible to predict the dynamical behavior of materials at short times, while atomistic simulations beyond microsecond remain a challenge. The energy landscape sampling methods have been suggested to predict materials behavior at long times. Herein, we show that by efficiently sampling the activation barriers of the high-dimensional energy hypersurface we were able to study the slow dynamics of supercooled ST2 water down to deeply supercooled temperatures. Furthermore, the method allows us to quantify the statistics of the activation barriers, yielding insight into the slow and fast dynamics of ST2 water at low temperatures. The computed transport coefficients across a wide temporal range are useful to bridge the gap between neutron scattering experiments and other bulk measurements.

P1.00003 Single-stranded DNA induced chirality and helical twist in achiral liquid crystals, RAJRATAN BASU, US Naval Academy — A small quantity of single-stranded DNA (Deoxyribonucleic acid—cellulose single-stranded from calf thymus DNA in lyophilized powder form) was doped in an achiral liquid crystal (LC), and the mixture was found to exhibit a weak degree of chirality. The induced chirality in the LC of DNA mixture is of the same sign as that of the LC without DNA mixture. The mixture showed significant pretransitional behavior on approaching the smectic-\(\alpha\)-smectic-\(C\) transition temperature from above. The same DNA was doped in an achiral nematic LC and the mixture was found to exhibit an average mechanical twist over macroscopic dimensions. The single-stranded DNA-induced chiral pitch length \(\lambda\) was determined by measuring the radius of curvature of reverse twist declination lines in 90° nematic twist cells. In the LC+DNA mixture, the LC’s benzene rings interact with the nucleobases of the DNA through \(\pi\pi\) stacking, which induces a molecular conformational deracemization in the LC.

P1.00004 Local environment of iron in garden soil Vs Plants

1 Sunil Dehipawala acknowledges financial support provided by PSC-CUNY.

P1.00005 Chemotaxing and haptotaxing random walkers having directional persistence, TAE GOO KWON, Korea Univ, KYOUNGJIN LEE TEAM, TAESEOK DANIEL YANG TEAM — Biological cell crawling is a rather complex process involving various biochemical and biomechanical processes, many of which are still not well understood. The difficulties in understanding the crawling are originating not just from cell-intrinsic factors but from their complex social interactions, cell-to-substrate interactions and nonlinear responses toward extrinsic factors. Here, in this report we investigate chemotactic behavior of mathematical model cells that naturally have directional persistence. A cell density is measured as a function of time and space, then the resulting steady state is compared with that of the well-known Keller-Segel model, which describes a population of chemotactic random walkers. Then, we add a cell-to-cell interaction, mimicking a “haptoaxis” mediated interaction, to the model and access its role as for altering the steady-state cell density profile. This mathematical model system, which we have developed and considered in this work, can be quite relevant to the chemotactic responses of interacting immune cells, like microglia, moving toward and around a site of wound, as for an example. We conclude by discussing some relevant experimental findings.

P1.00006 Aqueous Foam Stabilized by Tricationic Amphiphilic Surfactants, SETH HEERSCHAP, JOHN MARAFINO, KRISTIN MCKENNA, KEVIN CARAN, KLEBERT FEITOSA, M. Madison University, KEVIN CARAN’S RESEARCH GROUP COLLABORATION — The unique surface properties of amphiphilic molecules have made them widely used in applications where foaming, emulsifying or coating processes are needed. The development of novel architectures with multi-cephalic/tailed molecules have enhanced their anti-bacterial activity in connection with tail length and the nature of the head group. Here we report on the foamability of two triple head double, tail cationic surfactants (M-1,14,14, M-P, 14,14) and a triple head single tail cationic surfactant (M-1,11,14) and compare them with commercially available single headed, single tailed amionic and cationic surfactants (SDS,CTAB and DTAB). The results show that bubble rupture rate decrease with the length of the carbon chain irrespective of head structure. The growth rate of bubbles with surfactants (SDS) and longer, single tailed tricionic surfactants (M-1,11,14) was shown to be twice as high as those with longer tailed surfactants (CTAB, M-P,14,14, M-1,14,14). This fact was related to the size variation of bubbles, where the foams made with short tail surfactants exhibited higher polydispersivity than those with short tails. This suggests that foams with tricationic amphiphilics are closed linked to their tail length and generally insensitive to their head structure.

P1.00007 Reversible mechano-memory in sheared cross-linked actin networks, SAYANTAN MAJUMDAR, MARGARET L. GARDEL, MRSEC and the James Franck Institute, University of Chicago, IL 60637 — Is it possible to control the shear modulus of a material mechanically? We reconstitute a network of actin filaments cross-linked with Filamin A and show that the system has remarkable property to respond under shear in a deformation history dependent manner. When a large shear stress pulse is applied to the system, the system remembers the direction of deformation long after the stress pulse is removed. For the next loading cycle, shear response of the system becomes anisotropic; if the applied pulse direction is same as the previous one, the system behaves like a viscoelastic solid but a transient liquefaction is observed if the pulse direction is reversed. Imaging and imaging and force measurements under shear suggest that this anisotropic response comes from stretching and bending dominated deformation directions induced by the large shear deformation giving rise to a direction dependent mechano-memory. The long time scale over which the memory effect persists has relevance in various deformations in cellular and multicellular systems.

P1.00008 Understanding hydrodynamics in the cell at the molecular level, XIAOYU BAI, PETER WOLYNES, Rice Univ — Cellular collective motion is a result of complex coupling of nonequilibrium mechano-chemical events in the cytoskeleton, of which the underlying physics is far from completely understood. In an attempt to study the cytoskeletal dynamics, we develop analytical theories based on a coarse-grained model, Cat’s Cradle. Our current work highlights how the activated events due to energy-consuming molecular motors are coupled by hydrodynamic interaction and therefore reveals the modified cytoskeletal dynamics. Within our framework, we were able to find the stability limit of the uniformly flowing phase, which is consistent with the predictions from the well-studied continuum models. In the model we accounted for the effect of shear-stretching forces on the extended structure of molecular motors. The resulting influenced stochastic properties of motor power strokes provide us with further insights into the nonequilibrium aspects of cellular dynamics.
P1.00009 Behavior of Caulobacter Crescentus Diagnosed Using a 3-Channel Microfluidic Device1, JAY TANG, MICHAEL MORSE, Brown University, REMY COLIN, Max Planck Institute-Marburg, LAURENCE WILSON, University of York — Many motile microorganisms are able to detect chemical gradients in their surroundings in order to bias their motion towards more favorable conditions. We study the biased motility of Caulobacter crescentus, a singly flagellated bacteria, which alternate between forward and backward swimming, driven by its flagella motor, which switches in rotation direction. We observe the swimming patterns of C. crescentus in an oxygen gradient, which is established by flowing atmospheric air and pure nitrogen through a 3 parallel channel microfluidic device. In this setup, oxygen diffuses through the PDMS device and the bacterial medium, creating a linear concentration gradient. Using low magnification, dark field microscopy, individual cells are tracked over a large field of view, with particular interest in the cell's motion relative to the oxygen gradient. Utilizing observable differences between backward and forward swimming motion, motor switching events can be identified. By analyzing these run interval times between motor switches as a function of a cell's local oxygen level, we demonstrate that C. crescentus displays aerotactic behavior by extending forward swimming run times while moving up an oxygen gradient, resulting in directed motility towards oxygen sources. Additionally, motor switching response is sensitive to both the steepness of the gradient experienced and background oxygen levels with cells exhibiting a logarithmic response to oxygen levels.

1Work funded by the United States National Science Foundation and by the Rowland Institute at Harvard University.

P1.00010 Influence of Chirality in Ordered Block Copolymer Phases, ISHAN PRASAD, GREGORY GRASON, University of Massachusetts Amherst — Block copolymers are known to assemble into rich spectrum of ordered phases, with many complex phases driven by asymmetry in copolymer architecture. Despite decades of study, the influence of intrinsic chirality on equilibrium mesophase assembly of block copolymers is not well understood and largely unexplored. Self-consistent field theory has played a major role in prediction of physical properties of polymeric systems. Only recently, a polar orientational self-consistent field (oSCF) approach was adopted to model chiral BCP having a thermodynamic preference for cholesteric ordering in chiral segments. We implement oSCF theory for chiral nematic copolymers, where segment orientations are characterized by quipolar chiral interactions, and focus our study on the thermodynamic stability of bi-continuous network morphologies, and the transfer of molecular chirality to mesoscale chirality of networks. Unique photonic properties observed in butterfly wings have been attributed to presence of chiral single-gyroid networks, this has made it an attractive target for chiral metamaterial design.

P1.00011 Jamming, Self-Filteration and Cake Growth in Concentrated Particle Suspensions, JOYJINGGuo, Chemical Engineering, Tongji University, Shanghai, SHOUBO LI, DONGLEI YANG, YONGLI MI, Department of Chemistry, Tongji University, Shanghai, XIAORONG WANG, Institute for Advanced Study, Tongji University, Shanghai, P. R. China — We study the flows of concentrated particle suspensions driven through a hydrodynamic shear gradient. A pressure-driven flow in a microchannel generates a local fluid motion, which is enhanced by particle translation and rotation under non-polarized UV light irradiation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation.

P1.00012 Designing thermo-responsive nanocomposites with anti-fouling properties, YA LIU, GERALD MCFARLIN, University of Pittsburgh, XIN YONG, Binghamton University, OLGA KUKSENOK, ANNA BALAZS, University of Pittsburgh — Inspired by marine organisms that utilize active “defense” (such as active cilia) to prevent the biofouling of their surfaces, we use computational modeling to design synthetic gel-based composite films that provide dual “defense” for anti-fouling applications. We design a nanocomposite gel film that can be harnessed to repel a variety of particles via either a temperature change or an imposed shear. Incorporation of stiff hydrophobic posts into a gel composed of cross-linked poly(N-isopropylacrylamide) chains allows us to drastically alter the film’s surface properties when gel undergoes temperature-induced phase transitions. Depending on whether the system’s temperature is below or above the lower critical solution temperature (LCST) of the gel, the posts are hidden in the swollen gel or exposed to the external solution. We model our system using dissipative particle dynamics (DPD); we validate our model through comparisons with Flory-Rehner theory. We focus on the influence of shear and temperature on the position of the particle in the system and isolate the conditions under which adsorption of particles of different sizes to the substrate is effectively prevented.

P1.00013 Optically driven translational and rotational motions of micro-rod particles in a nematic liquid crystal, RALF STANNARIUS, ALEXEY EREMIN, HAJNALKA NADASI, HIDEO TAKEZOE, Otto von Guericke University, Magdeburg, PEMIKA HIRANKITWONG, NATTAPORN CHATTHAM, Kasetsart University, Bangkok, OSAMU HABA, KOICHIRO YONETAKE, Yamagata University, Yonezawa — Liquid crystals are self-organized mesomorphic materials with various symmetries and structures. Their unique features can be exploited for smart multifunctional materials. Colloidal dispersions of micro- and nano-particles in LCs have been widely studied. We demonstrate controlled light-driven translational and rotational motions of micro-rods in a nematic matrix. A small amount of azo-dendrimer molecules dissolved in a liquid crystal drives translation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation on a particle surface and transforms it into a mechanical torque.

P1.00014 Thermophoresis of micrometer-sized poly(N-isopropylacrylamide) microgel particles1, KEVIN APTOWICZ, West Chester University, TIM STILL, ARJUN YODH, University of Pennsylvania — We investigate the diffusion and thermophoresis of micrometer sized poly(N-isopropylacrylamide) (PNIPAM) gel particles in a temperature gradient. Recently published results of the thermophoretic mobility of PNIPAM systems are puzzling. Cross-linked microgel particles show unusually large thermophoretic mobility whereas the mobility of core-shell colloids and linear polymers are more consistent with other aqueous systems. Our experiments add to our empirical understanding of thermophoresis of PNIPAM particles. In particular, we study micrometer-sized PNIPAM particles, which are an order of magnitude larger than those previously studied. The size of the particles prohibits the use of the optical beam deflection, the standard measurement technique. Instead, the thermophoretic mobility of the particles is measured using a novel optical system utilizing video microscopy and ring traps generated with holographic techniques.

1KBA acknowledges support from grant DMR-1206231. AGY acknowledges support from grants PENN-MRSEC DMR11-20901, NASA NNX08AO09G, and DMR-1205463.

P1.00015 Nucleation Pathways of CO2 Condensation under Mesoporous Templated Glass, BO WANG, MATTHEW S. BYRAN, GARFIELD T. WARREN, PAUL E. SOKOL, Indiana University — Carbon capture and storage (CCS) are important elements in reducing greenhouse gas emission and combating global warming. The adsorption behavior of CO2 under mesoporous confinement at room temperature is particularly relevant. Small Angle Scattering of X-ray (SAXS) and Neutron (SANS) were used to probe the adsorption process of CO2 under such mesoporous confinement MCM-41 and details of nucleation pathways were mapped out by fitting the scattering intensities with adsorption models. From both experiments, the nucleation of CO2 on the inner pore surface of MCM-41 is found to be a two-step process; high density liquid phase CO2 first forms uniform layers following the long range translational symmetry of the porous matrix, above one CO2 filling, determined by the pore size and temperature, capillary condensation initiates. The nucleation sites formed during capillary condensation start to separate the long range symmetry from the one at uniform layers. Finally, SAXS and SANS techniques are compared and they both showed their unique properties of probing the filling-dependent structures of adsorbed CO2 under such mesoporous system.
P1.00016 Divergence of the Long Wavelength Collective Diffusion Coefficient in Quasi-one and Quasi-two-Dimensional Colloid Suspensions

Binhua Lin, University of Chicago; Bianxiaow Cui, Stanford University; Xinliang Xi, MIT; Ronen Zangi, Basque Foundation for Science, Spain; Haim Diament, Tel Aviv University; Stuart A. Rice, University of Chicago

We report the results of experimental studies of the short time-long wavelength behavior of collective particle displacements in q1D and q2D colloid suspensions. Our results are reported via the $q$-behavior of the hydrodynamic function $H(q)$ that relates the effective collective diffusion coefficient, $D_c(q)$, with the static structure factor $S(q)$ and the self-diffusion coefficient of isolated particles $D_o$. 

We find an apparent divergence of $H(q)$ as $q \to 0$ with the form $H(q) \sim (1.7 < q < 1.9)$ for both q1D and q2D colloid suspensions. Given that $S(q)$ does not diverge as we infer that $D_c(q)$ does. This behavior is qualitatively different from that of the three-dimensional $H(q)$ and $D_c(q)$ as $q \to 0$, and the divergence is of a different functional form from that predicted for the diffusion coefficient in one component 1D and 2D fluids not subject to boundary conditions that define the dimensionality of the system.


P1.00017 Predicting and measuring the effects of colloid polydispersity during spinodal decomposition

John Williamson, Georgetown University; Mike L. Evans, University of Leeds

Polydispersity pervades soft matter physics, but remains so poorly understood that its effects are often guessed at or ignored entirely. Significant progress has been made on the phase equilibria of polydisperse colloids, but practical understanding of the kinetics that govern real systems lags behind. We employ kinetic Monte Carlo simulation to study the gas-liquid spinodal decomposition of a size-polydisperse colloid, particularly focusing on fractionation (demixing) between the phases, an effect which causes the properties of the “daughter” phases to depart significantly from the overall “parent” particle distribution. We find that, even though the excitation is highly localized, a collective dance of colloidal particles results; these collective modes take the form of closed rings or open-ended strings, depending on the sequence of events which nucleate the rearrangements. Surprisingly, we find from Brownian Dynamics simulations that these cooperative dynamics are thermally-activated modes inherent to the crystal, and can even occur through a single, sufficiently large thermal fluctuation, resulting in the irreversible displacement of 100s of particles from their lattice sites.

P1.00018 Cooperative dynamics in ultrasmall 2D crystals

Joris Sprakel, Wageningen University; Berend van der Meer, Marjolein Dijkstra, Jasper Van der Gucht, Utrecht University

The creation, annihilation, and diffusion of defects in crystal lattices remains so poorly understood that its effects are often guessed at or ignored entirely. Significant progress has been made on the phase equilibria of polydisperse colloids, but practical understanding of the kinetics that govern real systems lags behind. We employ kinetic Monte Carlo simulation to study the gas-liquid spinodal decomposition of a size-polydisperse colloid, particularly focusing on fractionation (demixing) between the phases, an effect which causes the properties of the “daughter” phases to depart significantly from the overall “parent” particle distribution. We find that, even though the excitation is highly localized, a collective dance of colloidal particles results; these collective modes take the form of closed rings or open-ended strings, depending on the sequence of events which nucleate the rearrangements. Surprisingly, we find from Brownian Dynamics simulations that these cooperative dynamics are thermally-activated modes inherent to the crystal, and can even occur through a single, sufficiently large thermal fluctuation, resulting in the irreversible displacement of 100s of particles from their lattice sites.

P1.00019 ABSTRACT WITHDRAWN

P1.00020 Determination of colloidal particle surface charge from dielectrophoresis

Marko Chavez, Rittirong Nuansri, Jacob Mazza, H. Daniel Ou-Yang, Lehigh University

Electrophoresis (EP) is used to determine colloidal particle surface charge. However, when the Debye length is comparable to or larger than the particle size, electrophoresis cannot be reliably used to determine the surface charge due to counter ion retardation flow. Alexander et al. developed a theory relating colloidal osmotic pressure and particle surface charge. We use dielectrophoresis (DEP) to obtain a potential landscape based on the number density distribution of the particles in a non-uniform AC electric field. We determine the osmotic pressure from the DEP force and density profiles using Einstein’s osmotic equilibrium equation. Surface charge obtained by DEP (thermodynamics) will be compared to that obtained by EP (electrokinetics).

P1.00021 Fabrication of Uniform Janus Microparticles by Photopolymerization-Driven Phase Separation and their Asymmetric Hybridization with Metal Nanoparticles

Jangwoo Cho, Jeong Won Kim, Hanyang Univ

In the field of colloid science, there is growing interest in synthesis of anisotropic particles, since they are desirable for controlling light scattering. These anisotropic particles have been developed by using sophisticated techniques, including clustering, stamping, microfluidics, and controlled nucleation and precipitation. This study introduces a facile approach for fabrication of uniform Janus microparticles with anisotropic phases as a seed for the synthesis of metallic Janus nanoparticles. This method focused on controlling the ratio of metallic and nonmetallic components, which complete compartmentalization of the particles into two distinct phases occurred upon polymerizing the monomer-swollen droplets. Then, we patched nanoparticle, such as gold nanoparticles and magnetic nanoparticles, onto one of the compartmentalized phases of the Janus microparticles. Finally, we demonstrate that these asymmetrically hybridized Janus microparticles are of great importance and play a role in the designated colloidal 2D array.

P1.00022 Fabrication of Uniform Hydrogel Microparticles with Alternate Polyelectrolyte/Silica Shell Layers for Applications of Controlled Loading and Releasing

Eun Sook Jeong, Jin Woong Kim, Hanyang Univ

Hydrogel particles, also known as microgels, consist of cross-linked three-dimensional water-soluble polymer networks. They play an essential role in loading and delivering active ingredients in medicine, cosmetics, and foods. Despite their excellent biocompatibility as well as structural diversity, much wider applications are limited due mainly to their intrinsically loose network nature. This study introduces a practical and straightforward method that enables fabrication of hydrogel microparticles layered with a mechanically robust hybrid thin shell. Basically highly monodisperse hydrogel microparticles were produced in microcapillary devices. Then, their surface was coated with alternate polyelectrolyte layers through the layer-by-layer deposition. Finally, a thin silica layer was again formed by reduction of silicate on the amino-functionalized polyelectrolyte layer. We have figured out that these hybrid hydrogel microparticles showed controlled loading and releasing behaviors for water-soluble probe molecules. Moreover, we have demonstrated that they can be applied for immobilization of biomacromolecules, such as bacteria and living cells, and even for targeted releasing.

P1.00023 2D Colloidal Wigner crystals in confined geometries

Ruben Higler, Joris Sprakel, Wageningen University

Crystallization of bulk systems has been widely studied using colloids as a model system. However, study into colloidal crystallization in confined geometries has been sparse and little is known about the effects of strong confinement on the dynamics of colloidal crystal. In our research we prepare 2D crystals from charged colloids in an apolar solvent to study crystal dynamics, formation, and structure in circular confinements. These confining geometries are made using soft lithography techniques from SU-8. In order to broaden the parameter space we can reach in experiments we employ Brownian dynamics simulations to supplement our experimental results. Using single-particle tracking we have subpixel resolution positional information of every particle in the system. We study the vibrational modes of our confined crystals and find well defined modes unique to confined systems, such as a radially symmetric compression (or breathing) mode, a collective rotation mode, and distinct resonance modes. Furthermore, due to the circular nature of our constrictions, defectless crystals are impossible, we find, for sufficiently high area fractions, that the defects order at well defined points at the edge. The effect of this “defect-localization” has a clear influence on the vibrational modes.
P1.00024 Shear-induced demixing of glassy suspension, TIES VAN DE LAAR, JORIS SPRAKEL, KARIN SCHROEN, Wageningen University — The ground state of a binary suspension composed of particles of incommensurate size is that of two demixed crystal phases. However this has never been experimentally observed, due to the prohibitively long time scales associated with diffusion in a glass. Here we show that enhancing particle mobility in a glass, by means of flow, can lead to this type of solid-solid demixing. We study this phenomenon at the scale of single particles by means of high speed confocal imaging of suspensions flowing through microfluidic channels. By systematically varying the applied pressures and volume fractions we intend to bridge the gap between classical shear-induced migration at dilute concentrations and deformation of glasses.

P1.00025 Hyperuniformity of self-assembled soft colloidal spheres, COLINE BRETZ, University of Pennsylvania, YE XU, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn; University of Pennsylvania, TIM STILL, University of Pennsylvania, JEAN BAUDRY, ESPCI ParisTech/CNRS, LAWRENCE A. HOUGH, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn, ARJUN G. YODHI, University of Pennsylvania, SALVATORE TORQUATO, Princeton University, REMI DREYFUSS, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn, COMPLEX ASSEMBLIES OF SOFT MATTER TEAM1, DEPARTMENT OF PHYSICS AND ASTRONOMY TEAM2, LABORATOIRE DE COLLOIDES ET MATERIAUX DIVISES TEAM3 — Hyperuniformity characterizes a state of matter for which density fluctuations vanish on large scales. Hyperuniform materials are of technological importance as they exhibit interesting photonic properties. We have shown that such materials can be obtained by assembling spheres into a disordered jammed 2D-packing. To this end, we use a binary mixture of large and small Poly(NIPAM) particles confined between two cover slips. These soft spheres have been chosen for their temperature-sensitive properties. We can locally increase or decrease the volume fraction occupied by the spheres by finely tuning the temperature. By applying various temperature patterns, we are studying the spatial arrangements of the microgels and characterizing their hyperuniform properties through reconstruction and detection algorithms.

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P1.00026 Model colloidal system for interfacial adsorption kinetics, STEVEN HUDSON, PAUL SALIPANTE, NIST — An experimental colloidal model for sorption behavior may allow direct observation of the effects of particle shape and concentration on adsorption and desorption kinetics. Here we investigate spherical colloid adsorption to near a solid surface. The attraction is induced by depletion interaction. The colloid-interface interaction potential is tuned to be less than 10 kT using a combination of depletion, electrostatic, and gravitational forces. The colloids transition between an entropically trapped adsorbed state and a desorbed state through Brownian motion. High resolution particle tracking is made using LED-based Total Internal Reflection Microscopy (TIRM). The observed adsorption and desorption rates obey different distributions and are compared to theoretical predictions based on the measured interaction potential and near wall particle diffusivity. This experimental system also allows for the study of more complex dynamics such as nonphysical colloids and collective effects at higher concentrations.

P1.00027 ABSTRACT WITHDRAWN —

P1.00028 Interfacial Behavior of Polymer Coated Nanoparticle, LUQING QI, HADI SHAMSILIAZEYI, JASON MANN, RAFAEL VERDUZCO, GEORGE HIRASAKI, Rice Univ, RICE UNIVERSITY TEAM — Oxidized carbon black (OCB) nanoparticle is functionalized with different coatings, i.e. alkyl group, polyvinyl alcohol (PVA) and partially sulfonated polyvinyl alcohol (spVPA). In oil and water systems, the functionalized nanoparticle is found to have a versatile dispersion i.e. in lower aqueous phase, in upper oil phase, or in middle phase microemulsion. Oil substitute n-octane and commercial oil IOSPAR have been test as oil phase; series of commercially available surfactant, C12-4,5 orthoxylene sulfonate(OXS), i-C13-(PO)7 -SO4Na (S13B), surfactant blend of anionic Alfoterra with nonionic Tergitol have been test as additive to help with the OCB dispersion. It is found that the OCB with sulfonated polyvinyl alcohol attachment (spVPA-OCB) stays in microemulsion; with the increase of salinity, it follows the microemulsion to go from lower phase, to middle phase, and to upper phase. The dispersion of spVPA and alkyl functionalized OCB (Cn-OCB-spVPA) is the balance of the length of alkyl and spVPA and the degree of sulfonation of PVA, depending on which, it can either disperse into microemulsion or form a separate layer. The spVPA-OCB also indicates a tolerance of high salinity; this is shown by the stable dispersion of it in blend surfactant solution of anionic Alfoterra and nonionic Tergitol at high salinity API brine (8% NaCl and 2% CaCl2). The study of different functionality on OCB dispersion can help design appropriate modified nanoparticle as additive for enhanced oil recovery either to reduce the interfacial tension between oil and water, or to stabilize microemulsion.

P1.00029 Nematic Liquid Crystal reorientation with a Photosensitive layer, ADRIAN REYES, LAURA PALOMARES, PATRICIA GUTIERREZ, Universidad Nacional Autonoma de Mexico — We assume a nematic cell in a planar configuration for which one of their confining plates, is submitted to a hard-anchoring boundary condition and the other plate has a coating monolayer of azo dye molecules, such that the change of the orientation of azo dye isomers, due to light, causes changes in the nematic director. We find an approximated expression for the density of isomers, written in terms of the director angle, which allows us to close the equation for the director’s angle on the boundary having a photosensitive plate. We have managed to decouple the director’s angle and the isomer densities by assuming extremely different temporal time scales between them. We show that switching times inversely depend on trans-cis transition rate of photo-excitation meanwhile relaxation times do not depend on it, for a given sample. On the other hand, switching and relaxation times linearly depend on surface viscosity values.

P1.00030 Electric field variation within a nematic liquid crystal layer1, LINDA CUMMINGS, ENSELA MEMA, CHENJING CAI, LOU KONDIC, New Jersey Institute of Technology — A thin layer of Nematic Liquid Crystal (NLC) across which an electric field is applied is a setup of great industrial importance in Liquid Crystal Display devices, and there is a wide associated literature. A common assumption is that an electric field generated by constant-potential electrodes at the two bounding surfaces of the layer will produce a field that is uniform: the presence of NLC does not affect the electric field. We derive the equations that couple the electric potential to the orientation of the NLC’s director field and use asymptotic and computational methods to address the question: Under what conditions is the uniform field assumption justified, and when is it inappropriate?


1Supported by NSF Grant No. DMS-1211713.
P1.00031 Molecular dynamics simulations of liquid crystalline ordering in bulk and at interfaces, XIAOYU WEI, JUSTIN HOOPER, DMITRY BEDROV, Univ of Utah — The influence of induced polarization interactions in atomistic MD simulations on the thermodynamic and structural properties of 4-Cyano-4'-pentylbiphenyl (5CB) bulk systems have been systematically investigated utilizing both polarizable (POL) and non-polarizable (NP) version of the APPLiP force field (FF). The predicted densities for the nematic and isotropic phases of 5CB are in excellent agreement with available experimental data. However, the nematic-isotropic transition temperature Tw showed noticeable sensitivity to the details of FF. The NP FF showed a tendency to predict systematically higher Tw (by about 30K) and showed very little sensitivity to modifications of dihedral potential in the biphenyl unit. The POL FF showed a much stronger sensitivity to the details of biphenyl conformational properties and was able to predict Tw at around 313K, which is very close to the experimental Tw of 308K. Using the developed potentials we have also investigated the anchoring of nematic 5CB at the water interface as well as phase behavior and structure of the newly discovered twist-bend nematic phase of CB7CB. Detailed analysis of molecular scale correlations for both systems will be presented and discussed in light of available experimental data.

P1.00032 Polarized Raman Spectroscopic and Conoscopic study of twist-bend nematic liquid crystal CB7CB1, JINXIN FU, KARTHIK NAYANI, JUNG OK PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology — The liquid crystal CB7CB, which exhibits a new twist bend nematic phase, has aroused lots of interest recently. We use polarized Raman Spectroscopy to measure the liquid crystal order parameters, which are crucial to know the molecular orientation distribution and to understand the phase transition. It is found that in the twist-bend phase, both P<200> and P<400> increase with temperature before the nematic transition takes place at 103°C, and then decrease in the nematic region until the LC becomes isotropic at 116°C. Conoscopy is a convenient tool to determine the structure and orientation of crystals. We develop a monochromatic conoscopy method to study the uniaxial and biaxial behavior of CB7CB in the different phases.1This work was supported a grant from the U.S. Office of Basic Energy Sciences, Department of Energy; Grant No. DE-SC0001412.

P1.00033 Ground states of lyotropic chromonic liquid crystals in cylindrical capillaries1, RUI CHANG, School of Chemical and Biological Engineering, Georgia Institute of Technology, KARTHIK NAYANI, JINXIN FU, School of Material Science and Engineering, Georgia Institute of Technology, ELSA REICHMANIS, School of Chemical and Biological Engineering, Georgia Institute of Technology, JUNG OK PARK, MOHAN SRINIVASARAO, School of Material Science and Engineering, Georgia Institute of Technology — We investigate the ground states of nematic lyotropic chromonic liquid crystals (LCLCs) confined in cylindrical capillaries. Two line defects with double helical configuration is observed for Sunset Yellow FCF with the homeotropic anchoring being obtained by parylene-N coating. The striking features of nematic-isotropic phase transition is also studied, in which we find a coexistence of double helix configuration and escape radial configuration mediated with point defects in biphasic temperature range. However with Disodium Cromoglycate (DSCG) we observe that the anchoring is planar anchoring in both parylene-N coated and uncoated borosilicate capillaries.1We acknowledge the support from the U.S. Office of Basic Energy Sciences, Department of Energy; grant DE-SC-0001412.

P1.00034 ABSTRACT WITHDRAWN —

P1.00035 Lipid Nanodiscs as potential carriers of enzymes: a light scattering study, KIRIL STRELETZKY, GHAITH TAWALBEH, MEKKI BAYACHOU, Cleveland State University — The structure and dynamics of discoidal phospholipid protein complexes (nanodiscs) with and without endothelial nitric oxide synthase (eNOS) were studied with multilangle polarized and depolarized light scattering. Nanodiscs present a mobile system that is similar to enzyme's native microenvironment which allows to explore the potential effect of membrane phospholipids on the activity of eNOS. Light scattering revealed at least two different size distribution modes for empty nanodiscs, and nanodiscs loaded with eNOSoxy. In both cases, the first mode was diffusive (linear v = qa) with a small intercept (with apparent Rb = 4.5 nm for empty nanodiscs and 4.9 nm for loaded nanodiscs, sizes consistent with nanodisc dimensions. The second mode contributed only about 20% to the intensity and showed non-diffusive behavior which might correspond to coalesced nanodiscs present in solution. Studied concentration dependencies and depolarized scattering measurements on enzyme free and enzyme loaded nanodiscs corroborated these findings. Also, the specific activity of nanodiscs-bound eNOS was found to be significantly lower than the specific activity of free eNOS.

P1.00036 Active motion induced break-up of colloidal gels, MEGAN SZAKASITS, MICHAEL SOLOMON, University of Michigan — We found that fractal gel networks of polystyrene colloids can be broken up by active motion of Janus colloids that have been incorporated into them. Janus particles were synthesized by electron beam deposition of platinum onto one micron carbomate modified polystyrene particles. Through addition of the divalent salt magnesium chloride, an initially stable suspension of Janus and polystyrene colloids, present in equal proportion, underwent aggregation to yield a fractal gel. The Janus colloids were activated by addition of 30% v/v hydrogen peroxide through a porous hydrogel membrane. Changes in structure and dynamics were visualized by two channel confocal laser scanning microscopy (CLSM). By means of image analysis, we calculated the mean squared displacement (MSD) and radial distribution function (RDF) for gel samples before and after addition of hydrogen peroxide. The MSD confirmed the Janus particles we synthesized undergo active motion. The RDF and cluster size distribution of gel samples before and after addition of peroxide demonstrate how active motion broke apart the gel network into smaller clusters.

P1.00037 Direct visualization of photoinduced glassy dynamics on the amorphous silicon carbide surface by STM movies, DUC NGUYEN, LEA NIENHAUS, RICHARD T. HAAUCH, JOSEPH LYDING, MARTIN GRUEBELE, Univ of Illinois - Urbana — Glassy dynamics can be controlled by light irradiation. Sub- and above-bandgap irradiation cause numerous phenomena in glasses including photorelaxation, photoexpansion, photodarkening and photoinduced fluidity. We used scanning tunneling microscopy to study surface glassy dynamics of amorphous silicon carbide irradiated with above-bandgap 532 nm light. Surface clusters of ~ 4-5 glass forming unit in diameter hop mostly in a two-state fashion, both without and with irradiation. Upon irradiation, the average hopping activity increases by a factor of 3. A very long (~1 day) movie of individual clusters with varying laser power density provides direct evidence for photoinduced enhanced hopping on the glass surfaces. We propose two mechanisms: heating and electronic for the photoinduced surface dynamics.

P1.00038 A Simulation Study on Translation-Rotation Decoupling and its Dependence on Tracer Shape in Two Dimensional Colloids, JEONGMIN KIM, BONG JUNE SONG, Department of Chemistry and Research Institute for Basic Science, Sogang University — Near the glass transition, translation is often faster than expected from the viscosity of liquids unlike rotation. It is the well-known translation-rotation decoupling phenomenon. In this poster, we present the dependence of the decoupling on tracer shape in two-dimensional (2D) colloids using three representative tracer shapes (diamond, distorted diamond and square). We find that near the freezing (liquid-hexatic) transition, the translation-rotation decoupling occurs for all tracers regardless of shapes, but trends are different for different shape. In 2D, there exists an orientationally ordered liquid phase called a hexatic phase between isotropic liquid and solid phases. Entering the hexatic phase, 2D colloids exhibit the heterogeneous dynamics with several dynamic regions of different mobility like glass-forming liquids [1]. We find that the observed decoupling of tracer diffusion is attributed to the dynamic heterogeneity of 2D colloids. To our surprise, the shape-dependence of decoupling trend relate closely to the rotational diffusion of tracers. Square shape tracer disturbs the hexagonal ordering of 2D colloids, thus resulting in faster rotation of square tracers, which is not observed for diamond shape tracers.

P1.00039 Trimerization of Phenyl Cyanate Ester, MADHUSUDHAN REDDY PALLAKA, SINDEE L. SIMON, Texas Tech Univ — The kinetics of phenyl cyanate ester trimerization is studied in the bulk using differential scanning calorimetry. Dynamic experiments for different heating rates are analyzed for the activation energy using the model-free Kissinger-Akahira-Sunose (KAS) isoconversion method. The activation energy and other kinetic parameters are also obtained by fitting the data to a first order autocatalytic reaction model, which well describes the experimental data. The activation energy obtained from the KAS isoconversion method (70.1 kJ/mol) is in good agreement with that obtained from the kinetic model (73.2 kJ/mol) and is much lower than the more bulky cyanate esters studied in our laboratory, which have activation energies of approximately 95 kJ/mol. In addition, the rate constant for the phenyl cyanate ester is one to two orders higher than the bulkier cyanate esters in the temperature range of 200 to 300°C. Further elucidation of the dynamic experiments revealed a strong dependence of the reaction kinetics on the sample weight. Future work aims to understand this finding.

P1.00040 FEL approach to the crystallization of super-cooled liquids1, TAKASHI ODAKAGI, ANJU OKADA, Tokyo Denki University — The crystallization time of most super-cooled liquids as a function of temperature (time-temperature transformation (TTT) diagram) show a nose-shaped form, namely near the melting temperature it is an increasing function of temperature and at much lower temperatures it becomes a decreasing function of temperature. The former behavior is believed to be controlled by the thermodynamics and the latter is governed by the slow dynamics. Exploiting the merit of the free energy landscape (FEL) approach which can handle both thermodynamic and dynamic processes in the same frame work, we investigate the crystallization of super-cooled liquids as the first passage process of a representative point to the crystalline basin in the FEL. We first show that the crystallization time can be related to the eigenvalues of the transition matrix which governs the stochastic dynamics of the representative point in the FEL. We apply this formalism to various structures of the FEL which include the small world and the scale free network. We show that the TTT diagram is sensitive to the structure of the FEL, indicating the possibility of obtaining the structural information from the TTT diagram.

1This work was supported in part by KAKENHI (25400429).

P1.00041 Critical adsorption and colloidal interaction in binary liquid mixtures1, SHARMINE ALAM, RAMI OMARI, CHRISTOPHER GRABOWSKI, ASHIS MUKHOPADHYAY, Wayne State Univ — We studied critical adsorption on colloidal nanoparticles in binary liquid mixture system of 2,6 lutidine + water by using fluorescence correlation spectroscopy (FCS). Our results indicated that the adsorbed film thickness is of the order of correlation length associated with concentration fluctuations. The excess adsorption per unit area increases following a power law in reduced temperature with an exponent of -1, which is the mean-field value for the bulk susceptibility exponent. The measurements at higher particle volume fractions, where particle-particle interaction becomes important, will be presented.

1Acknowledgements are made to the Donors of the American Chemical Society Petroleum Research fund (PRF # 51694-ND10) for support of this research.

P1.00042 Control of nanoparticle formation using the constrained dewetting of polymer brushes, THOMAS LEE1, School of Chemistry, The University of Sydney, Camperdown, NSW 2006, Australia, SHAUN C. HENDY, MacDiarmid Institute for Advanced Materials and Nanotechnology, Department of Physics, University of Auckland, Auckland 1142, New Zealand, CHIARA NETO, School of Chemistry, The University of Sydney, Camperdown, NSW 2006, Australia — We have used coarse-grained molecular dynamics simulations to investigate the use of pinned micelles formed by the constrained dewetting of polymer brushes to act as a template for nanoparticle formation. The evaporation of a thin film containing a dissolved solute from a polymer brush was modeled to study the effect of solubility, concentration, grafting density, and evaporation rate on the nucleation and growth of nanoparticles. Control over particle nucleation could be imposed when the solution was dilute enough such that particle nucleation occurred following the onset of constrained dewetting. We predict that nanoparticles with sizes on the order of 1 nm to 10 nm could be produced from a range of organic molecules under experimentally accessible conditions. This method could allow the functionality of organic materials to be imparted onto surfaces without the need for synthetic modification of the functional molecule, and with control over particle size and aggregation, allowing for the preparation of surfaces with useful optical, pharmaceutical, or electronic properties.

1Now at Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA

P1.00043 STATISTICAL AND NON LINEAR PHYSICS —

P1.00044 Critical behavior of the disordered three-color Ashkin-Teller Model – A Monte Carlo study, QIONG ZHU, XIN WAN, Zhejiang University, RAJESH NARAYANAN, Indian Institute of Technology, Madras, JOSÉ A. HOYOS, Instituto de Física de São Carlos, Universidade de São Paulo, THOMAS VOJTA, Missouri University of Science and Technology — The impact of quenched disorder on systems undergoing first-order phase transitions has received less attention than its effects on critical points. A notable exception is the seminal work by Aizenman and Wehr1 predicting that disorder rounds the critical value diverges proportionally to the mass. By increasing the inertia the transition becomes more hysteretic and within the hysteretic region clusters of locked oscillators form. We study the transition from incoherence to coherence for increasingly large system size and inertia. For sufficiently large inertia the transition is hysteretic and within the hysteretic region clusters of locked oscillators of various sizes and different levels of synchronization coexist. A modification of the mean field theory developed by Tanaka, Lichtenberg, and Oishi allows to derive the synchronization curve associated to each of these clusters. We have also investigated numerically the limits of existence of the coherent and the incoherent solutions. The minimal coupling required to observe the coherent state is largely independent of the system size and it saturates to a constant value for moderately large inertia values. The incoherent state is observable up to a critical coupling whose value saturates for large inertia and for finite system sizes, while in the thermodynamic limit this critical value diverges proportionally to the mass. By increasing the inertia the transition becomes more complex, and the synchronization occurs via the emergence of clusters of coherently drifting oscillators.

1Financial support has been provided by the Italian Ministry of University and Research within the project CRISIS LAB PNR 2011-2013

P1.00045 Hysteretic transitions in the Kuramoto model with inertia, ALESSANDRO TORCINI, SIMONA OLMI, Istituto dei Sistemi Complexi, CNR, Sesto Fiorentino, Italy, ADRIAN NAVAS, Centre for Biomedical Technology (UPM) 28922 Pozuelo de Alarcon, Madrid, Spain, STEFANO BOCCALETTI, Istituto dei Sistemi Complexi, CNR, Sesto Fiorentino, Italy — We report finite size numerical investigations and mean field analysis of a Kuramoto model with inertia for fully coupled and diluted systems. In particular, we examine the transition from incoherence to coherence for increasingly large system size and inertia. For sufficiently large inertia the transition is hysteretic and within the hysteretic region clusters of locked oscillators of various sizes and different levels of synchronization coexist. A modification of the mean field theory developed by Tanaka, Lichtenberg, and Oishi allows to derive the synchronization curve associated to each of these clusters. We have also investigated numerically the limits of existence of the coherent and the incoherent solutions. The minimal coupling required to observe the coherent state is largely independent of the system size and it saturates to a constant value already for moderately large inertia values. The incoherent state is observable up to a critical coupling whose value saturates for large inertia and for finite system sizes, while in the thermodynamic limit this critical value diverges proportionally to the mass. By increasing the inertia the transition becomes more complex, and the synchronization occurs via the emergence of clusters of coherently drifting oscillators.
P1.00046 Discontinuous phase transitions via cooperative contagion. FAKHTEH GHANBARNEJAD, Max-Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany, WEIRAN CAI, TU Dresden, Germany, LI CHEN, Robert Koch-Institute, 13353 Berlin, Germany, PETER GRASSBERGER, Forschungszentrum Juelich, 52425 Juelich, Germany — We study the spreading of two diseases that interact cooperatively (the presence of one helps the other to spread) on different network topologies, and with two microscopic realizations, both of which are stochastic versions of an SIR type studied by us recently in mean field approximation. We had shown that cooperativity can lead to discontinuous transitions (DT). However, due to the rapid mixing implied by the mean field assumption, DTs were seen only when there were finite (non-zero) densities of sick individuals in the initial state. In this paper we find that the results of the stochastic model depend strongly on the underlying network. In particular, DTs are found when there are few short but many long loops: (i) No DTs exist on trees, due to the absence of loops; (ii) On 2-d lattices with local contacts there are no DTs either, but because of too many short loops; (iii) We do find DTs on Erdos-Renyi (ER) networks, on d-dimensional lattices with $d \geq 4$, and on 2-d lattices with sufficiently long-ranged contacts; (iv) On 3-d lattices with local contacts the results depend on the microscopic details of the implementation. All found discontinuous transitions are of “hybrid” type, i.e. they display also scaling features usually associated with continuous transitions.

P1.00047 ABSTRACT WITHDRAWN

P1.00048 Origin of the $1/f^\alpha$-Spectral-Noise in Chaotic and Regular Quantum Systems. LEONARDO A. PACHON, Instituto de Física, Universidad de Antioquia. Department of Chemistry and Chemical Biology, Harvard University, ARMANDO RELAÑO, Departamento de Física Aplicada I and GISC, Universidad Complutense de Madrid, Spain., BORJA PERÓPÆDRE, ALAN ASPURÚ-GUZIK, Department of Chemistry and Chemical Biology, Harvard University. — Based on the recent connection between the spectral form factor and the probability to return [Phys. Rev. Lett. 102, 150401 (2009)], the origin of the $1/f^\alpha$-noise in fully chaotic and fully integrable systems is tracked to the quantum interference between invariant manifolds of the classical dynamics and the dimensionality of those manifolds. This connection and the order-to-chaos transition are analyzed in terms of the statistics of Floquet’s quasienvironments of a classically chaotic driving non-linear system. The direct connection established here allows for predicting that in the presence of decoherence, the statistics of the spectral correlations of both, chaotic and integrable, coincide.

P1.00049 Enhanced rare-region effects in the contact process with long-range correlated disorder. AHMED K. IBRAHIM, HATEM BARGHATHI, THOMAS VOJTA, Missouri Univ of Sci & Tech — We investigate the nonequilibrium phase transition in the disordered contact process in the presence of long-range spatial disorder correlations. These correlations greatly increase the probability for finding rare regions that are locally in the active phase while the bulk system is still in the inactive phase. Specifically, if the correlations decay as a power of the distance, the rare-region probability is a stretched exponential of the rare-region size rather than a simple exponential as is the case for uncorrelated disorder. As a result, the Ginzburg-Landau exponent $\gamma$ is related to the non-power-law form of the $1/f^\alpha$-noise.

P1.00050 Critical Initial Slip Scaling for Driven-dissipative Bose-Einstein Condensation. WEIGANG LIU, UWE TAUBER, Department of Physics, Virginia Tech — We investigate the universal non-equilibrium critical behavior at the driven-dissipative Bose-Einstein condensation phase transition by means of the perturbative field-theoretic renormalization group method. Such criticality may be realized experimentally in driven open systems on the interface of quantum optics and many-body physics, ranging from exciton-polariton condensates in optically pumped semiconductor wells to cold atomic gases. We describe the critical dynamics through a noisy and dissipative Gross-Pitaevskii or time-dependent Ginzburg-Landau equation with complex coefficients. We focus on the universal critical behavior of this system in the early stages of the relaxation process following a quench from an initially (Gaussian distributed) disordered state that is characterized by broken time translation invariance and governed by the “critical” exponent $\theta$. We compute $\theta$ to first order in the dimensional $\epsilon = 4-d$ expansion with respect to the upper critical dimension $d=4$, and find that its one-loop value is identical to that of the classical relaxation model $A$ for a two-component non-conserved order parameter.

P1.00051 Energy flow between two hydrodynamically coupled particles kept at different effective temperatures. SERGIO CILIBERTO, ENSL-CNRS, ANTOINE BERUT, ENSL, ARTYOM PETROSYAN, ENSL-CNRS, EQ 2 TEAM — We measure the energy exchanged between two hydrodynamically coupled micron-sized Brownian particles trapped in water by two optical tweezers. The system is driven out of equilibrium by random forcing the position of one of the two particles. The forced particle behaves as if it has an “effective temperature” higher than that of the other bead. This driving modifies the variance ratios and cross-correlations of the bead positions: We measure an energy flow between the particles and an instantaneous cross-correlation, proportional to the effective temperature difference between the two particles. A model of the interaction which is based on classical hydrodynamic coupling tensors is proposed. The theoretical and experimental results are in excellent agreement.

P1.00052 Effect of Graphene in Quenching Fluorescence from Strained Conjugated Polymer Doped Polystyrene Composite Films. XUAN LONG HO, YAN-HAO CHEN, JONATHON DAVID WHITE, NEN-WEN PU, Yuan Ze University, Taiwan, ARNOLD CHANG-MOU YANG, National Tsing Hua University, Taiwan — Introduction of graphene into films and solutions of conjugated polymers has been observed to dramatically quench photoluminescence (PL) of MEH-PPV. In other work, the PL of MEH-PPV well dispersed in an optically inert matrix was seen to be dramatically increased when the individual molecular strands were fully stretched. Strong polarization effects indicated that stretching individual polymer chains was responsible for the observed enhancement. We examined the combined effect of stress and the addition of reduced graphene oxide (rGO) on PL. We found that the addition of a small amount of rGO (0.3%) into polystyrene films lightly doped with 1% MEH-PPV quenched 40% of the PL. Stretching resulted in the creation of local deformation zones (LDZ) of high stress and strain. Within these zones, while the PL efficiency increased dramatically, the results depend on the microscopic details of the implementation. All found discontinuous transitions are of “hybrid” type, i.e. they display also scaling features usually associated with continuous transitions.

P1.00053 Mechanical Properties of Hydrogel Beads. KEELY CRIDDLE, THOMAS BENNS, DAN SHORTS, KLEBERT FEITOSA, James Madison University — Fragile solids made of dense disordered packing of bubbles, droplets and grains are able to withstand small stresses by virtue of system-wide force chains that lock the system into a jammed state. The nature of the jamming transition in such soft materials has been the subject of intense research, but despite much effort, a deep understanding remains elusive. In this experiment we study the mechanical properties of hydrogel beads to exploit them as force transducers in densely packed systems. The experiment consists of applying uniaxial planar compressions on the beads, and correlating the force to the bead’s strain and contact area. The results show that while the strain scales linearly with the diameter of the contact area, the force and strain are found to obey a power law relation with two distinct exponents at small and large strains. This result leads to a power law dependence of the force on the contact area diameter of the compressed bead.
P1.00054 The nature of long-ranged forces between pinned particles in a jammed system. JUAN-JOSE LIETOR-SANTOS, JUSTIN BURTON, Emory University — We explore the interaction between two fixed-position particles immersed in a binary, two-dimensional jammed system of disks at T=0. In our simulations, the two pinned particles develop an interaction along their alignment direction. At short distances, their interaction can be described by a mean-force potential derived from the particle-particle correlation function, g(r), and thus have a repulsive and attractive nature which depends on separation. However, there is an additional repulsive force that dominates at large particle separation or when the ambient jammed disks are much smaller than the pinned particles. We will show that the nature of this repulsive force stems from fluctuations near the jamming transition, in analogy with other fluctuation-induced forces, such as the thermal Casimir effect. We expect these results will be relevant to other studies of pinned particles near the glass transition [1]. The dependence of the long-ranged force on packing fraction, particle separation, and the size ratio of pinned to free particles will be discussed.

P1.00055 “Anti-Equilibrium”: The limiting frozen state of kappa distributions. GEORGE LIVADIOTIS, Southwest Research Institute, USA — The kappa distribution of particle velocities provides an unambiguous replacement of the Maxwell distribution for systems out of thermal equilibrium. The kappa index is a measure of how far the system of particles is from thermal equilibrium. This “thermodynamic distance” is inversely proportional to the kappa index; it becomes zero at thermal equilibrium where the kappa index is infinite, while it obtains its maximum at the furthest state from thermal equilibrium, where the kappa index is zero, a state called “anti-equilibrium.” By keeping fixed the temperature and decreasing the kappa index, the particles approach this peculiar state of anti-equilibrium and are characterized by a power-law distribution density with spectral index $\sim 1.5$; this constitutes a universal behavior, independent of the system’s number of particles or degrees of freedom. As the kappa decreases and the system approaches the anti-equilibrium state, the particles lose their kinetic energy. This procedure of “kappa-freezing” by decreasing the kappa index at a fixed temperature is similar to the more familiar freezing procedure of decreasing temperature and approaching the “absolute zero” for a fixed kappa index.

P1.00056 The price of anarchy is maximized at the percolation threshold. BRIAN SKINNER, Argonne National Laboratory — When many independent users try to route traffic through a network, the flow can easily become suboptimal as a consequence of congestion in the most efficient paths. The degree of this suboptimality is quantified by the so-called “price of anarchy” (POA), but so far there are no general rules for when to expect a large POA in a random network. Here I address this question by introducing a simple model of flow through a network with randomly-placed “congestible” and “incongestible” links. I show that the POA is maximized precisely when the fraction of congestible links matches the percolation threshold of the lattice. Both the POA and the total cost demonstrate critical scaling near the percolation threshold.

P1.00057 Four Parameter Characterization of Network Reliability and Analysis of Critical Point Phenomenology. MADHURIMA NATH, STEPHEN EUBANK, MINA YOUSSEF, YASAMIN KHORRAMZADEH, SHAHIR MOWLAEI, Virginia Tech — A new characterization of network structure as represented by the reliability polynomial is introduced that requires only four parameters. Exact evaluation of the polynomial is not feasible for large graphs. Approximation to within a specified error is feasible, but a complete specification of the polynomial still requires many parameters. However, it turns out that a two-parameter family of functions fits the non-trivial part of the reliability polynomial to within approximation error. We demonstrate this by fitting the reliability polynomials of both random graphs with different sizes and synthetic social networks to the error function. The network reliability can be viewed as a partition function of a physical system, for example percolation on a network. This method produces a good analytical approximation to the partition function for a given network and suggests a way to explore critical point phenomenology.

P1.00058 Diffusion theory of Brownian particles moving at constant speed in D dimensions. FRANCISCO J. SEVILLA, Instituto de Física, Universidad Nacional Autónoma de México — The propagation of Brownian-active particles that move at constant speed in the limit of short times, differs from wave-like propagation in that active particles propagate without leaving a wake trailing characteristic of wave propagation in even dimensions. In the long time regime, normal diffusion is expected due to random fluctuations that disperse the particle direction of motion. A phenomenological equation that describe the transition from the behavior free of effects of wake, to the normal diffusion of the particles is proposed. A comparison of the results predicted by such equation with those obtained from models using Langevin equations is presented in the spherically symmetric case.

P1.00059 ABSTRACT WITHDRAWN

P1.00060 Nature of the Congested Traffic and Quasi-steady States of the General Motor Models. BO YANG, Institute of High Performance Computing, XIHUA XU, National University of Singapore, JOHN Z.F. PANG, CHRISTOPHER MONTOROLA, Institute of High Performance Computing — We look at the general motor (GM) class microscopic traffic models and analyze some of the universal features of the (multi-)cluster solutions, including the emergence of an intrinsic scale and the quasisoliton dynamics (arXiv:1407.3177). We show that the GM models can capture the essential physics of the real traffic dynamics, especially the phase transition from the free flow to the congested phase, from which the wide moving jams emerges (the F-S-J transition pioneered by B.S. Kerner). In particular, the congested phase can be associated with either the multi-cluster quasi-steady states, or their more homogeneous precursor states. In both cases the states can last for a long time, and the narrow clusters will eventually grow and merge, leading to the formation of the wide moving jams. We present a general method to fit the empirical parameters so that both quantitative and qualitative macroscopic features can be reproduced with a minimal GM model. We present numerical results for the traffic dynamics both with and without the bottleneck, including various types of spontaneous and induced “synchronized flow,” as well as the evolution of wide moving jams. We also discuss its implications to the nature of different phases in traffic dynamics.

P1.00061 New Analysis Techniques for Avalanches in a Conical Bead Pile with Cohesion. CATHERINE TIEMAN, SUSAN LEHMÁN, Department of Physics, College of Wooster, Wooster, OH — Avalanche statistics and pile geometry for 3 mm steel spheres dropped on a conical bead pile were studied at different drop heights and different cohesion strengths. The pile is initially built on a circular base and is subsequently slowly driven by adding one bead at a time to the apex of the pile. We investigate the dynamic response of the pile by recording avalanches off the pile over the course of tens of thousands of bead drops. The level of cohesion is tuned through use of an applied uniform magnetic field. Changes in the pile mass and geometry were investigated to determine the effect of cohesion and drop height on the angle of repose. The angle of repose increased with cohesion strength, and decreased somewhat for higher drop heights. The packing density of beads is expected to decrease as magnetic cohesion increases, but for our 20 000-bead pile, this effect has not been observed. The proportion of beads removed from the pile by different avalanche sizes was also calculated. Although larger avalanches are much rarer occurrences, they carry away a larger fraction of the total avalanche mass than small avalanches. As the pile cohesion increases, the number of small and medium avalanches decreases so that this mass loss distribution shifts more strongly to large sizes.
P1.00062 Use of a magnetic field to modify and detect avalanche behavior on a conical bead pile. NATHAN JONATHAN, SUSAN LEHMAN, Department of Physics, College of Wooster, Wooster, OH — A conical bead pile subject to slow driving and an external magnetic field is used to test the effects of drop height and cohesion on avalanche statistics. Magnetically susceptible beads were dropped onto a pile from different heights and into different strengths of magnetic field. Avalanches were recorded by the change in mass as beads fall off the pile. For beads dropped from a low drop height with no cohesion, the avalanche size distribution follows a power law. As cohesion increases, we observe an increase in the probability of very large avalanches and decreases in the mid-size avalanches. The resulting bump in the avalanche distribution moves to larger avalanche size as the cohesion in the system is increased, matching the prediction by an analytic theory from a mean-field model of slip avalanches. The model also makes predictions for avalanche duration, which is not measurable with our current system. Since the steel beads are magnetized while in the applied magnetic field, their motion during an avalanche creates a change in magnetic field. To detect this motion, we have placed a large-diameter pick-up coil around the pile. Results of the testing and calibration of this coil to measure avalanche duration are presented.

P1.00063 Granular gas mediated attraction of intruders in a granular Casimir effect. GEORGE WILKES, BRIAN UTTER, James Madison University — When two objects are submerged in a granular gas, entropic effects due to inelastic collisions lead to attractions between the objects. This has been referred to as an analog to the Casimir effect, though arises via a different mechanism. In this experiment, we place two objects (such as vertical plates or spheres) in either a strongly driven granular gas or dense fluid. We find that when the plates are closely spaced, there is a net attractive force. By analyzing high-speed video, we track the distance between these plates and characterize the effective force versus distance with changes in the vibration parameters and initial separation. A 2D simulation is also used to further explore parameter space.

P1.00064 Fingerprinting in Confined Elastic Layers. JOHN BIGGINS, University of Cambridge, L. MAHADEVAN, Harvard, Z. WEI, Stanford, BAUDOUIN SAINTYVES, Harvard, ELIZABETH BOUCHAUD, Commissariat à l’énergie atomique et aux énergies alternatives — Fingerprinting has recently been observed in soft highly elastic layers that are confined between and bonded to two rigid bodies. In one case an injected fluid invades the layer in finger-like protrusions at the layer’s perimeter, a solid analogue of Saffman-Taylor viscous fingering. In a second case, separation of the rigid bodies (with maintained adhesion to the layer) leads air to the formation of similar fingers at the layer’s perimeter. In both cases the finger formation is reversible: if the fluid is removed or the separation reduced, the fingers vanish. In this talk I will discuss a theoretical model for such elastic fingers that shows that the origin of the fingers is large-strain geometric non-linearity in the elasticity of soft solids. Our simplified elastic model unifies the two types of fingerprinting and accurately estimates the amplitudes and wavelengths of the fingers.

P1.00065 Non-equilibrium relaxation between two quasi-stationary states in a stochastic lattice Lotka-Volterra model. SHENG CHEN, UWE C. TÄUBER, Department of Physics, Virginia Tech — Spatially extended stochastic models for predator-prey competition and coexistence display complex, correlated spatio-temporal structures and are governed by remarkably large fluctuations. Both populations are characterized by damped erratic oscillations whose properties are governed by the reaction rates. Here, we specifically study a stochastic lattice Lotka-Volterra model by means of Monte Carlo simulations that impose spatial restrictions on the number of occupants per site. The system tends to relax into a quasi-stationary state, independent of the imposed initial conditions. We investigate the non-equilibrium relaxation between two such quasi-stationary states, following an instantaneous change of the predation rate. The ensuing relaxation times are measured via the peak width of the population density Fourier transforms. As expected, we find that the initial state only influences the oscillations for the duration of this relaxation time, implying that the system quickly loses any memory of the initial configuration.

P1.00066 Implications of lack-of-ergodicity in 2D Potts model. SMITA OTA, None — Microcanonical Monte Carlo simulation is used to study two dimensional (2D) q state Potts model. We consider a 2D square lattice having N x N spins with periodic boundary condition and simulated the system with N=15 and q=10. The demon energy distribution is found to be exponential for high system energy and large system size. For smaller system size and above the first order transition the demon energy distribution is found to deviate from exp(-βE_d) and has the form exp(-βE_d + γD^2). Here γ = 1/k_B T and k_B is the Boltzmann constant. It is found that γ is finite at higher temperatures. As the system energy is reduced γ becomes zero near the first order transition. It is found that during cooling γ changes sign from negative to positive and then to negative again near the 1st order transition. Therefore the demon energy distribution becomes exp(-βE_p) (or ergodic) at two values of system energy near the 1st order transition. Further cooling or at still lower temperatures the system shows lack of ergodicity. However, difference in heating cooling curves are apparent in E vs γ. The system energies for which γ is zero during cooling can represent the ‘ergodic’ states. This can be related to the two-level systems observed in glasses at low temperatures.


P1.00068 Static and Dynamic Finite-Size Scaling for Kuramoto Model with Generalized Form of Unimodal Natural Frequency Distribution. CHULHO CHOI, HYUNGYU PARK, Korea Inst for Advanced Study, KIAS TEAM — Synchronization phase transitions of collective phase oscillators have been studied actively for decades. The natural frequency distribution p(ω) of oscillators plays an important role in determining the phase transition’s types, properties and its universality class. Kuramoto model, a basic framework for synchronization, with unimodal and symmetric natural frequency distribution exhibits a second-order phase transition with critical exponent β = 1/2 whereas uniform distribution or bimodal and symmetric distribution make it a first-order phase transition, i.e., β = 0. We present a case in which β has other values than 1/2 or 0 even though it still has a unimodal natural frequency distribution and generalize it to obtain any values of β as we want. Therefore, we need to describe the unimodality more precisely. As a result, the critical exponent β and dynamic exponent α also have different values than the known values. We derive those exponents analytically and confirm them using static and dynamic finite-size scaling in numerical simulation.
P1.00069 Signatures of the Berezinskii-Kosterlitz-Thouless transition on the zeros of the canonical partition function for the 2D XY-model. JULIO ROCHA, LUCAS MOL, BISMARCK COSTA, Universidade Federal de Minas Gerais — In this work we show that the canonical partition function zeros, the Fisher zeros, can be used to uniquely characterize a transition as being in the Berezinskii-Kosterlitz-Thouless (BKT) class of universality. By studying the zeros map for the 2D XY model we found that its internal border coalesces into the real positive axis in a finite region corresponding to temperatures smaller than the BKT transition temperature. This behavior is consistent with the predicted existence of a line of critical points below the transition temperature, allowing one to distinguish the BKT class of universality from other ones.

1This work was partially supported by CNPq and Fapemig, Brazilian Agencies.

P1.00070 Nonlinear dynamics of three gravitating rods. ZIYI SANG, JOHN LINDNER, The College of Wooster — As a generalization of Newton’s three body problem, we explore the dynamics of three massive line segments interacting gravitationally. The extension of each line segment or slash (/) provides extra degrees of freedom that enable the interplay between rotation and revolution in an especially simple example while still elucidating the dynamics of non spherical objects like asteroids and space stations. Fortunately, Newton’s laws imply exact algebraic expressions for the force and torque between the slashes, and this greatly facilitates analysis of this slash-slash-slash (///) body problem. We provide exact solutions to several symmetrical orbits and numerically study three slashes moving in a figure-8 orbit.

P1.00071 Balancing Newtonian gravity and spin to create localized structures. MICHAEL BUSH, JOHN LINDNER, The College of Wooster — Using geometry and Newtonian physics, we design localized structures that do not require electromagnetic or other forces to resist implosion or explosion. In two-dimensional Euclidean space, we find an equilibrium configuration of a rotating ring of massive dust whose inward gravity is the centripetal force that spins it. We find similar solutions in three-dimensional Euclidean and hyperbolic spaces, but only in the limit of vanishing mass. Finally, in three-dimensional Euclidean space, we generalize the two-dimensional result by finding an equilibrium configuration of a spherical shell of massive dust that supports itself against gravitational collapse by spinning isoclinically in four dimensions so its three-dimensional acceleration is everywhere inward. These Newtonian “atoms” illuminate classical physics and geometry.

P1.00072 BIOLOGICAL PHYSICS —

P1.00073 Single-molecule optical study of cholesterol-mediated dimerization process of EGFRs in different cell lines. CHIEN YU LIN, JUNG Y. HUANG, Department of Photonics, Chiao Tung University, LEU-WEI LO, Institute of Biomedical Engineering and Nanomedicine, National Health Research Institutes — A growing body of data reveals that the membrane cholesterol molecules can alter the signaling pathways of living cells. However, the understanding about how membrane cholesterol modulates receptor proteins remains lacking. In this study we applies single-molecule optical tracking on ligand-induced dimerization process of EGFRs in the plasma membranes of several cancer and normal cell lines. We tracked individual EGFR and dual correlated receptors in the plasma membranes of live cells. We developed an energetic model based on the generalized Langevin equation and the Cahn-Hilliard equation to help extracting information from single-molecule trajectories. From the study, we discovered that ligand-bound EGFRs move from non-raft areas into lipid raft domains. This ligand-induced motion is a common behavior for all cell lines under study. By manipulating the total amount of cholesterol with methyl-β-cyclodextrin and the local concentration of cholesterol with nystatin, we found that the amount of cholesterol can affect the stability of EGFR dimers. The EGFR dimers in the plasma membrane of normal cells are more sensitive to the local concentration changes of cholesterol than EGFR dimers in the cancer cells.

P1.00074 Conformational transitions of plasmid ds-DNA on ultrathin films of alkylamines on graphite. CAROLINE FALK, HUA LIANG, NIKOLAI SEVERIN, WEI ZHUANG, Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, STEFAN ZAUSCHER, Mechanical Engineering and Materials Science, Duke University, JÜRGEN P. RABE, Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin — DNA replication is an important process in the human body. Replication of double-stranded (ds)-DNA requires its local melting into two single strands [1]. DNA, when stretched in solution, overwinds and melts [2]. This was argued to give insight onto the replication mechanism. It is difficult, however, to access the direct conformational changes during stretching in solution. Recent work demonstrated that this transition can be imaged with scanning force microscopy on a graphite surface that is coated with an alkylamine layer [3]. ds-DNA can be controlled by an amphiphilic layer, since the DNA conformation depends on the amphiphile concentration. In particular we analyzed different DNA lengths on the same surface, and we found that at a specific concentration of octadecylamine the ds-DNA pUC19 plasmid ring splits into two single strands at one position. We will discuss methods to mark the DNA to determine the exact location at which the plasmid rings split.


P1.00075 Modification of protein structure and function using photoactivated porphyrin ligands. GABRIEL MORENO, University of Texas at San Antonio — The tremendous advances in genomic research have sparked an interest in investigating the possibility to “manipulate” the structure of proteins that modify existing functionality. This study makes use of small molecules (e.g., porphyrins) to photosensitize proteins and modify the higher order structure of the polypeptide with the goal of engineering novel functions, or affecting/eliminating native functions. The irradiation of non-covalently bound ligands prompts charge transfer events that have the potential to locally modify the structure of the host protein. The characterization of photinduced conformational changes in the protein/porphyrin complex is carried out using a combination of electronic spectroscopy and kinetics (e.g., fluorescence spectroscopy, fluorescence decay, circular dichroism). This study is focused primarily on human serum albumin (HSA) as a model. The structure of HSA is well established, the binding sites for an array of ligands are well characterized (including one for protoporphyrins), and HSA provides a series of functions (including some allosteric activity) that can be tested.

P1.00076 Bacterial Chemotaxis with a Moving Target. COREY DOMINICK, Univ of Pittsburgh — Most chemotaxis studies so far have been conducted in a quiescent fluid with a well-defined chemical gradient. Such experiments may be appropriate for studying enteric bacteria, such as Escherichia coli, but the environment it provides is very different from that typically encountered by marine bacteria. Herein we describe an experiment in which marine bacterium Vibrio alginolyticus is subject to stimulation by a small moving target. A micropipette of the tip size <1 μm is used to slowly release a chemoattractant, serine, at different concentrations. The pipette is moved to make different patterns and speeds, ranging from 0 to 100 μm/s; the latter is about twice the bacterial swimming speed. We found that if the pipette is moved slowly, with 1/4 of bacterial swimming speed, cells accumulate near the tip region but when it is moved with speed greater than 1/2 the bacterial swimming speed, cells trail behind the pipette over a large distance. The behaviors observed in V. alginolyticusare significantly different from E. coli, suggesting that the former is a better chemotaxer in a changing environment.
P1.00077 Bacterial Growth in Weak Magnetic Field . SAMINA MASOOD, University of Houston Clear Lake — We study the growth of bacteria in a weak magnetic field. Computational analysis of experimental data shows that the growth rate of bacteria is affected by the magnetic field. The effect of magnetic field depends on the strength and type of magnetic field. It also depends on the type of bacteria. We mainly study gram positive and gram negative bacteria of rod type as well as spherical bacteria. Preliminary results show that the weak magnetic field enhances the growth of rod shape gram negative bacteria. Gram positive bacteria can be even killed in the inhomogeneous magnetic field.

P1.00078 Phase Transitions in the Nucleus: the functional implications of concentration-dependent assembly of a Liquid-like RNA/Protein Body . AMILA ARIYARATNE, University of California Los Angeles, CHENHAO WU, University of California, Irvine. We explore enzyme conformational dynamics at sub - A resolution, specifically temperature effects. The ensemble averaged mechanical response of the folded enzyme is viscoelastic in the whole temperature range between the warm and cold denaturation transitions. The dissipation parameter γ of the viscoelastic description decreases by a factor 2 as the temperature is raised from 10 °C to 45 °C; the elastic parameter K also show, qualitatively, a small softening for increasing temperature. Equilibrium mechanical experiments with the DNA spring (and a different enzyme) also show, qualitatively, a small softening for increasing temperature.

P1.00079 Kinesin-1 Translocation along Human Breast Cancer Cell Microtubules in Vitro . MITRA SHOJANIA FEIZABADI, Physics Department, Seton Hall University, YONGGUN JUN, Developmental and Cell Biology, School of Biological Sciences, University of California, Irvine, CA — A principle approach to better understand intra-cellular microtubule based transport is to study such in vitro. Such in vitro examinations have predominantly used microtubules polymerized from bovine brain tubulin, but motor function can also in principle be affected by the specific tubulin isotypes present in different cells. The human breast cancer cells carry different beta tubulin isotype distribution. However, it is entirely unknown whether transport along the microtubules is different in these cells. In this work we have characterized, for the first time, the translocation specifications of kinesin-1 along human breast cancer cell microtubules polymerized in vitro. We found that as compared with the translocation along bovine brain microtubules, kinesin-1 shows a fifty percent shorter protractive run length and slightly longer velocity under similar experimental conditions. These first time results support the regulatory role of tubulin isotypes in regards to motor protein translocations, and quantify the translocation specifications of kinesin-1 along microtubules of human breast cancer cells.

P1.00080 Dissipative Dynamics of Enzymes , AMILA ARRIYARATNE, University of California Los Angeles, CHENHAO WU, University of California San Diego, CHIAO-YU TSENG, GIOVANNI ZOCCHI, University of California Los Angeles, ZOCCHI LAB FOR MOLECULAR BIOPHYSICS TEAM — We explore enzyme conformational dynamics at sub - A resolution, specifically temperature effects. The ensemble averaged mechanical response of the folded enzyme is viscoelastic in the whole temperature range between the warm and cold denaturation transitions. The dissipation parameter γ of the viscoelastic description decreases by a factor 2 as the temperature is raised from 10 °C to 45 °C; the elastic parameter K shows a similar decrease. Thus when probed dynamically, the enzyme softens for increasing temperature. Equilibrium mechanical experiments with the DNA spring (and a different enzyme) also show, qualitatively, a small softening for increasing temperature.

P1.00081 Effects of solvent (effective medium versus explicit) on the structure of a protein (H3.1) . RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Structure and dynamics of a histone (H3.1) are studied in the presence of effective medium and explicit solvent over a range of temperatures with coarse-grained Monte Carlo simulations. The protein is represented by a coarse-grained chain of residues whose interactions are described by knowledge-based residue-residue and hydrophathy-index-based residue-solvent interactions. Each empty lattice site acts as a solvent in effective medium while a fraction of sites are occupied by mobile solvent constituents in explicit solvent medium. The presence of fluctuations with explicit solvent may affect the structure and dynamics of protein differently than that in effective solvent medium. Large scale simulations are performed to analyze the structure of the protein for a range of residue-solvent interactions and temperature, and a number of local and global physical quantities are analyzed. Differences due to type of solvent on the response of some of these quantities as a function of temperature will be presented.

P1.00082 ABSTRACT WITHDRAWN –

P1.00083 ABSTRACT WITHDRAWN –

P1.00084 Effect of Nanodiamond Surfaces on tRNA Dynamics Studied by Neutron Scattering and MD Simulations . GURPREET DHINDSA, DEBSINDHU BHOWMIK, Wayne State University, PANCHAPAKESAN GANESH, MONOJOY GOSWAMI, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, VADYN M. MOCHALIN, Drexel University, HUGH O’NEILL, Biology and Soft Matter Division, Oak Ridge National Laboratory, USA, YURY GOGOTSI, Drexel University, EUGENE MAMONTOV, SNS OakRidge National Laboratory, USA, XIANG QIANG CHU, Wayne State University — Nanodiamond (ND) inherits most of the superior properties of bulk diamond and delivers them at the nanoscale. ND is non-toxic and possesses excellent mechanical and optical properties with large surface area and surface functionality. ND mixed with biomolecules can be a good platform for drug delivery. Here we demonstrate the adsorption of tRNA on the ND surface and investigate the change in the tRNA dynamics using neutron scattering technique and molecular dynamics (MD) Simulations. We compare the dynamics of hydrated tRNA on ND surfaces with that of freestanding hydrated tRNA molecules and dry tRNA on ND surfaces. Both experiments and simulations show that the relaxational dynamics of tRNA on ND surface is faster than that of the freestanding tRNA molecules and dry tRNA on ND surfaces. Our results suggest that the tRNA on the ND surfaces has fewer hydration water molecules on it due to the water adsorption on the ND hydrophilic surface. Therefore fewer hydrogen bonds formed on its surface results in the tRNA faster motion. The MD simulations also show a “caged” dynamics of the water molecules adsorbed on the ND surfaces.

P1.00085 Fast loop modeling for protein structures1 . JIONG ZHANG, SON NGUYEN, YI SHANG, DONG XU, IOAN KOSZTIN, University of Missouri — X-ray crystallography is the main method for determining 3D protein structures. In many cases, however, flexible loop regions of proteins cannot be resolved by this approach. This leads to incomplete structures in the protein data bank, preventing further computational study and analysis of these proteins. For instance, all-atom molecular dynamics (MD) simulation studies of structure-function relationship require complete protein structures. To address this shortcoming, we have developed and implemented an efficient computational method for building missing protein loops. The method is database driven and uses deep learning and multi-dimensional scaling algorithms. We have implemented the method as a simple stand-alone program, which can also be used as a plugin in existing molecular modeling software, e.g., VMD. The quality and stability of the generated structures are assessed and tested via energy scoring functions and by equilibrium MD simulations. The proposed method can also be used in template-based protein structure prediction.

1Work supported by the National Institutes of Health [R01 GM100701]. Computer time was provided by the University of Missouri Bioinformatics Consortium.
P1.00086 Bio-inspired metal-coordination dynamics: A unique tool for engineering novel properties in soft matter systems. SCOTT GRINDY, QIAOCHU LI, ABIGAIL HALIM, ROBERT LEARSC, NIELS HOLSEN-ANDERSEN, Massachusetts Inst of Tech-MIT — In soft material systems, material properties are generally governed by transient, dynamic interactions of many types over many hierarchical length- and time-scales. However, explicit control over these dynamics is not always possible, leaving open questions into how transient interactions can be exploited to design soft materials with unique and exceptional properties. Inspired by the adhesive chemistry and tough character of mussel byssal threads, we present several studies on both the mechanical properties of soft materials and templated crystallization kinetics to show the diverse array of materials properties that can be generated using bio-inspired metal-coordination. By studying our model systems, we can determine the explicit effects of metal-coordination dynamics on various bulk properties, further adding to the set of tools we can use to design soft material systems.

P1.00087 Examining the role of finite reaction times in swarming models KATHERINE COPENHAGEN, University of California Merced, DAVID QUINT, Stanford University, AJAY GOPINATHAN, University of California Merced — Modeling collective behavior in biological and artificial systems has had much success in recent years at predicting and mimicking real systems by utilizing techniques borrowed from modeling many particle systems interacting with physical forces. However unlike inert particles interacting with instantaneous forces, living organisms have finite reaction times, and behaviors that vary from individual to individual. What constraints do these physiological effects place on the interactions between individuals in order to sustain a robust ordered state? We use a self-propelled agent based model in continuous space based on previous models by Vicsek and Couzin including alignment and separation maintaining interactions to examine the behavior of a single cohesive group of organisms. We found that for very short reaction times the system is able to form an ordered state even in the presence of heterogeneities. However for larger more physiological reaction times organisms need a buffer zone with no cohesive interactions in order to maintain an ordered state. Finally swarms with finite reaction times and behavioral heterogeneities are able to dynamically sort out individuals with impaired function and sustain order.

P1.00088 High Intensity Pressure Noise Transmission in Human Ear: A Three Dimensional Simulation Study†, TAKUMI HAWA, RONG GAN, KEGAN LECKNESS, The University of Oklahoma — High intensity pressure noise generated by explosions and jet engines causes auditory damage and hearing loss of the military service personal, which are the most common disabilities in the veterans. Authors have investigated the high intensity pressure noise transmission from the ear canal to middle ear cavity. A fluid-structure interaction with a viscoelastic model for the tympanic membrane (TM) as well as the ossicular chain has been considered in the study. For the high intensity pressure simulation the geometry of the ear was based on a 3D finite element (FE) model of the human ear reported by Gan et al. (Ann Biomed Eng 2004). The model consists of the ear canal, TM, ossicular chain, and the middle ear cavity. The numerical approach includes two steps: 1) FE based finite-volume method simulation to compute pressure distributions in the ear canal and the middle ear cavity using CFX; and 2) FE modeling of TM and middle ear ossicles in response to high intensity sound using multi-physics analysis in ANSYS. The simulations provide the displacement of the TM/ossicular chain and the pressure fields in the ear canal and the middle ear cavity. These results are compared with a human temporal bone experimental data obtained in our group.

† This work was supported by DOD W81XWH-14-1-0228

P1.00089 Computational Characterization of Type I collagen-based Extra-cellular Matrix†, LONG LIANG, Department of Physics, Arizona State University, CHRISTOPHER ALLEN RUCKSACK JONES, DANIEL LIN, Department of Physics, Oregon State University, YANG JIAO, Department of Materials Science and Engineering, Arizona State University, BO SUN, Department of Physics, Oregon State University — A model of extracellular matrix (ECM) of collagen fibers has been built, in which cells could communicate with distant partners via fiber-mediated long-range-transmitted stress states. The ECM is modeled as a spring-like fiber network derived from skeletonized confocal microscopy data. Different local and global perturbations have been performed on the network, with the network followed by an optimized global Monte-Carlo (MC) energy minimization leading to the deformed network in response to the perturbations. In the optimization, a highly efficient local energy update procedure is employed and force-directed MC moves are used, which results in a convergence to the energy minimum state 20 times faster than the commonly used random displacement trial moves in MC. Further analysis and visualization of the distribution and correlation of the resulting force network reveal that local perturbations can give rise to global impacts: the force chains formed with a linear extent much further than the characteristic length scale associated with the perturbation sites and average fiber length. This behavior provides a strong evidence for our hypothesis of fiber-mediated long-range force transmission in ECM networks and the resulting long-range cell-cell mechanical signaling.

† ASU Seed Grant

P1.00090 Hidden Markov models for the analysis of single particle trajectories containing multiple mobile states. DYLAN YOUNG, JAN SCRIMGEOUR, Clarkson Univ — Single particle tracking offers significant insight into the molecular mechanics that govern the behavior of living cells. The analysis of trajectories that transition between different motive states, such as diffusive, driven and tethered modes, is of considerable importance, with even single trajectories containing significant amounts of information about a molecule’s environment and its interactions with structures such as the cell cytoskeleton, membrane or extracellular matrix. Traditional analysis of particle trajectories has relied heavily on evaluation of the mean squared displacement, but often struggles to extract information reliably from small quantities of data or when multiple mobile states are present. Here, we present hidden Markov models for the analysis of complex multi-mobility tracks, focusing on transitions between states exhibiting free diffusion and either driven or tethered motion. The models were tested using simulated trajectories and practical limitations on the track length and state switching probabilities needed for accurate extraction of the physical parameters in the model are identified. These results provide critical information for the design of particle tracking experiments where trajectories containing multiple mobile states are expected.

P1.00091 A theoretical analysis of inferring molecular interactions from single particle trajectories†, ZIYA KALAY, Kyoto University — Single molecule/particle tracking has become a valuable tool in microscopy that allows for recording trajectories of probes such as individual biological molecules with high temporal and spatial resolution. With the trajectory of a particle, mesoscale transport properties such as diffusion coefficients and first-passage times can be calculated. With the trajectories of two particles that interact, we can investigate the kinetics of reactions by analyzing the statistics of overlap between trajectories. This approach is useful for single molecule biophysics in exploring the kinetics of reversible binding among molecules in biological membranes and on the DNA. Nevertheless, extracting information from noisy trajectories, where the noise stems from a combination of thermal fluctuations and uncertainty introduced by measuring apparatus, is a challenging task. In this work, we consider an exactly solvable model of diffusion and reversible binding in a 1-D structure, such as the DNA, and present a mathematical analysis of how much information about the binding kinetics can be reliably extracted from experimental data. With insight gained from this low-dimensional model, we discuss the analysis of trajectory pairs in two-dimensional systems such as biological membranes.

†This research was supported by JSPS Grant-in-Aid for Young Scientists (B) (26730150)
P1.00092 Stochastic Movement of Multiple Motor Transported Cargo, DAVID ANDO, AJAY GOPINATHAN, JING XU, UC Merced — Experimental observations of cargo position during transport by multiple motors are determined by several coupled stochastic processes. During collective transport, each motor can transition between multiple kinetic states, with the state of each motor influencing the states of the others via mechanical coupling through a common cargo. We measured the motion of a micron sized bead as it is transported by two kinesin motors along a single microtubule track, focusing on cargo displacements which are both axial and transverse to the microtubule. We model the effects of inter-motor interference and the state of each motor throughout time, and back out motor properties using a systematic comparison of experimental observations with simulated model traces over a wide parameter space. Our model captures a surface-associated mode of kinesin, which is only accessible via inter-motor interference in groups, in which kinesin diffuses along the microtubule surface and rapidly “hops” between protofilaments without dissociating from the microtubule. This enhances local exploration of the microtubule surface, possibly enabling cellular cargos to overcome macromolecular crowding and to navigate obstacles along microtubule tracks without sacrificing overall travel distance.

P1.00093 Light, Imaging, Vision: An interdisciplinary undergraduate course1, PHILIP NELSON, Univ Pennsylvania — The vertebrate eye is a fantastically sensitive instrument, capable of registering the absorption of a single photon, and yet generating very low noise. Using eyes as a common thread helps motivate undergraduates to learn a lot of physics, both fundamental and applied to scientific imaging and neuroscience. I’ll describe an undergraduate course, for students in several science and engineering majors, that takes students from the rudiments of probability and the state of each motor throughout time, and back out motor properties using a systematic comparison of experimental observations with simulated model traces over a wide parameter space. Our model captures a surface-associated mode of kinesin, which is only accessible via inter-motor interference in groups, in which kinesin diffuses along the microtubule surface and rapidly “hops” between protofilaments without dissociating from the microtubule. This enhances local exploration of the microtubule surface, possibly enabling cellular cargos to overcome macromolecular crowding and to navigate obstacles along microtubule tracks without sacrificing overall travel distance.

1Work supported by NSF grants EF–0928048 and DMR–0832802.

P1.00094 A new course and textbook on Physical Models of Living Systems, for science and engineering undergraduates1, PHILIP NELSON, Univ Pennsylvania — I’ll describe an intermediate-level course on “Physical Models of Living Systems.” The only prerequisite is first-year university physics and calculus. The course is a response to rapidly growing interest among undergraduates in a broad range of science and engineering majors. Students acquire several research skills that are often not addressed in traditional courses:

- Basic modeling skills
- Probabilistic modeling skills
- Data analysis methods
- Computer programming using a general-purpose platform like MATLAB or Python
- Dynamical systems, particularly feedback control.

These basic skills, which are relevant to nearly any field of science or engineering, are presented in the context of case studies from living systems, including:

- Virus dynamics
- Bacterial genetics and evolution of drug resistance
- Statistical inference
- Superresolution microscopy
- Synthetic biology
- Naturally evolved cellular circuits.

1Work supported by NSF grants EF–0928048 and DMR–0832802.

P1.00095 Analytical framework for modeling of long-range transport of fungal plant epidemics, OLEG KOGAN, KEVIN O'KEEFFE, DAVID SCHNEIDER, CHRISTOPHER MYERS, Cornell University, ANALYTICAL FRAMEWORKS FOR INFECTIOUS DISEASES DYNAMICS TEAM — A new framework for the study of long-range transport of fungal plant epidemics is proposed. The null nonlinear model includes advective transport through the free atmosphere, spore production on the ground, and transfer of spores between the ground and the advective atmospheric layer. The competition between the growth wave on the ground and the effect of the wind is most strongly reflected in upwind fronts, which can propagate into the wind for exponential initial conditions. If the rate of spore transfer into the advective layer is below critical, this happens for initial conditions with arbitrary steepness. Upwind fronts from localized initial conditions will propagate in the direction of the wind above this critical parameter, and will not propagate below it. On the other hand, the speed of the downwind front does not have a strong dependence on the rate of spore transfer between the advective layer and the ground. Thus, even vanishingly small, but finite transfer rates result in a substantial epidemic wave in the direction of the wind. We also consider the effect of an additional, random-walk like mechanism of transport through the near-ground atmospheric boundary layer, and attempt to understand which route dominates the transport over long distances.

P1.00096 Interstitial flows promote an amoeboid cell phenotype and motility of breast cancer cells1, CHIH-KUAN TUNG, YU LING HUANG, ANGELA ZHENG, MINGMING WU, Department of Biological and Environmental Engineering, Cornell University — Lymph nodes, the drainage systems for interstitial flows, are clinically known to be the first metastatic sites of many cancer types including breast and prostate cancers. Here, we demonstrate that breast cancer cell morphology and motility is modulated by interstitial flows in a cell-ECM adhesion dependent manner. The average aspect ratios of the cells are significantly lower (or are more amoeboid like) in the presence of the flow in comparison to the case when the flow is absent. The addition of exogenous adhesion molecules within the extracellular matrix (type I collagen) enhances the overall aspect ratio (or are more mesenchymal like) of the cell population. Using measured cell trajectories, we find that the persistence of the amoeboid cells (aspect ratio less than 2.0) is shorter than that of mesenchymal cells. However, the maximum speed of the amoeboid cells is larger than that of mesenchymal cells. Together these findings provide the novel insight that interstitial flows promote amoeboid cell morphology and motility and highlight the plasticity of tumor cell motility in response to its biophysical environment.

1Supported by NIH grant R21CA138366
P1.00097 Robust Nonlinear Neural Codes\textsuperscript{1}. QIANLI YANG, Rice Univ, XAQ PITKOW, Rice Univ. Baylor College of Medicine — Most interesting natural sensory stimuli are encoded in the brain in a form that can only be decoded nonlinearly. But despite being a core function of the brain, nonlinear population codes are rarely studied and poorly understood. Interestingly, the few existing models of nonlinear codes are inconsistent with known architectural features of the brain. In particular, these codes have information content that scales with the size of the cortical population, even if that violates the data processing inequality by exceeding the amount of information entering the sensory system. Here we provide a valid theory of nonlinear population codes by generalizing recent work on information-limiting correlations in linear population codes. Although these generalized, nonlinear information-limiting correlations bound the performance of any decoder, they also make decoding more robust to suboptimal computation, allowing many suboptimal decoders to achieve nearly the same efficiency as an optimal decoder. Although these correlations are extremely difficult to measure directly, particularly for nonlinear codes, we provide a simple, practical test by which one can use choice-related activity in small populations of neurons to determine whether decoding is suboptimal or optimal and limited by correlated noise. We conclude by describing an example computation in the vestibular system where this theory applies.

\textsuperscript{1} QY and XP was supported by a grant from the McNair foundation.

P1.00098 Spatiotemporal discrimination in neural networks with short-term synaptic plasticity. BENJAMIN SHLAER, PAUL MILLER, Brandeis Univ. — Cells in recurrently connected neural networks exhibit bistability, which allows for stimulus information to persist in a circuit even after stimulus offset, i.e. short-term memory. However, such a system does not have enough hysteresis to encode temporal information about the stimuli. The biophysically described phenomenon of synaptic depression decreases synaptic transmission strengths due to increased presynaptic activity. This short-term reduction in synaptic strengths can destabilize attractor states in excitatory recurrent neural networks, causing the network to move along stimulus dependent dynamical trajectories. Such a network can successfully separate amplitudes and durations of stimuli from the number of successive stimuli\textsuperscript{[1]} and so provides a strong candidate network for the encoding of spatiotemporal information. Here we explicitly demonstrate the capability of a recurrent neural network with short-term synaptic depression to discriminate between the temporal sequences in which spatial stimuli are presented.

P1.00099 The Brain Physics: Multi Laser Beam Interaction with the Brain Topions (the Brain Neurocenters)\textsuperscript{2}. V. ALEXANDER STEFAN, Institute for Advanced Physics Studies, Stefan University, La Jolla, California 92037 — A novel method for the treatment of the neurological diseases is proposed. The multi-energy laser photon\textsuperscript{[1]} (the blue scanning photons and ultraviolet focusing photons) interact with the specific DNA molecules within the topion (such as Parkinson’s and Alzheimer’s brain topion) via the matching of laser frequency with the oscillation eigen-frequency of a particular molecule\textsuperscript{[1]} within the DNA\textsuperscript{[1]}. In this way, the corrupt molecules (the structure of molecules) can be manipulated so as to treat (eliminate) the neurological disease.

\textsuperscript{1} Supported by Nikola Tesla Labs, Stefan University.

\textsuperscript{2} V. Alexander Stefan, NEUROPHYSICS, STEM CELL PHYSICS, and GENOMIC PHYSICS: Beat-Wave-Driven-Free Electron Laser Beam Interactions with the Living Matter (S-U-Press, La Jolla, CA, 2012)

P1.00100 Network oscillations of inferior olive neurons: entrainment and phase-locking of locally-coupled oscillators. THOMAS CHARTRAND, MARK S. GOLDMAN, TIMOTHY J. LEWIS, University of California, Davis — Although the inferior olive is known to contribute to the generation of timing and error signals for motor control, the specific role of its distinctive spatiotemporal activity patterns is still controversial. Olfactory neurons display regular, sometimes synchronized oscillations of subthreshold membrane potential, driven in part by the highest density of electrical coupling of any brain region. We show that a reduced model of coupled phase oscillators is sufficient to reproduce and study experimental observations previously only demonstrated in more complex models. These include stable phase differences, variability of entrainment frequency, wave propagation, and cluster formation. Using the phase-response curve (PRC) of a conductance-based model of olivary neurons, we derive our phase model according to the theory of weakly-coupled oscillators. We retain the heterogeneity of intrinsic frequencies and heterogeneous, spatially constrained coupling as weak perturbations to the limit-cycle dynamics. Generalizing this model to an ensemble of coupled oscillator lattices with frequency and coupling disorder, we study the onset of entrainment and phase-locking as coupling is strengthened, including the scaling of cluster sizes with coupling strength near each phase transition.

P1.00101 Temporal Evolution Of Information In Neural Networks With Feedback\textsuperscript{1}. ARAM GIAHI SARAVANI, Baylor College of Medicine, XAQ PITKOW, Baylor College of Medicine/Rice University — Recurrent neural networks are pivotal for information processing in the brain. Here we analyze how the information content of a neural network is altered by dynamic feedback of a stimulus estimated from the network activity. We find that the temporal evolution of the Fisher information in the model with feedback is bounded by the Fisher information in a network of pure integrators. The available information in the feedback model saturates with a time constant and to a final level both determined by the match between the estimator weights and the feedback weights. This network then encodes signals specifically from either the beginning or the end of the stimulus presentation, depending on this match. These results are relevant to recent experimental measurements of psychophysical kernels indicating that earlier stimuli have a stronger influence on perceptual discriminations than more recent stimuli. We discuss consequences of this description for choice correlations, a measure of how individual neuronal responses relate to perceptual estimates.

\textsuperscript{1} McNair Foundation, Baylor College of Medicine, Rice University

P1.00102 ABSTRACT WITHDRAWN —

P1.00103 The Deterministic Information Bottleneck. D.J. STROUSE, Princeton University, DAVID SCHWAB, Northwestern University — A fundamental and ubiquitous task that all organisms face is prediction of the future based on past sensory experience. Since an individual’s memory resources are limited and costly, however, there is a tradeoff between memory cost and predictive payoff. The information bottleneck (IB) method (Tishby, Pereira, & Bialek 2000) formulates this tradeoff as a mathematical optimization problem using an information theoretic cost function. IB encourages storing as few bits of past sensory input as possible while selectively preserving the bits that are most predictive of the future. Here we introduce an alternative formulation of the IB method, which we call the deterministic information bottleneck (DIB). First, we argue for an alternative cost function, which better represents the biologically-motivated goal of minimizing required memory resources. Then, we show that this seemingly minor change has the dramatic effect of converting the optimal memory encoder from stochastic to deterministic. Next, we propose an iterative algorithm for solving the DIB problem. Additionally, we compare the IB and DIB methods on a variety of synthetic datasets, and examine the performance of retinal ganglion cell populations relative to the optimal encoding strategy for each problem.
P1.00104 Modeling the Kinetics of a Memory-Associated Immediate Early Gene's Compartmental Expression After Sensory Experience\textsuperscript{1}, ADAM WILLATS, Georgia Institute of Technology and Emory University: Dept. of Biomedical Engineering, TAMARA IVANOVA, ASTRID PRINZ, ROBERT LIU, Emory University: Dept. of Biology — Immediate Early Genes (IEGs) are rapidly and transiently transcribed in neurons after a sensory experience. Some of these genes act as effector IEGs, which mediate specific effects on cellular function. Arc is one such effector IEG that is essential for synaptic plasticity and memory consolidation in hippocampus and cortex. The expression of Arc in neurons has previously been examined using an imaging method known as Compartamental Analysis of Temporal Fluorescent In-Situ Hybridization. Previous work found that the time course of Arc expression within the nuclear and perinuclear cytoplasmic compartments of a neuron is altered by prior sensory experience. We explore a simple model of the kinetics of IEG transcription and nuclear export, with the aim of eventually uncovering possible mechanisms for how experience alters expression kinetics. Thus far, we characterize our compartmental model using phase-plane analysis and validate it against several IEG expression data sets, including one where prior experience with vocalizing mice alters the time course of call-induced Arc expression in the auditory cortex of a listening mouse. Our model provides a framework to explore why Arc expression may change depending on a receiver’s past sound experience and internal state.

\textsuperscript{1}Adam Willats was supported by NIH Training grant 5T90DA032466. This research was also supported by NIDCD R01 DC8343

P1.00105 The brain as a complex system: plasticity at multiple scales and criticality , TONY NG, PAUL MILLER, Brandeis University — As a complex system, a successful organism is one that can react effectively to environmental fluctuations. Not only should its response repertoire be commensurate with the number of independent conditions that it encounters, behavioral and environmental variations need to be matched at the appropriate scales. In the cortex, neuronal clusters, not individual cells, operate at the proper scale that is necessary to generate appropriate responses to external states of the world. Single neurons, however, serve on a finer scale to mediate interactions between neuronal assemblies. The distinction of scales is significant, as plasticity mechanisms can operate on various spatial and temporal scales. The brain has apparently evolved complex-system strategies to calibrate its own dynamics at multiple scales. This makes the joint study of local balance and global homeostasis fundamentally important, where criticality emerges as a signature of a computationally powerful system. We show via simulations how plasticity mechanisms at multiple scales are inextricably tied to spike-based neuronal avalanches, which are microscopic in origin and poorly predictive of animal behavior, and cluster-based avalanches, which are manifest macroscopically and are relevant to cognition and behavior.

P1.00106 Marginalization in Random Nonlinear Neural Networks , RAJKUMAR VASUDEVA RAJU, Rice University, XAQ PITKOW, Rice University, Baylor College of Medicine — Computations involved in tasks like causal reasoning in the brain require a type of probabilistic inference known as marginalization. Marginalization corresponds to averaging over irrelevant variables to obtain the probability of the variables of interest. This is a fundamental operation that arises whenever input stimuli depend on several variables, but only some are task-relevant. Animals often exhibit behavior consistent with marginalizing over some variables, but the neural substrate of this computation is unknown. It has been previously shown (Beck et al. 2011) that marginalization can be performed optimally by a deterministic nonlinear network that implements a quadratic interaction of neural activity with divisive normalization. We show that a simpler network can perform essentially the same computation. These Random Nonlinear Networks (RNN) are feedforward networks with one hidden layer, sigmoidal activation functions, and normally-distributed weights connecting the input and hidden layers. We train the output weights connecting the hidden units to the output population, such that the output model accurately represents a desired marginal probability distribution without significant information loss compared to optimal marginalization. Simulations for the case of linear coordinate transformations show that the RNN model has good marginalization performance, except for highly uncertain inputs that have low amplitude population responses. Behavioral experiments, based on these results, could then be used to identify if this model does indeed explain how the brain performs marginalization.

P1.00107 Investigating structural details of lipid-cholesterol-\(A_{\beta}\) interactions , DURGESH RAI, DIVINA ANUNCIADO, WILLIAM HELLER, HUGH O'NEILL, VOLKER URBAN, SHUO QIAN, Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Alzheimer's disease (AD) is the most common form of dementia and is predicted to affect 1 in 85 people around the world by 2050. Amyloid beta (A\(\beta\))-peptide, a peptide composed of 40–42 amino acids that is the product of cleavage from the amyloid precursor protein (APP), is regarded to play a major role in the development of AD. In addition, accumulating evidence points to a positive association between cholesterol and AD. Here, we present results from our studies about A\(\beta\)-peptide and cholesterol in bilayer by small-angle neutron scattering (SANS) using a combination of dimeristoyl, phosphocholine (DMPC) and partially deuterated cholesterol (cholesterol-d7) with and without A\(\beta\). We compare the results using gracing incidence and transmission SANS on lipid bilayer films and unilamellar vesicles respectively. The structural details on vesicles and bilayers work in conjunction with the circular dichroism on peptide in solution and oriented circular dichroism in bilayer films. The studies confirm a positive association of A\(\beta\) with the membrane layers. The results from different studies will be compared and contrasted in presentation.

P1.00108 Using Small Angle Neutron Scattering on Glucose Oxidase immobilized on Single Layer Graphene , DURGESH RAI, Oak Ridge National Lab, M. GURUSARAN, IISC Bangalore, S. QIAN, K. WEISS, V. URBAN, Oak Ridge National Lab, P. LI, Harvard Medical School, L. MA, P. AJAYAN, Rice University, T. NARAYANAN, TRIF Hyderabad, K. SEKAR, IISC Bangalore, S. VISWANATHAN, Newton Wellesley Hospital, V. RENU GOPALAKRISHANAN, Harvard Medical School — Reliable blood glucose monitoring using biosensors is valuable for health evaluations and medication in wake of chronic diabetic issues accompanying deviations from evolutionary human lifestyle. Glucose oxidase (GOx) is an ideal enzyme because of its specificity and the ability to electrochemically transduce from the enzymatic reaction. We use graphene-based electrode with GOx sensor matrix so that the emitted electrons from sensor matrix can flow across graphene nearly without scattering; crucial for constructing ultrasensitive-sensors. Thereafter, establishing a structure-property based relationships to tune the sensor topology with electrochemically output forms the main focus of the device development process. We have developed a methodology to obtain low-resolution hierarchical models of the aggregate matrix using Small Angle Neutron Scattering (SANS) technique. A Unified Fit model is used in tandem with GNOM, DAMMIN and DAMAVER to construct low-resolution models for GOx matrices. A detailed explanation of a general methodology for obtaining quantitative details aggregate structures along with qualitative models will be presented.

P1.00109 Interatomic Coulombic Decay Effects in Theoretical DNA Recombination Systems Involving Protein Interaction Sites\textsuperscript{1}, E.L. VARGAS, D.A. RIVAS, A.C. DUOT, R.T. HOVEY, V.M. ANDRIANARIAJONA, Department of Physics, Pacific Union College, Angwin, CA 94508 — DNA replication is the basis for all biological reproduction. A strand of DNA will “unzip” and bind with two complementary strands to create two new strands. In this study, we are considering how this process is affected by interactions for the enzyme DNA polymerase. Understanding how ICD affects DNA molecules can give us invaluable insight into the human genetic code and the processes behind cell mutations that can lead to cancer.

\textsuperscript{1}Authors wish to give special thanks to Pacific Union College Student Senate in Angwin, California, for their financial support.
P1.00110 Gramicidin Induce Local Non-Uniform Distribution of Lipids in Multi-Component Membrane Domains , YU MAO, FAZLE HUSSAIN, JUYANG HUANG, Texas Tech University — In lipid membranes, gramicidin form transmembrane channels that are specific for monovalent cations. We performed Molecular Dynamics simulations of gramicidin in coexisting liquid-ordered (Lo) and liquid disordered (Ld) domains using GROMACS. The lipid compositions of Lo and Ld domains are DOPC/DSPC/Cholesterol = 6.5/52.6/40.9 and 74.4/10.6/15, respectively. In the Ld domain, the membrane thickness matches the hydrophobic length of gramicidin quite well, and water molecules can diffuse through the gramicidin channels. However, in the Lo lipid domain, the bilayer thickness is far greater than the hydrophobic length of gramicidin and majority of gramicidin do not form conducting channel. The simulation result explained our experimental finding that gramicidin partition favorably into the Ld domains. The calculated radial distribution functions of lipids indicate that gramicidin recruit a layer of short DOPC surrounding each protein and keep cholesterol and taller DSPC away from the protein-bilayer interface. Our result indicates that membrane proteins are capable of inducing non-uniform distributions of lipids and creating a local bilayer environment, which favors protein function.

P1.00111 Directly mapping the surface charge density of lipid bilayers under physiological conditions , THOMAS FUHS, LASSE HYLDGAARD KLAUSEN, FLEMMING BESENBACKER, MINGDONG DONG, Interdisciplinary Nanoscience Center, Aarhus University, Denmark — The surface charge density of lipid bilayers governs the cellular uptake of charged particles and guides cell-cell and cell-surface interactions. Direct probing of the potential requires sub nanometer distances as the electrostatic potential is screened by high physiological salt concentrations. This prevented direct measurement of the SCD under physiological conditions. In this study we investigate supported bilayers of lipid mixtures that form domains of distinct surface charges, submerged in 150mM NaCl. We use a scanning ion-conductance microscope (SCM) setup to measure the ionic current through a nanopipette as the pipette is scanned several nanometers above the sample. The charged headgroups of the lipids attract counter ions leading to a charge dependent enhancement of the ion concentration near the surface. This creates a measurable change of conductivity in the vicinity of the surface. As the dependency of the current on the SCD and pipette potential is non-trivial we characterized it using numerical solutions to Poisson and Nernst-Planck equations. Based on the simulation results we propose an imaging method. We confirm feasibility of the proposed method by experimentally mapping the local surface charge density of phase separated lipid bilayers.

P1.00112 Lipid mobility in supported lipid bilayers by single molecule tracking, MARYAM KOHRAM, University of Akron, Department of Physics, XIAOJUN SHI, ADAM SMITH, University of Akron, Department of Chemistry — Phospholipid bilayers are the main component of cell membranes and their interaction with biomolecules in their immediate environment is critical for cellular functions. These interactions include the binding of polycationic polymers to lipid bilayers which affects many cell membrane events. As an alternative method of studying live cell membranes, we assembled a supported lipid bilayer and investigate its binding with polycationic polymers in vitro by fluorescently labeling the molecules of the supported lipid bilayer. To study the internal mobility of labeled lipids by utilizing single molecule tracking total internal reflection fluorescence microscopy (TIRF) to study phosphatidylinositol phosphate (PIP) lipids with and without an adsorbed polycationic polymer, quaternized polyvinylpyridine (QPVP). Individual molecular trajectories are obtained from the experiment, and a Brownian diffusion model is used to determine diffusion coefficients through mean square displacements. Our results indicate a smaller diffusion coefficient for the supported lipid bilayers in the presence of QPVP in comparison to its absence, revealing that their binding causes a decrease in lateral mobility.

P1.00113 Nanoparticle size and shape characterization with Solid State Nanopores, SANTOSHI NANDIVADA, MOURAD BENAMARA, JIALI LI, University of Arkansas — Solid State Nanopores are widely used in a variety of single molecule studies including DNA and biomolecule detection based on the principle of Resistive Pulse technique. This technique is based on electrophoretically driven charged particles through 35-60 nm solid state nanopores. The translocation of these particles produces current blockage events that provide an insight to the properties of the translocation particles and the nanopore. In this work we study the current blockage events produced by ~ 30nm negatively charged PS nanoparticles through Silicon Nitride solid state nanopores. We show how the current blockage amplitudes and durations are related to the ratio of the volume of the particle to the volume of the pore, the shape of the particle, charge of the particle and the nanopore surface, salt concentration, solution pH, and applied voltage. The solid-state nanopores are fabricated by a combination of Focus Ion Beam and low energy Ion beams in silicon nitride membranes. High resolution TEM is used to measure the 3D geometry of the nanopores and a finite element analysis program (COMSOL) is used to simulate the experimental results.

P1.00114 ABSTRACT WITHDRAWN —

P1.00115 Characterizing detergent mediated reconstitution of viral protein M2 in large unilamellar vesicles1, MARIEL FREYRE, CARL GROSSMAN, CATHERINE CROUCH, KATHLEEN HOWARD, Swarthmore College — Influenza M2 is a model membrane protein whose function is to induce curvature and vesicle formation in the process of viral infection. To study embedded M2 in synthetic phospholipid vesicles (large unilamellar vesicles or LUVs), a concentration of detergent and buffer is optimized to balance protein solubility, proteolipid concentration, and LUV stability. Adding detergent also causes the LUVs to partially disassemble and form micelles, which warrants detergent removal to restore LUV integrity. We explore methods of measuring the coexistence of detergent micelles and LUVs to track the different phases of the system as detergent is removed. A combination of Fluorescence Correlation Spectroscopy, Dynamic Light Scattering, and chemical analysis are used to measure the properties of this system. With detergent/LUV number densities as high as 5 we find coexistence of micelles and LUVs at 50% to 60%. As the detergent is removed, the micelle concentration drops to lower than 30% while detergent levels drop to nearly zero. These results may indicate a polydispersed LUV size distribution after detergent mediated reconstitution.

1Supported by HHMI and Swarthmore College

P1.00116 Preventing drug resistance in severe influenza , HANA DOBOVOLNY, Texas Christian Univ, LUCAS DEECKE, University of Cologne — Severe, long-lasting influenza infections are often caused by new strains of influenza. The long duration of these infections leads to an increased opportunity for the emergence of drug resistant mutants. This is particularly problematic for new strains of influenza since there is often no vaccine, so drug treatment is the first line of defense. One strategy for trying to minimize drug resistance is to apply periodic treatment. During treatment the wild-type virus decreases, but resistant virus might increase; when there is no treatment, wild-type virus will hopefully out-compete the resistant virus, driving down the number of resistant virus. We combine a mathematical model of severe influenza with a model of drug resistance to study emergence of drug resistance during a long-lasting infection. We apply periodic treatment with two types of antivirals: neuraminidase inhibitors, which block release of virions; and adamantanes, which block replication of virions. We compare the efficacy of the two drugs in reducing emergence of drug resistant mutants and examine the effect of treatment frequency on the emergence of drug resistant mutants.

P1.00117 Simultaneous influenza and respiratory syncytial virus infection in human respiratory tract, LUBNA JAHAN Rashid Pinky, HANA DOBOVOLNY, Texas Christian University — Studies have shown that simultaneous infection of the respiratory tract with at least two viruses is not uncommon in hospitalized patients, although it is not clear whether these infections are more or less severe than single infections. We use mathematical models to study the dynamics of simultaneous influenza (flu) and respiratory syncytial virus (RSV) infection, two of the more common respiratory viruses, in an effort to understand simultaneous infections. We examine the roles of initial viral inoculum, relative starting time, and cell regeneration on the severity of the infection. We also study the effect of antiviral treatment on the course of the infection. This study shows that, unless treated with antivirals, flu always takes over the infection no matter how small the initial dose and how delayed it starts with respect to RSV.
P1.00118 Determining Mechanism of Action of Antivirals for Respiratory Illness

IRMA RODRIGUEZ, HANA DOBROVOLNY, Texas Christian Univ — Viral infections in the respiratory tract are common in humans and can cause serious illness and death. Drug treatment is the principal line of protection against many of these illnesses and many compounds are tested as antivirals. Often the efficacy of these antivirals is determined before a mechanism of action is understood. We use mathematical models to represent the evolution of these diseases and establish which experiments can help determine the mechanism of action of antivirals.

P1.00119 Object-adapted trapping and shape-tracking to probe a bacterial protein chain motor

JULIAN ROTH, MATTHIAS KOCH, ALEXANDER ROHRBACH, University of Freiburg — The helical bacterium Spiroplasma is a motile plant and anthropod pathogen which swims by propagating pairs of kinks along its cell body. As a well suited model system for bacterial locomotion, understanding the cell’s molecular motor is of vital interest also regarding the combat of bacterial diseases. The extensive deformations related to these kinks are caused by a contractile cytoskeletal protein ribbon representing a linear motor in contrast to common rotary motors as, e.g., flagella. We present new insights into the working of this motor through experiments with object-adapted optical traps and shape-tracking techniques. We use the given laser irradiation from the optical trap to hinder bacterial energy (ATP) production through the production of O_2 radicals. The results are compared with experiments performed under the influence of an O_2-scavenger and ATP inhibitors, respectively. Our results show clear dependences of the kinking properties on the ATP concentration inside the bacterium. The experiments are supported by a theoretical model which we developed to describe the switching of the ribbon’s protein subunits.

P1.00120 Modeling the Lymphocytic Choriomeningitis Virus: Insights into understanding its epidemiology in the wild

CHRISTY CONTRERAS, College of Liberal Arts and Sciences – Physics Department, Arizona State University, JOHN MCKAY, Applied Mathematics for the Life and Social Sciences, Arizona State University, JOSEPH BLATTMAN, SUSAN HOLECHEK, The Biodesign Institute, Arizona State University — The lymphocytic choriomeningitis virus (LCMV) is a rodent-spread virus commonly recognized as causing neurological disease that exhibits asymptomatic pathology. The virus is a pathogen normally among rodents that can be transmitted to humans by direct or indirect contact with the virus in excretions and secretions from rodents and can cause aseptic meningitis and other conditions in humans. We consider an epidemiological system with rodent and human populations modeled by a system of ordinary differential equations that captures the dynamics of two |the dynamics of the diseases transmission and present our findings. The asymptotic nature of the pathogen plays a large role in its spread within a given population, which has motivated us to expand upon an existing SIRC model (Holechek et al in preparation) that accounts for susceptible-, infected-, recovered-, and carrier-mice on the basis of their gender. We are interested in observing and determining the conditions under which the carrier population will reach a disease free equilibrium, and we focus our investigation on the sensitivity of our model to gender, pregnancy related infection, and reproduction rate conditions.

P1.00121 ABSTRACT WITHDRAWN

P1.00122 Feeding strategies as revealed by the section moduli of the humerus bones in bipedal theropod dinosaurs

SCOTT LEE, ZACHARY RICHARDS, University of Toledo — The section modulus of a bone is a measure of its ability to resist bending torques. Carnivorous dinosaurs presumably had strong arm bones to hold struggling prey during hunting. Some theropods are believed to have become herbivorous and such animals would not have needed such strong arms. In this work, the section moduli of the humerus bones of bipedal theropod dinosaurs (from Microceratotherium to Tyrannosaurus rex) are studied to determine the maximum bending loads their arms could withstand. The results show that bending strength is not of uniform importance to these magnificent animals. The predatory theropods had strong arms for use in hunting. In contrast, the herbivorous dinosaurs had weaker arms.

P1.00123 Microrheology of single microtubule filaments and synthesized cytoskeletal networks

MATTHIAS KOCH, ALEXANDER ROHRBACH, Lab for Bio- and Nano-Photonics, University of Freiburg — The ability to sense and respond to external mechanical forces is crucial for cells in many processes such as cell growth and division. Common models on mechanotransduction rely on the conversion of mechanical stimuli to chemical signals in the cell periphery and their translocation by diffusion (passive) or molecular motors (active). These processes are rather slow (~ seconds) and it has been argued that the cytoskeleton itself might be able to transport a mechanical signal within microseconds via stress waves. Microtubules are the stiffest component of the cytoskeleton and thus ideal candidates for this purpose. We study the frequency dependent response of single microtubule filaments and small networks thereof in a bottom-up approach using several (N=2–10) time-multiplexed optical tweezers together with back focal plane interferometry. Small synthesized networks with a defined geometry are constructed using trapped Neutravidin beads as anchor points for biotinylated filaments. The network is then probed by a defined oscillation of one anchor (actor). The frequency dependent response of the remaining beads (sensors) is analyzed experimentally and modeled theoretically over a wide frequency range.

P1.00124 Biviscous blood flow and a new method for velocity profile adjustment

CARLOS VE-LAZQUEZ, ADRIAN REYES, Universidad Nacional Autonoma de Mexico — In this paper we describe our proposal of a new numerical procedure for the adjusting of the velocity profile of body fluids with two viscosities. We have focused on the relevant case of the human blood and we have selected a particular model, the biviscous blood model, with the purpose of proving the convenience of our method. We start by describing the convenience of the biviscous stress equation as a model for the blood constitutive equation, then we solve it in the particular case of a stationary flow and use this solutions as the basis of our numerical procedure, which is described afterwards. Then, we present its implementation for analyzing in vivo measurements and exhibit its pertinence. Finally, we explain the design of a programmatic code of an automatic routine which is capable of applying our method and therefore could be used as the basis of an automatic implementation in new diagnosis software within a measurement device.

P1.00125 Femoral bone strength in large theropod dinosaurs: A study by genus

SCOTT LEE, University of Toledo — The locomotion of bipedal theropod dinosaurs is controlled by the strength of the femur to resist bending torques (caused by the foot striking the ground and the action of muscles on the femur). The section modulus at the narrowest part measures the ability of the femur to resist such torques. We present the results of our study of the femoral section moduli for six genus of large theropods: *Tyrannosaurus*, Nanotyrannus, Gorgosaurus, and *Albertosaurus* of the Late Cretaceous, *Acrocanthosaurus* of the Early Cretaceous, and *Allosaurus* of the Late Jurassic. These animals had femora of lengths between 65 and 134 cm. The corresponding section moduli varied between 23 and 570 cm². Some species of *Tyrannosaurus*, Gorgosaurus, *Allosaurus*, and *Albertosaurus* had femora with lengths in the same 75 to 90 cm range. The section moduli of these animals are all in the same range, showing that the animals had the same abilities of locomotion. That is, *Allosaurus* of the Late Jurassic could locomote just as well as the Late Cretaceous *Tyrannosaurus*, Gorgosaurus, and *Albertosaurus*. There is no evidence that these later theropods had evolved to be any faster than similarly-sized theropods living about 80 million years earlier.
P1.00126 Allometry in dinosaurs and mammals, SCOTT LEE, University of Toledo — The proportions of the leg bones change as the size of an animal becomes larger since the mass of the animal increases at a faster rate than the cross-sectional area of its leg bones. For the case of elastic similarity (in which the longitudinal stress in the legs remains constant in animals of all sizes), the diameter d and length L of the femur should be related as $d = A L^{3/2}$. For geometric similarity (in which all dimensions are scaled by the same factor), $d = A L$. For animals with femora longer than 20 cm, we find the power law relationship to be $d = A L^b$ with $b = 1.13 \pm 0.06$ for extant mammals (the largest mammal being *Loxodonta africana* with a 1.00-m-long femur) and $b = 1.18 \pm 0.02$ for dinosaurs (the largest dinosaur being *Brachiosaurus brancai* with a 2.03-m-long femur). These data show that extinct dinosaurs and extant animals scale in the same basic manner. The large sauropods (with femora twice as long as found in elephants) scale in a manner consistent with extrapolation of the scaling shown by extant mammals. These results argue that extinct dinosaurs moved in a manner very similar to extant mammals.

P1.00127 Direct Osmolyte-Macromolecule Interactions Confer Entropic Stability to Folded States, FRANCISCO RODRIGUEZ-ROPERO, NICO F.A. VAN DER VEGT, Tech Univ Darmstadt — Protective osmolytes are chemical compounds that shift the (bio)macromolecule folding/unfolding equilibrium toward the folded state under osmotic stresses. Traditionally it has been considered that osmolytes are depleted from the macromolecule first solvent shell, leading to entropic stabilization of the folded state. Recent theoretical and experimental studies suggest that protective osmolytes may directly interact with the macromolecule. As an exemplary and experimentally well-characterized system, we herein discuss poly(N-isopropylacrylamide) (PNIPAM) in water whose folding/unfolding equilibrium shifts toward the folded state in the presence of urea. Based on Molecular Dynamics simulations we show that urea preferentially accumulates in the first solvation shell of PNIPAM driven by attractive van der Waals dispersion forces leading to the formation of urea clouds around the polymer. Solvation thermodynamics analysis of the folded and unfolded states discards direct urea/macromolecule interactions as driving force of the folding mechanism. Our data shows that entropic penalization of unfolded polymer chains upon increasing urea concentration drives the collapse of the polymer chain.

P1.00128 Quantifying macromolecular conformational transition pathways, SEAN SEYLER, AVISHEK KUMAR, MICHAEL TORPHE, OLIVER BECKSTEIN, Arizona State University — Diverse classes of proteins function through large-scale conformational changes that are challenging for computer simulations. In this work, we introduce a comprehensive method (pathway similarity analysis, PSA) for quantitatively characterizing and comparing macromolecular pathways. The Hausdorff and Fréchet metrics (known from computational geometry) are used to identify the degree of similarity between polygonal curves in configuration space. A strength of PSA is its use of the full information available from the 3N-dimensional configuration space trajectory without requiring additional specific knowledge about the system. We compare a sample of eleven different methods for the closed-to-open transitions of the apo enzyme adenylate kinase (AdK) and also apply PSA to an ensemble of 400 AdK trajectories produced by dynamic importance sampling MD and the Geometrical Pathways algorithm. We discuss the method’s potential to enhance our understanding of transition path sampling methods, validate them, and help guide future research toward deeper physical insights into conformational transitions.

P1.00129 Interaction of Human Serum Albumin with Metal Protoporphyrins, JIE HU, URTSA, LORENZO BRANCLEON, Physics Dept. URTSA — Fluorescence spectroscopy is widely used in biotechnology, nanotechnology, and molecular biophysics, since it can probe the interactions of macromolecules with fluorophores, conformational changes, and binding interactions. In this study, we present the photophysical properties of various interactions of human serum albumin (HSA) with metal protoporphyrin IX (ZnPPIX), including ZnPPIX, FePPIX, MgPPIX, MnPPIX and SnPPIX respectively, as well as the free base PPIX. Binding constants were retrieved independently using the Benesi-Hildebrand analysis of the porphyrin emission or absorption spectra and the fluorescence quenching (i.e. Stern-Volmer analysis) and reveal that the two methods yield a difference of approximately one order or magnitude between the two. Fluorescence lifetimes was used to identify the degree of similarity between polygonal curves in configuration space. A strength of PSA is its use of the full information available from the 3N-dimensional configuration space trajectory without requiring additional specific knowledge about the system. We compare a sample of eleven different methods for the closed-to-open transitions of the apo enzyme adenylate kinase (AdK) and also apply PSA to an ensemble of 400 AdK trajectories produced by dynamic importance sampling MD and the Geometrical Pathways algorithm. We discuss the method’s potential to enhance our understanding of transition path sampling methods, validate them, and help guide future research toward deeper physical insights into conformational transitions.

P1.00130 Replica-exchange Wang-Landau simulations of the H0P model of protein folding, GUANGJIE SHI, DAVID P. LANDAU, Center for Simulational Physics, The University of Georgia, THOMAS WÜST, Scientific IT Services, ETH Zurich — The hydrophobic-polar (HP) model has served as a coarse-grained lattice protein folding, validating them, and help guide future research toward deeper physical insights into conformational transitions.

P1.00131 Ergodic protein dynamics underlie the universal shape of protein distribution in populations, NAAMA BRENNER, EREZ BRAUN, Technion-Israel Institute of Technology, JAMES ROTELLA, HANNA SALMAN, University of Pittsburgh, NAAMA BRENNER COLLABORATION, EREZ COLLABORATION, JAMES ROTELLA AND HANNA SALMAN COLLABORATION — We have previously shown that protein fluctuations in cell populations exhibit a universal distribution shape under a broad range of biological realizations. Here we report new results based on continuous measurement in individual bacteria for over ~70 generations, which show that single-cell protein trajectories sample the available states with the same distribution shape as the population, i.e. protein fluctuations are ergodic. Analysis of temporal trajectories reveals that one effective random variable, sampled once each cell cycle, suffices to reconstruct the distribution from the trajectory. This in turn implies that cellular microscopic processes are strongly buffered and population-level protein distributions are insensitive to details of the intracellular dynamics. Probing them thus requires searching for novel universality-breaking experimental perturbations.
Besides pore diameter, the relative hydrocarbon loading in the controlled-pore glass is evaluated. The findings suggest that the bubble point is dramatically
of 4.3 to 38.1 nm pore diameter. Differential scanning calorimetry is used to measure the temperature at which the gas phase begins to form (i.e. bubble point).

Phase behavior in shale remains a challenging problem in the petroleum industry due to many complexities. One complexity is the
strong surface-fluid interactions in shale nano-scale pores. These interactions can lead to a heterogeneous distribution of molecules, which conventional bulk-

P1.00133 FLUIDS —

P1.00134 Effect of Confinement on the Bubble Points of Hydrocarbons in Controlled-Pore Glasses †, SHENG LUO, Harold Vance Department of Petroleum Engineering, Texas A&M University, JODIE LUTKENHAUS, Artie McFerrin Department of Chemical Engineering, Texas A&M University, HADI NASRABADI, Harold Vance Department of Petroleum Engineering, Texas A&M University, HADI NASRABADI TEAM — Phase behavior in shale remains a challenging problem in the petroleum industry due to many complexities. One complexity is the
strong surface-fluid interactions in shale nano-scale pores. These interactions can lead to a heterogeneous distribution of molecules, which conventional bulk-

P1.00135 Liquid Crystals under Photo-patterned Spatially Varying Boundary Conditions †, MIAO JIANG, YU-BING GUO, QI-HUO WEI, Liquid Crystal Institute, Kent State Univ, Kent, OH — Liquid crystals under geometric confinements are of not only fundamental interest but also practical importance to applications such as chemical sensing and smart windows. Orientations of liquid crystal molecules
in most geometric confinements are uniform at the boundaries and not highly controllable. In this paper, we will present a novel photoalignment technique to
pattern spatially varying complex orientation fields, and discuss experimental studies on nematic liquid crystals under confinements of two parallel plates with
various well designed molecular orientation fields.

P1.00136 Two-dimensional Yukawa fluids ‡, †, MINERVA GONZALEZ-MELCHOR, Instituto de Fisica “Luis Rivera Terrazas,” Benemerita Universidad Autonoma de Puebla, Apdo. Postal J-48, Puebla, 72570, Puebla, Mexico, ARLETTE MENDEZ, JOSE ALEJANDRE, Departamento de Quimica, Universidad Autonoma Metropolitana-Iztapalapa, Av. San Rafael Atlicoc 186, Col. Vicentina, 09340 Mexico Distrito Federal, Mex — When the
movement of particles is performed predominantly in two dimensions, the systems can be considered at a good extent as two-dimensional. For instance the
lipsid in a bilayer, micrometric particles in a quasi-two-dimensional colloidal suspension, colloids in a monolayer deposited on the air-water interface, and DNA complexes trapped at the water surface can be described at first approach as bidimensional fluids. These systems are important for many applications in
surface and colloidal science. In simulations where the explicit interface between liquid and vapor is present, the line tension can be directly computed. In this
work we present molecular dynamics results obtained for the liquid/vapor coexistence curve of 2D Yukawa fluids and for the line tension. A comparison with
the three-dimensional case is also presented.

P1.00137 Heat Transfer Enhancement in Forced Convective Boiling in Microchannels by Periodic Electrospun Nanofiber Coatings †, ALEXANDER YARIN, University of Illinois at Chicago, MARTIN FREYSTEIN, FELIX KOLBERG, Technische Universität Darmstadt, SUMIT SINHA-RAY, RAKESH SAHU, University of Illinois at Chicago, LUCAS SPIEGEL, TATIANA GAMBARYAN-ROISMAN, PETER STEPHAN, Technische Universität Darmstadt — To enhance heat transfer in forced convective boiling the microchannel bottom was amended by a nano-texture - periodic rectangular mats of electrospun polymer nanofibers. The fibers were ~ 300-500 nm in diameter and the mat thickness was about 6-15 µm. The test fluid was FC-72 and the flow in microchannels contained trains of Taylor bubbles. The role of the nanofibers was to retain the warm microchannel bottom wet, to prevent dry-out and thus to enhance the heat removal rate. In the present experiments the time-average heat flux and heat
transfer coefficient at the nanofiber-coated domains were found to be 1.5-2 times higher than those at the uncoated ones. Accordingly, a significant decrease (by 5-8 K) in the superheat was observed at the same Re of 387 and power supply of 36.1 kW/m2. At a higher Re of 432 and lower power supply of 28.1 kW/m2 similar trends in the heat removal rate and surface superheat were found. The significant enhancement of the heat transfer results from the fact that nanofiber mats facilitate wetting of surface under passing Taylor bubbles, thus delaying formation of vapor flow at the channel bottom. The interstices of the nanofiber mat act as the nucleation sites facilitating formation of tiny bubbles, which eventually results in a higher heat removal rate from the surface at a reduced superheat.

P1.00138 A simulation study of flow dynamics of erythrocytes through diverging and converging bifurcations †, TONG WANG, Nanjing University of Aeronautics and Astronautics, ZHONGWEN XING, Nanjing University — A numerical model has been developed to predict the cells deformation and motion in a symmetric diverging and converging bifurcation of a microchannel. Fluid dynamics and membrane mechanics are incorporated. The model was utilized to evaluate the effect of different biophysical parameters, such as: initial cell position, membrane stiffness and shape of the cells on deformation and motion of the erythrocytes in the bifurcating curved microchannel. The numerical results demonstrate that erythrocytes in microvessels blunt velocity profiles in both straight section and daughter branches, and the transit velocity of erythrocytes is strongly influenced by cell deformability, shape of the cells, and the vessel geometry. These results may provide fundamental knowledge for a better understanding of hemodynamic behavior of microscale blood flow.

P1.00139 Fluid flow calculations of Graphene Composites †, AMIRESSAM TAHMASSEBI, ALPER BULDUM, University of Akron, Department of Physics — The flow of fluids through carbon nanotubes was investigated in order to get a better understanding of the unique properties and phenomena of nano-fluidics. The previous modeling and simulation efforts were based on diffusion of atoms or molecules that were thrown to the nanotubes with initial velocities. This talk has shed some light on the flow of fluids using molecular dynamic simulations of different types of carbon nanotubes that were embedded in liquid argon using a moving wall piston of graphene. We focused on analyzing pressure difference, velocities, and momentum conservation in different regions.

3Work supported by NSF CMMI-1436565

1The authors acknowledge the support of the State Key Program for Basic Researches of China (2014CB921103 and 2010CB923404), the National “Climbing” Program of China (91021003), and the National Science Foundation of Jiangsu Province (BK2010012).
The effects of surface roughness on the contact line friction coefficients of water droplets on micro/nano-patterned surfaces, JIANGTAO CHENG, University of North Texas — We report the effects of surface roughness on contact line friction coefficient (CLFC) of water droplets on micro- and nano-patterned surfaces. Both advancing and receding CLFCs have been measured on smooth, one-tier (with micropillars), and two-tier (with CNTs grown on micropillars) surfaces. In comparison with smooth surface, superhydrophobic surfaces can decrease both the advancing and receding CLFCs by more than 10 times. However, droplets on one-tier surfaces exhibit different dynamic behaviors in advancing and receding movements. We investigated the Wenzel-Cassie state transition on micropillar structures and found that the receding motion of a droplet on micropillars is dominated by the Wenzel model with significant receding contact line pinning, which leads to higher receding CLFC. However, rolling mechanism of liquid particles near the advancing contact line controls the advancing motion of a droplet on micropillars. There is a high tendency for an advancing droplet to exhibit Cassie-type behavior on one-tier surfaces and hence advancing CLFC is considerably mitigated. On two-tier superhydrophobic surfaces, it is the Cassie-Baxter behavior that dominates both the advancing and receding contact line motions giving rise to less friction coefficients.

Patterns, Instabilities, Colors, and Flows in Vertical Foam Films, SUBINUER YILI XIATI, EWELINA WOJCIK, YIRAN ZHANG, COLLIN PEARSELL, VIVEK SHARMA, Chemical Engineering, University of Illinois Chicago — Foams find use in many applications in daily life, industry and biology. Examples include beverages, firefighting foam, cosmetics, foams for oil recovery and foams formed by pollutants. Foams are collection of bubbles separated by thin liquid films that are stabilized against drainage by the presence of surfactant molecules. Drainage kinetics and stability of the foam are strongly influenced by surfactant type, addition of particles, proteins and polymers. In this study, we utilize the thin film interference colors as markers for identifying patterns, instabilities and flows within vertical foam films. We experimentally study the emergence of thickness fluctuations near the borders and within thinning films, and study how buoyancy, capillarity and gravity driven instabilities and flows, are affected by variation in bulk and interfacial physicochemical properties dependent on the choice of constituents.

Diving dynamics of seabirds, SUNGHWAN JUNG, BRIAN CHANG, MATT CROSON, Virginia Tech, LORIAN STRAKER, CARLA DOVE, Smithsonian Museum — Diving is the activity of falling from air into water, which is somewhat dangerous due to the impact. Humans dive for entertainments less than 20 meters high, however seabirds dive as a hunting mechanism from more than 20 meters high. Moreover, most birds including seabirds have a slender and long neck compared to many other animals, which can potentially be the weakest part of the body upon axial impact compression. Motivated by the diving dynamics, we investigate the effect of surface and geometric configurations on structures consisting of a beat-like cone and a neck-like elastic beam. A transition from non-buckling to buckling is characterized and understood through physical experiments and an analytical model.

POLYMER PHYSICS —

Orthogonal gradient networks via post polymerization reaction, PANDYARAJAN CHINNAYAN KANNAN, JAN GENZER, North Carolina State University — We report a novel synthetic route to generate orthogonal gradient networks through post polymerization reaction using pentafuroporphylmethacrylate (PFPMac) active ester chemistry. These chemoselective monomers were successfully copolymerized with 5 mol% of the photo (methacryloyloxybenzophenone) and thermal (styrenesulfonynalzide) crosslinkers. Subsequently, the copolymers were modified by a series of amines having various alkyl chain lengths. The conversion of post polymerization reaction was monitored using Fourier Transform Infrared Spectroscopy (FT-IR) and noticed that almost all pentafurophenyl moiities are substituted by amines within in an hour without affecting the crosslinkers. In addition, the incorporation of photo and thermal crosslinkers in the polymer enabled us to achieve stable and covalently surface-bound polymer gradient networks (PGN) in an orthogonal manner, i.e. complete control over the crosslinking density of the network in two opposite directions (i.e. heat vs photo). The network properties such as wettability, swelling and tensile modulus of the gradient coatings are studied and revealed in the paper.

Enthalpy Relaxation of a DGEBA Epoxy as a function of Time, Temperature, and Cooling Rate, CAITLYN M. CLARKSON, JOHN D. MCCOY, New Mexico Tech, JAMIE M. KROPKA, Sandia National Laboratories — Enthalpy relaxation resulting from physical aging of a DGEBA epoxy, Epon 828, cross-linked with an amine curative, Jeffamine T-403, was studied for two isothermal aging temperatures at sequential aging times up to two weeks. Results were analyzed using the peak shift method to obtain the relaxation parameters $β$, $δ$ ($H^*$), and $χ$. The individual effects of cooling rate from the equilibrated state, aging time, and aging temperature were isolated to understand the initial state of the glassy epoxy and its evolution during physical aging. [Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.]

Frank-Kasper and other superlattice formations in a set of giant molecules having ABn type of Janus particles, XUEYAN FENG, YIWEN LI, MINGJUN HUANG, HI-HAO HSU, STEPHEN Z.D. CHENG, University of Akron — A novel serial of precisely defined giant molecules having ABn type of Janus particles has been designed and synthesized. They are consisted of one functionalized hydrophilic polyhedral oligomeric silsesquioxane (POSS) (A) connected with different number of hydrophobic POSS cages (B, n=2-6). With variation of the interaction functional groups on A and the number of the coordinated hydrophobic POSS B, different superlattice structures could be formed at a sub-10-nm scale. For example, the superlattice structure of DPOSS-BPOSS2 (DPOSS represents seven hydroxyl group functionalized POSS and BPOSS represents isobutyl POSS) could change from a double-dyroids phase to a hexagonally packed cylinder phase with increasing temperature, due to an order-order transition in the weak segregation region. For DPOSS-BPOSS3 and DPOSS-BPOSS4, both of these giant molecules could form A15 phase, which is a Frank-Kasper phase. With deep understanding of this set of model Janus type giant molecules based on the POSS nano atoms, it may be promising to construct new generations of giant molecules for further development of functional materials with desired structures and macroscopic properties.

Strain Rate Dependence of Compressive Yield and Relaxation in DGEBA Epoxy , GABRIEL K. ARECHEDERRA, RILEY C. RÉPROGLE, CAITLYN M. CLARKSON, JOHN D. MCCOY, New Mexico Tech, JAMIE M. KROPKA, KEVIN N. LONG, ROBERT S. CHAMBERS, Sandia National Laboratories — The mechanical response in uniaxial compression of two diglycidyl ether of bisphenol-Α epoxy were studied. These were 828DEA (Epon 828 cured with diethanolamine (DEA)) and 828T403 (Epon 828 cured with Jeffamine T-403). Two types of uniaxial compression tests were performed: A) constant strain rate compression and B) constant strain rate compression followed by a constant strain strain relaxation. The peak (yield) stress was analyzed as a function of strain rate from Eyring theory for activation volume. Runs at different temperatures permitted the construction of a mastercurve, and the resulting shift factors resulted in an activation energy. Strain and hold tests were performed for a low strain rate where a peak stress was lacking and for a higher strain rate where the peak stress was apparent. Relaxation from strains at different places along the stress-strain curve was tracked and compared. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
P1.00148 Template-directed synthesis of structurally-defined branched polymer architectures, AMANDA MARCIEL, UIUC — In this work, we describe a hybrid synthetic strategy to produce structurally-defined branched polymer architectures based on chemically-modified DNA. Overall, this approach enables precise control over branch placement, grafting density, and chemical identity of side branches. We utilize a two-step scheme based on polymerase chain reaction (PCR) for site-specific incorporation of non-natural nucleotides, followed by copper-free click chemistry for grafting side branches at specific locations along the main polymer backbone. Linear DNA backbones are first synthesized via PCR utilizing the promiscuity of a high yield thermostable DNA polymerase to incorporate nucleotides containing bioorthogonal dibenzocyclooctyne functional groups at precise locations along one strand of a double stranded DNA backbone. Following PCR, copper-free click chemistry is used to attach synthetic polymer branches or oligonucleotide branches to the DNA backbone, thereby allowing for the design and synthesis of a variety of precise polymer architectures, including three-arm stars, H-polymers, and graft block copolymers.

P1.00149 Light scattering measurement of sodium polyacrylate products, NISHA LAMA, DAVID NORWOOD, Southeastern Louisiana Univ, STEVEN BOONE, VALERIE MASSIE-BROWN, Bercen Inc. — In the presentation, we will describe the use of a multi-detector HPLC incorporating the DAWN EOS multi-angle laser light scattering (MALLS) detector to measure the properties such as molecular weight, RMS radius, contour and persistence length and polydispersity of sodium polyacrylate products. The samples of sodium polyacrylate are used in various industries as thickening agents, coating dispersants, artificial snow, laundry detergent and disposable diapers. Data and results obtained from the experiment will be presented.

P1.00150 Kinetics of the coil-to-globule transition in aqueous solution of poly (N-isopropylacrylamide), REZA FARASAT, University of Alabama at Birmingham — In an aqueous solution, poly (N-isopropylacrylamide) (PNIPAM) undergoes a reversible coil-to-globule phase transition that occurs above the lower critical solution temperature (LCST). The transition is driven by temperature-dependent molecular interactions that include hydrogen bonding and hydrophobic association. By increasing the temperature above LCST, the PNIPAM-water bonds break, and the polymer coils collapse to globules. The process is accompanied by an endothermic thermal effect which is detectable by Differential Scanning Calorimetry (DSC). A 10 wt. % solution of PNIPAM in water was prepared and subjected to DSC experiments under different heating rates (from 0.5 to 16°C min⁻¹). With increasing the heating rate, the transition temperature as well as the DSC peak shift to higher temperature. The DSC data have been analyzed by an isocconversional method to evaluate the temperature dependence of the effective activation energy of the process. The resulting data have been interpreted in terms of a nucleation kinetics model. The process has also been studied under nanoconfinement by introducing the PNIPAM solution into the silica nanopores. The results obtained under nanoconfinement are compared to those obtained for the bulk solution.

P1.00151 SEMI CRYSTALLINE POLYMERS

P1.00152 Effect of Crystallinity on Melt Memory of Random Ethylene Copolymers, XUEJIAN CHEN, AL MAMUN, ALAMO G. RUFINA, FAMU-FSU College of Engineering, Department of Chemical and Biomedical Engineering, Tallahassee, Fl 32310 — A strong melt memory effect of crystallization has been observed in random ethylene copolymers even above the equilibrium melting temperature. Melt memory is associated with seeds that increase the crystallization rate of copolymers in a range of comonomer content between 0.5 and 4.5 mol%. The seeds are taken as molten ethylene sequences that remain in close proximity and are unable to diffuse fast to the randomized melt state. Fast diffusion is restricted by topological chain constraints (loops, knots, and other entanglements) that build in the intercrystalline region during crystallization. The molten nature of the self-seeds is supported by a linear variation of T_N with T_melt. n NMR experiments in a range from 180 to 240°C, covering both the homogeneous and heterogeneous melt regions. The effect of topological constraints on melt memory, or on number of seeds that remain in the melt, was analyzed studying copolymers with different levels of crystallinity. There is a threshold level of crystallinity, which depends on type and concentration of comonomer, below which copolymers do not display strong melt memory. Increasing 1-hexene content from 0.5 to 3.5 mol%, the crystallinity threshold decreases from 39 to 4%, while decreasing branch length from hexyl to ethyl, the threshold crystallinity decreases from 18% to 5% in agreement with stronger melt memory in copolymers with increasing comonomer content and with shorter branches.

P1.00153 Structural Analysis of Semiconducting Polymers Exposed to High Energy Radiation, SAEED AHMADI VASELABADI, University of Poole, NIKHLA MAHABDEVAPURAM, Intel Corporation, DAVID SHAKARISAZ, University of Houston, JOSEPH STRZALKA, Argonne National Laboratory, PAUL RUCHHOEFT, GLA STEIN, University of Houston — Semicrystalline polymers are used in low-cost electronics such as solar cells, thin film transistors, and light-emitting diodes. Their optoelectronic performance in these devices is partly dictated by molecular ordering and nanoscale structure, where the latter is particularly difficult to control. We used atom-beam radiation to crosslink the polymer poly(3-hexylthiophene) into nanoscale and microscale patterns. Ionizing radiation sources generate intermolecular cross-links that render the polymer insoluble in organic solvents. Grazing-incidence Wide-angle X-ray Scattering (GIWAXS) was used to investigate the effects of irradiation on molecular ordering of poly(3-hexylthiophene). We found that crosslinking will disrupt intermolecular ordering (reduce crystallinity and crystalline grain sizes). We also found that X-ray exposure during the WAXS measurements can induce the crosslinking through a similar mechanism, and we propose a simple method to test for the damage caused by these measurements. As an example, we find that poly (3-hexylthiophene) has measurable cross-links after 20 sec exposure to 7.35 keV radiation with flux of 1 \* 10¹¹ photons/sec at an incident angle of 0.5°.

P1.00154 Mechanical properties of syndiotactic polypropylene (sPP) gels: the effects of temperature and solute concentration, RYUSUKE OKOSHI, ATUSHI HOTTADA, Department of Mechanical Engineering, Keio University — The effects of the solute concentration on the microstructures and the mechanical properties of quenched syndiotactic polypropylene (sPP) gels were investigated. Our group has previously reported a highly resilient sPP gel quenched using liquid nitrogen (Gel LN). In this research, sPP/decahydronaphthalene gels were prepared varying the sPP concentrations from 5 to 20 wt%. Compression test was carried out to evaluate the mechanical properties. Scanning electron microscopy (SEM) was conducted to analyze the microstructures. Gel LN with the sPP concentration of 20 wt% presented a high fracture stress of 2400 kPa. A high fracture strain of 70% was also observed for all Gel LN samples. By contrast, sPP gels with the sPP concentration of 20 wt% cooled at 25 degrees C (Gel 25) showed lower fracture stress of 480 kPa. The fracture strain of Gel 25 ranged from 21 to 37% depending on the sPP concentrations. The SEM results revealed that the Gel LN samples had homogeneous networks regardless of the sPP concentrations. The Gel 25, however, possessed inhomogeneous networks with spherulites. It was therefore concluded that the strengthening of the sPP gels could be effectively achieved by Gel LN regardless of the sPP concentrations.
P1.00155 Structural Characterization of Layered Morphologies in Precise Copolymers, Edward B. Trigg, L. Robert Middleton, Univ of Pennsylvania, Taylor W. Gaines, Kenneth B. Wagener, Univ of Florida, Karen I. Winey, Univ of Pennsylvania — Layered morphologies have been observed in precise polyethylene-based copolymers that contain acid, charged, or polar functional groups precisely spaced along a linear alkane chain. Sufficiently long alkane segments form structures resembling orthorhombic polyethylene crystals, while the functional groups form 2-D layers that disrupt the alkane crystal structure to varying degrees. Here, layered morphologies in precise copolymers containing acrylic acid, phosphonic acid, imidazolium bromide, and sulfone groups are studied via X-ray scattering. Specifically, the composition profiles of the layered structures are obtained by Fourier synthesis, and the coherence length is investigated using peak width analysis. This analysis indicates that the layers of functional groups are frequently bordered by two crystallites, which suggests different dynamics relative to layers bordered by one crystalline and one amorphous microdomain. Detailed understanding of the structure of the layered morphologies will allow for a systematic investigation of proton and ion conductivity mechanisms, which are expected to occur through the high-dielectric layers.

P1.00156 Polymer Crystals Formed at Liquid-Liquid Interface Show Broken Symmetry, Wenda Wang, Hao Qi, Ziyin Huang, Christopher Y. Li, Drexel University, Soft Matter Research Group Team — Curved space is incommensurate with typical ordered structures with three-dimensional translational symmetry. However, upon assembly, soft matter, including colloids, amphiphiles, and block copolymers, often form structures depicting curved surface/interface. On the other hand, twisted and curved crystals are often observed in crystalline polymers. Various mechanisms have been proposed for these non-flat crystalline morphologies. In this presentation, we will discuss the recent development of crystallization at flat and curved liquid/liquid (L/L) interface. We show that structure, morphology and chain folding behaviors are strongly affected by L/L interfacial energy and polymer chain ends. Both polyethylene and poly-L-lactic acid single crystal shells have been obtained using curved L/L interface. Polymer crystallization behavior at L/L interface will be compared with solution and bulk crystallization.

P1.00157 POLYMER MELTS AND SOLUTIONS —

P1.00158 Correlating solubility parameters and solvatochromatic parameters with the self-assembly of poly(3-hexylthiophene) in mixtures of organic solvents, Madeleine Gordon, David Boucher, College of Charleston — We have studied the assembly and crystallinity of poly(3-hexylthiophene) (P3HT) \( M_w \approx 28.2 \text{ kDa}, \text{ regioregularity} > 96\%, \text{ PDI} \approx 1.3 \) in >100 binary solvent mixtures using UV-Vis absorption spectroscopy, and it is clear that the identity of the poor solvent used to drive aggregation has a significant impact on the structural order and crystallinity of the P3HT aggregates in solution. Here we report our findings using Hansen solubility parameters (HSPs), specifically the solubility distance vector, \( R_\alpha \), and the Kamlet-Taft solvatochromatic parameters of the solvent mixtures to better understand the dominant solvent forces driving the self assembly of P3HT. We find that the directionality of the \( R_\beta \) vector provides a better measure of the crystallinity of the P3HT assemblies formed in the solvent mixtures than does the magnitude of the \( R_\alpha \) vector. Our analysis of the Kamlet-Taft \( (\alpha, \beta, \pi^*) \) and \( E_1(30) \) solvatochromatic parameters reveals that the \( \beta \) parameter correlates best with the crystallinity of P3HT and that, in general, assemblies having higher structural order are formed in solvent mixtures with lower values of \( \beta \).

P1.00159 Demixing transition and molecular interactions in Poly(N-isopropyl acrylamide) solutions compared to its monomer, Moritz Futschker, Martine Philipp, Peter Mueller-Buschbaum, Technical University Munich, Alfonso Schulte, University of Central Florida — Temperature-sensitive hydrogels such as poly(N-isopropyl acrylamide) (PNIPAM) exhibit a coil to globule transition of the polymer chains with a lower critical solution temperature (LCST) near 305 K. The cooperative dehydration of bound water molecules upon heating plays a significant role. The hydrogen bonding with the amide groups in the side chains has to be contrasted with the hydration interaction of the hydrophobic main chain hydro-carbons. Employing FTIR spectroscopy we probe molecular changes in the various chemical groups. PNIPAM and its monomer NIPAM are investigated at a concentration of 20% in aqueous solution. We observe a nearly discontinuous shift of the 30 peak frequencies and the intensities of vibrational bands (amides, CH) in PNIPAM, whereas in NIPAM there is a continuous linear shift with temperature. The results are discussed with respect to hydration changes in the amide group and cooperative interactions with bound water along the backbone chain.

P1.00160 Pressure and temperature response of Poly(N-isopropyl acrylamide) in aqueous solution probed with Raman microscopy, Coleman Cariker, Alfonso Schulte, University of Central Florida — Poly(N-isopropylacrylamide) (PNIPAM) is a thermo-responsive hydrogel that exists in a hydrated state beneath its lower critical solution temperature (LCST) near 305 K. Above this temperature water is expelled by the polymer as it undergoes a coil to globule collapse. High pressure is an important variable as it influences the strength of hydrogen bonding and can destabilize hydrophilic contacts. We present results from optical imaging on a micron scale and Raman spectroscopic measurements as a function of temperature (295 - 315 K) and hydrostatic pressure (0.1 - 400 MPa). Samples consisted of 25% PNIPAM in aqueous solution in micro-capillaries with 100 micron cross section. Our experiments reveal differences in the spatial evolution of the phase change across the temperature and pressure transitions. These are corroborated by bond specific and hydration changes observed in the Raman spectra.

P1.00161 POLYMERIC ELASTOMERS AND GELS —

P1.00162 ABSTRACT WITHDRAWN —

P1.00163 Systematic Investigation of the Mechanical and Surface Properties of Poly(dimethylsiloxane) Networks, Matthew Melillo, Zoe Klein, Edwin Walker, Jan Genzer, North Carolina State Univ — Poly(dimethylsiloxane) (PDMS) is one of the most common elastomers. Its applications range broadly from medical devices to absorbents for water treatment, and recently it has been used rapidly in the use of microfluidic devices. Despite extensive research and characterization of PDMS networks, the static water contact angles of these elastomers reported in the literature range broadly from a low near 90 degrees upwards to greater than 120 degrees. To investigate this large gap in reported surface properties, we have systematically studied the effects of polymer molecular weight, degree of tetra-functional crosslinker loading, end-group chemical functionality, and the extent of dilution of the curing mixture on the mechanical and surface properties of end-linked PDMS networks. The gel and sol fractions, mechanical properties, and water contact angles have been shown to vary greatly based on the aforementioned variables. This study provides insight to the factors that contribute to such a wide range of surface properties reported in the literature. Furthermore, these results demonstrate the need to fully and carefully consider the manner and environment in which PDMS networks are formed when preparing them for specific applications.
P1.00164 Effect of system compliance and indenter geometry on puncture mechanics of soft materials , SHRUTI RATTAN, SAMI FAKHOURI, ALFRED CROSBY, Univ of Mass - Amherst — Puncture mechanics in soft materials is critical for the development of new surgical instruments as well as new materials used in personal protective equipment. However, fundamental knowledge of how geometry and material properties control the nucleation of a crack, i.e. puncture, at large deformations in a soft material is currently limited. We describe a simple experimental method to study the resistive forces and failure of a soft gel being indented and punctured with a small needle. We show that puncture stresses can reach two orders of magnitude greater than the material modulus and that the force-deformation response is insensitive to the geometry of indenter at large indentation depths. We determine a transition between stress-limited and energy-limited failure modes, which is governed by the indenter size and the balance between fracture energy and cohesive stress. In addition, we examine the influence of system compliance on puncture of soft gels. It is well-known that system compliance influences the peak force in adhesion and traditional fracture experiments; however, its effect on crack nucleation is unresolved. We find that as the system becomes more compliant lower peak puncture forces were measured, which is associated with increased energy available for fracture.

P1.00165 Rheology of Poly(N-isopropylacrylamide)-Clay Nanocomposite Hydrogels , JACK LOMBARDI, DI XU, DIVYA BHATNAGAR, DILIP GERSAPPE, JONATHAN SOKOLOV, MIRIAM RAFAILOVICH, Materials Science and Engineering Department, Stony Brook University, Stony Brook, NY 11790, USA — The stiffness of PNIPA Gels has been reported could be significant improved by gelation with clay fillers. Here we conducted systematic rheology study of synthesized PNIPA-Clay Composites at different clay concentration, in a range from fluid to strong gel, where C" dominant changed to C' dominant. Molecular dynamics simulation was employed to analyze the structure of composites and corresponding mechanical changes with increased clays. Where we found viscoelastic behavior become significant only 1.5 times above percolation threshold. The yield stress extrapolated from our rheology results shows good fitting to modified Mooney's theory of suspension viscosity.

P1.00166 Self-Assembly and Relaxation Behavior of Graphene Containing Acrylic Triblock Copolymer Gels , MAHLA ZABET, SEYEDMEYSAM HASHEMNEJAD, SANTANU KUNDU, Dave C. Swalm School of Chemical Engineering, Mississippi State University, MS State, MS — Investigation of gel mechanical properties as a function of their structure is a significant research interest. This study presents the effect of graphene (or few-layer graphene) on the self-assembly and the relaxation behavior of a thermoreversible gel consists of a physically cross-linked poly (methyl methacrylate)-poly (n-butyl acrylate)-poly (methyl methacrylate) [PMMA-PnBA-PMMA] triblock copolymer in 2-ethyl-1-hexanol, a midblock selective solvent. Graphene was obtained by sonicating exfoliated graphite in 2-ethyl-1-hexanol at various concentrations. Filtration technique and spectrophotometry were utilized to measure the graphene concentration in the dispersions. The dispersed graphene was then incorporated in a series of gels and the effect of graphene on mechanical properties, including the relaxation behavior were studied. Small angle X-ray scattering (SAXS) was used to investigate the microstructure of these gels at room temperature. SAXS data were analyzed to estimate the number of end blocks per junction zone, the average spacing between the junctions, and the change of these properties as a function of graphene concentration. The results indicate that the presence of graphene affects the self-assembly process.

P1.00167 POLYMER BLENDS —

P1.00168 Bottlebrush additives drive formation of vesicle chains in polymer blends , HUI ZHEN MAH, PANTEA AFZALI, Univ of Houston, RAFAEL VERDUCO, Rice University, GILA STEIN, Univ of Houston — The effects of bottlebrush polymer additive with poly(styrene-r-methyl methacrylate) side-chains on the thin film morphology of polystyrene (PS) and poly (methyl methacrylate) (PMMA) blends were studied. Results were compared to PS/PMMA blends with diblock copolymer PS-b-PMMA compatibilizer and without any additive. Thin films were spin casted from toluene onto a “neutral” silicon surface and then annealed at a fixed temperature of 150°C for a range of times (up to 85 mins). The morphology of the films was characterized using optical microscopy and atomic force microscopy. In the absence of any additive, the PS/PMMA blend rapidly de-mixes to form macroscale domains, while high loads of the PS-b-PMMA additive can compatibilize the blend and suppress phase separation. However, the bottlebrush polymer additive drives the formation of well-organized vesicle chains in the PS/PMMA blend films. This morphology is favored by entropic considerations as the bottlebrush polymers are more stable than linear chains at the PS/PMMA interface and the brush like surface attracts.

P1.00169 Phase Equilibria in Ternary Blends of Two Linear Homopolymers and A Ring Gradient Copolymer , DACHUAN SUN, JUNHAN CHO, Dankook Univ — Phase equilibria in a ternary blend of linear A/B homopolymers of equal sizes and a symmetric A-co-B ring gradient copolymer as an amphipile with α as the ratio of their chain sizes are investigated in the mean-field picture. The monomer sequence on the copolymer chain is taken as either a step gradient or a fully linear gradient, to which a gradient number λ = 0 or 1 is assigned, respectively. Along the isopleth of equal homopolymer amounts, the resultant phase diagrams for the blends are to be built from multicritical points such as Lifshitz or bulk tricritical point depending on α and λ. The stabilization of lamellar mesophase or its equilibrium with A and B-rich bulk phases is accordingly controllable by the pair of α and λ.

This work was supported by the Basic Science Research Program (No. 2014023297) from National Research Foundation of Korea. The authors also acknowledge the support from the Center for Photofunctional Energy Materials, which is funded by Gyeonggi Regional Research Center Program (GRRC-dankook2011-001).

P1.00170 ABSTRACT WITHDRAWN —

P1.00171 COPOLYMERS —

P1.00172 Characteristic Phase Behaviors for Symmetric PS-b-PAMAs (n= 1?6) and Their Pressure Dependence , YONGOON LEE, HOYEON LEE, Yonsei University, DONG HYUN LEE, Dankook University, DU YEOL RYU, Yonsei University, YONSEI UNIVERSITY COLLABORATION, DANKOOK UNIVERSITY COLLABORATION — A series of polystyrene-b-poly(alkyl methacrylates) (PS-b-PAMAs) that pertain to the weakly interacting BCP homologues exhibited a variety of phase behaviors by varying alkyl chain length (n) in methacrylate unit. The enthalpic and volumetric changes at phase transitions were measured by the differential scanning calorimetry (DSC) and in-situ spectroscopic ellipsometry with increasing pressure. Together with the overview on the characteristic phase behaviors for symmetric PS-b-PAMAs (n = 1 ? 6), the pressure coefficient (dT/dP) of transition temperatures was calculated on the basis of the Clausius-Clapeyron equation and compared with the reference values. The strong baroplastic character of the closed-loop transitions could be attributed to the significant negative volume changes on mixing at both phase transitions.
P1.00173 Orienting Nanostructured Block Copolymer Thin Films via Entropy, TING-YA LO, Department of Chemical Engineering, National Tsing Hua University, ASHKAN DEGHGHAN, Department of Physics and Astronomy, McMaster University, PROKOPIOS GEORGOPANOS, APOSTOLOS AVGEROPOULOS, Department of Materials Science & Engineering, University of Ioannina, AN-CHANG SHI, Department of Physics and Astronomy, McMaster University, RONG-MING HO, Department of Chemical Engineering, National Tsing Hua University — Controlling the orientation of nanostructured thin films of block copolymers (BCPs) is essential for next generation lithography using BCPs. According to conventional wisdom, the orientation of BCPs is mainly determined by molecular interactions (enthalpy-driven orientation). Here, we demonstrate that entropic effect can be used to control the orientation of BCP thin films. Specifically, the architecture of star-block copolymers consisting polystyrene (PS) and poly(dimethylsiloxane) (PDMS) blocks is used to regulate the entropic contribution to the self-assembled nanostructures. Our experimental and theoretical results unequivocally demonstrate that entropy-driven perpendicular orientation of BCP nanostructures can be induced by increasing the arm number of the star-block copolymers with the same volume fractions of PS and PDMS.

P1.00174 A Facile Method to Fabricate Double Gyroid as a Polymer Template for Nanohybrids, HSIAO-FANG WANG, RONG-MING HO, Department of Chemical Engineering, National Tsing Hua University — Here, we suggest a facile method to acquire double gyroid (DG) phase from the self-assembly of chiral block copolymers (BCPs*), polystyrene-b-poly(L-lactide) (PS-PLLA). A wide region for the formation of DG can be found in the phase diagram of the BCPs*, suggesting that helical phase (H*) from the self-assembly of BCPs* can serve as a stepping stone for the formation of the DG due to an easy path for order-order transition from two-dimensional to three-dimensional (network) structure. Moreover, the order-order transition from metastable H* to stable DG can be expedited by blending the PS-PLLA with compatible entity. Moreover, PS-PLLA blends are prepared by using styrene oligomer (S) to fine-tune the morphologies of the blends at which the molecular weight ratio of the S and compatible PS block (r) is less than 0.1. Owing to the use of the low-molecular-weight oligomer, the increase of BCP chain mobility in the blends significantly reduces the transformation time for the order-order transition from H* to DG. Consequently, nanoporous gyroid SiO$_2$ can be fabricated using hydrolyzed PS-PLLA blends as a template for sol-gel reaction followed by removal of the PS matrix.

P1.00175 Selective Permeating Properties of Butanol and Water through Polystyrene-b-polydimethylsiloxane-b-polystyrene Pervaporation Membranes, CHAEYOUNG SHIN, ZACHARY BAER, X. CHELSEA CHEN, A. EVREN OZCAM, DOUGLAS CLARK, NITASH BALSARA, University of California, Berkeley — Polystyrene-b-polydimethylsiloxane-b-polystyrene (SDS) membranes have been studied in butanol-water binary pervaporation experiments and pervaporation experiments integrated with viable fermentation broths. Polymethylsiloxane has been widely known to be a suitable material for separating organic chemicals from aqueous solutions, and it thus provides a continuous matrix phase in SDS membranes for permeation of small molecules. The polystyrene block provides mechanical stability to maintain the membrane structure in the pervaporation membranes. We take advantage of these features to fabricate a thin and butanol-selective SDS membrane for in situ product removal in fermentation.

P1.00176 Effect of Asymmetric Confinement on the Microdomain Morphology of Block Copolymers, YOUNGKOE KIM, Seoul Natl Univ, GUIDUK YU, Samsung Electro-Mechanics, KOOKHEON CHAR, Seoul Natl Univ — Nanometer scale confinement could impose constraints to change the bulk equilibrium behavior of block copolymers (BCPs). The self-assembly of BCPs confined by two parallel surfaces (one-dimensional confinement) has been both theoretically and experimentally studied. More recently, cylindrical pores where the diameter of the pores are only several repeat periods of the copolymers have been employed to investigate the influence of two-dimensional confinement on the behavior of BCPs. However, the analysis on confinement by asymmetric geometry has not been thoroughly studied yet. Given the size of confining channels, singularity arising from the asymmetric geometry such as triangles and squares, could have a significant effect on the structure and symmetry of BCP morphologies self-assembled within such confinement. We prepared AAOs with triangular pores based on aluminum substrates with inverse-hexagonal packing pattern. Based on the detailed observation of BCP self-assembly within porous triangular columns, we analyzed the structural transition of BCPs induced by asymmetric confinement. Furthermore, we found that the packing frustration imposed by such confinement could be released by adding homopolymers into the BCP system.

P1.00177 Synthesis of zwitterionic polymer-based amphiphilic triblock copolymers by atom transfer radical polymerization for production of extremely stable nanoemulsions, JIN YONG LEE, JI EUN KIM, JIN WOONG KIM, Hanyang Univ — In fields of soft matter, there have been growing interests in utilizing amphiphilic block copolymers due to their intriguing properties, such as surface activity as well as self-assembly. In this work, we synthesize a series of poly (2-(methyleneoxyloxy) ethyl phosphorylcholine)-b-poly (-caprolactone)-b-poly (2-(methyleneoxyloxy) ethyl phosphorylcholine) (PMPC-b-PCL-b-PMPC) triblock copolymers by using atom transfer radical polymerization (ATRP). They have a particular interest in using poly (2-(methyleneoxyloxy) ethyl phosphorylcholine) (PMPC) as a hydrophilic block, since it can have both electrostatic repulsion and steric repulsion in complex fluid systems. Assembling them at the oil-water interface by using the phase inversion method enables production of highly stable nanoemulsions. From the analyses of the crystallography and self-assembly behavior, we have found that the triblock copolymers assemble to form a flexible but tough monomolecular thin film at the interface, which is essential for the remarkable improvement in the emulsion stability.

P1.00178 Ab initio molecular dynamics simulations of the thermal degradation of model compounds of industrially relevant copolymers, EROL YILDIRIM, Fiber and Polymer Science Program, North Carolina State University, ANDREW T. DETWILER, CURT CLEVEN, Eastman Chemical Company, AHMED EL-SHAFEI, MELISSA A. PASQUINELLI, Fiber and Polymer Science Program, North Carolina State University — The thermal degradation of copolymers can be impacted by a variety of factors beyond the chemical composition of the polymer, including the solvent and processing conditions, as well as the presence of oxygen, moisture, additives, and dyes. Thus, we investigated the role that these factors play for a series of model compounds of industrially relevant copolymers using ab initio molecular dynamics simulations. The results reveal some interesting trends and correlations to experiments, which can be applied to improve the exterior longevity of copolymers.

P1.00179 Resonant Soft X-ray Scattering for Soft Materials, CHENG WANG, ATHONY YOUNG, ALEXANDER HEXEMER, HOWARD PADMORE, Lawrence Berkeley National Laboratory — Over the past a few years, we have developed Resonant Soft X-ray Scattering (RSoXS) and constructed the first dedicated resonant soft x-ray scattering beamline at the Advanced Light Source, LBNL. RSoXS combines soft x-ray spectroscopy with x-ray scattering thus offers statistical information for 3D chemical morphology over a large length scale range from nanometers to micrometers. Its unique chemical sensitivity, large accessible size scale, molecular bond orientation sensitivity with polarized x-rays and high coherence have shown great potential for chemical/morphological structure characterization for many classes of materials. Some recent development of in-situ soft x-ray scattering with in-vacuum sample environment will be discussed. In order to study sciences in naturally occurring conditions, we need to overcome the sample limitations set by the low penetration depth of soft x-rays and requirement of high vacuum. Adapting to the evolving environmental cell designs utilized increasingly in the Electron Microscopy community, customized designed liquid/gas environmental cells will enable soft x-ray scattering experiments on biological, electro-chemical, self-assembly, and hierarchical functional systems in both static and dynamic fashion. Recent RSoXS results on organic electronics, block copolymer thin films, and membrane structure will be presented.

P1.00180 CHARGED AND ION-CONTAINING POLYMERS —
P1.00181 Complexation between Charged Dendrimers and Polyelectrolytes, GUNJA PANDAV, VENKAT GANESAN, University of Texas at Austin — We extend the single chain in mean field simulation framework to treat charged nanoparticles in polyelectrolyte solution in presence of explicit counterions and salt. We use two models to depict nanoparticles, viz., soft nanoparticles in the form of dendrimers and hard nanoparticles having impenetrable core and penetrable outer shell. For both models, a systematic analysis of properties of complexes formed due to electrostatic interactions is carried out using radial distribution functions, charge distribution, complex size distribution, etc. In addition, we also comment on the structure of complexes formed as a function of charge on nanoparticles and polyelectrolytes.

P1.00182 The effect of multivalent ions on the thermal transition of hydrated polyelectrolyte multilayers, DARIYA REID, JODIE LUTKENHAUS, Texas A&M University, Department of Chemical Engineering — Layer-by-layer (LbL) assembly is a commonly studied technique in the production of uniform thin films. Hydrate LbL assemblies made of model polyelectrolytes, poly(diallyldimethylammonium chloride) (PDAC) and poly(styrene sulfonate) (PSS), exhibit a thermal transition with features of a glass transition and a lower critical solution temperature transition when assembled in the presence of sodium chloride. The question remains as to how multivalent cations affect the nature of the transition. Here, we present results on the thermal transition of PDAC/PSS LbL assemblies exposed to various multivalent salts. Quartz crystal microbalance (QCM-D) and modulated differential scanning calorimetry (MDSC) is used to assess the transition.

P1.00183 Phase Behavior and Conductivity of Phosphonated Block Copolymers Containing Ionic Liquids, HA YOUNG JUNG, SUNG YEON KIM, MOON JEONG PARK, Pohang Univ of Sci & Tech — As the focus on proton exchange fuel cells continues to escalate in the era of alternative energy systems, the rational design of sulfonated polymers has emerged as a key technique for enhancing device efficiency. While the sulfonic acid group guarantees high proton conductivity of membranes under humidified conditions, the growing need for high temperature operation has discouraged their practical uses in fuel cells. In this respect, phosphonated polymers have drawn intensive attention in recent years owing to their self-dissociation ability. In this study, we have synthesized a set of phosphonated block copolymers, poly(styrenephosphonate-methylbutylene) (PSP-b-PMB), by varying phosphonation level (PL). A wide variety of self-assembled morphologies, i.e., disordered, lamellar, hexagonally perforated lamellae and hexagonally packed cylindrical phases, were observed with PL. Remarkably, upon comparing the morphology of PSP-b-PMB and that of sulfonated analog, we found distinctly dissimilar domain sizes at the same molecular weight and composition. A range of ionic liquids (ILs) were incorporated into the PSP-b-PMB block copolymers and their ion transport properties were examined. It has been revealed that the degree of confinement of ionic phases (domain size) impacts the ion mobility and proton dissociation efficiency of IL-containing polymers.

P1.00184 Molecular Dynamics of Coarse-grained Ionomers Showing Aggregate Morphology During Deformation, JANANI SAMPATH, LISA M. HALL, The Ohio State University — Ionomers are polymers with a small fraction of charged monomers that have a wide range of applications from dental fixtures and packaging to actuators. We consider dense melts of ionomers and counterions with no solvent. An important aspect of their performance is the aggregation of ions, since ionic aggregates act to hold polymer chains together like temporary cross-links. Because of the size scales involved, it is difficult to obtain a complete 3D microscopic picture of polymer aggregation experimentally; typically the thickness of a sample used in transmission electron microscopy is such that multiple overlapping aggregates appear together. How aggregate structure changes under strain and affects mechanical properties is even less clear. We perform molecular dynamics simulations of ionomers of various architectures, and show aggregate morphology and scattering profiles. We apply uniaxial tensile strain and observe the aggregates align, in qualitative agreement with experimental findings. We also obtain stress-strain curves and will discuss effects of degree of neutralization of the ionomers.

P1.00185 Effects of Acid and Ionic Aggregation on the Polymer Dynamics in Precise Ionomers, LURI ROBERT MIDDLETON, University of Pennsylvania, JACOB TARVER, National Institute of Standards and Technology, JASON AZOULAY, DUSTIN MURTAGH, Sandia National Laboratory, KAREN WINEY, University of Pennsylvania — Interest in acid- and ion-containing polymers arises from applications as single-ion conductors for selectively transporting a counter ion of the opposite charge for energy applications. The relatively low dielectric constant of the organic polymer and strong ionic interactions leads to ion aggregation. Ion aggregation anchors the polymer chain, decreasing the mobility of the ionic and the polymer. In precise poly(ethylene-acrylic acid) copolymers and ionomers (pAAA-%Li) we report on the effect of carbon spacer length (x=9, 15, 21) between the acid groups and the effect of the percent of acid groups neutralized with Li on backbone dynamics. The polymer backbone motion is investigated through quasi-elastic neutron scattering measurements. At nano-second timescales a single relaxation fits the data. Systematic changes in dynamics were observed with increasing neutralization percent where polymer dynamics are confined due to anchoring effects. Intriguingly, systematic changes in the spacer lengths did not result in similar behavior. At pico-second timescales multiple overlapping relaxations are observed but even at these short timescales systematic changes in atomic motion are observed with ion content.

P1.00186 Structure and Proton Conductivity in Mixtures of Poly(acrylic acid) and Imidazole, HAN-CHANG YANG, PHILIP J. GRIFFIN, KAREN I. WINEY, University of Pennsylvania, UNIVERSITY OF PENNSYLVANIA TEAM — Proton conductivity in polymer electrolyte membranes (PEMs) typically involves water, which requires that during operation the humidity of the PEM be carefully controlled. In contrast, anhydrous protic polymer membranes promote proton transport by incorporating heterocyclic molecules, such as imidazole and its derivatives, into acid-containing polymers. In this work, we explore the interplay between nanoscale-structure and proton conduction of poly(acrylic acid) (PAA) blended at varying compositions with 2-ethyl-4-methylimidazole (EMI). We present the glass transition temperature from differential scanning calorimetry, morphology characterization from X-ray scattering, and proton conductivity from electrical impedance spectroscopy.

P1.00187 pH-Responsive Behavior of Poly(acrylic acid) Brushes of Varying Thickness, VIVEK YADAV, MEGAN ROBERTSON, JACINTA CONRAD, Univ of Houston — We have investigated the pH-dependent response of polyelectrolyte brushes of varying thickness. Our model system consists of poly(acrylic acid) brushes, which change from hydrophobic and neutral at low pH to hydrophilic and negatively charged at high pH, synthesized using a grafting-from approach at constant grafting density. As the polymer brush thickness increased, the brushes exhibited greater hysteresis in static water contact angle as a function of pH. We extracted the pKa of the polymer brushes from contact angle measurements. The relationship between the pKa and brush thickness was observed to change with the bromine content and increasing in pKa as the brushes were exposed to solutions of varying pH: pKa decreased on increasing bromine content when going from acidic to basic medium. We speculate that the origin of hysteresis can be explained by pH-dependent conformational changes in these polyelectrolyte brushes.
P1.00188 Influence of Hydration Level on Polymer and Water Dynamics in Alkaline Anion Exchange Fuel Cell Membranes, JACOB TARVER, JENNY KIM, MADHU TYAGI, CHRISTOPHER SOLES, National Institute of Standards and Technology, TSUNG-HAN TSAI, BRYAN COUGHLIN, University of Massachusetts - Amherst — Triblock copolymers based on poly(chloromethylstyrene)-b-poly(ethylene)-b-poly(chloromethylstyrene) can be quenched to different extents to yield anion exchange membranes for alkaline fuel cells. In the absence of moisture, these membranes demonstrate bilayer lamellar morphology. Upon high levels of hydration, however, in-situ small angle neutron scattering reveals the emergence of higher-order diffraction peaks. This phenomena has previously been observed in analogous diblock copolymer-based membranes and has been attributed to the induction of a multilamellar morphology in which selective striping of water occurs in the center of the ion-rich domain. By conducting humidity-resolved quasielastic neutron scattering (QENS) measurements using deuterated water, we are able to isolate differences in the pico- to nanosecond timescale dynamics of the hydrogenated membrane upon hydration. QENS measurements in the presence of a hydrogenated water source subsequently permit deconvolution and isolation of the translational and rotational dynamics of water as a function of relative humidity, revealing spatial and temporal changes in polymer and water motion at high levels of hydration.

P1.00189 Understanding the impact of nanoscale aggregation on charge transport and structural dynamics in room temperature ionic liquids, PHILIP GRIFFIN, University of Pennsylvania, ADAM HOLT, University of Tennessee, YANGYANG WANG, Oak Ridge National Lab, ALEXEI SOKOLOV, University of Pennsylvania — Amphiphilic room temperature ionic liquids (ILs) segregate on the nanoscale, forming intricate networks of charge-rich ionic domains intercalated with charge-poor aliphatic domains. While this structural phenomenon has been well established through x-ray diffraction studies and atomistic MD simulations, the precise effects of nanophase segregation on ion transport and structural dynamics in ILs remains poorly understood. Using a combination of broadband dielectric spectroscopy, light scattering spectroscopy, and rheology, we have characterized the ion conductivity, structural dynamics, and shear viscosity of a homologous series of quaternary ammonium ionic liquids over a wide temperature range. Upon increasing the length and volume fraction of the alkyl side chains of these quaternary ammonium ILs, ionic conductivity decreases precipitously, although no corresponding slowing of the structural dynamics is observed. Instead, we identify the dynamical signature of supramolecular aggregates. Our results directly demonstrate the role that chemical structure and ionic aggregation plays in determining the charge transport properties of amphiphilic ILs.

P1.00190 Spray-assisted layer-by-Layer (LbL) assembly of anisotropic materials, SOUVIK DE, PILAR SUAREZ MARTINEZ, AVANTI KAVARTHAPU, JODIE LUTKENHAUS, Department of Chemical Engineering at Texas A&M University — Layer-by-Layer (LbL) assembly has gained tremendous interest as it allows one to incorporate a large variety of molecules with nano-scale precision and very good reproducibility. In addition to charged polymers, the technique has become extremely popular to fabricate tailor-made thin films containing anisotropic nanomaterials (e.g., graphene oxide sheets). The challenge is that a standard protocol to fabricate “all-polyelectrolyte” LbL films may not necessarily give rise to satisfactory film growth when applied to LbL assembly where one of the adsorbing components is an anisotropic nanomaterial. Therefore, in this contribution, we combine polymers and anisotropic nanomaterials via dip- and spray-assisted LbL assembly and investigate the effect of charge density, exfoliation, concentration of the components on the growth behavior and the film quality. The end result is a conformal, pin-hole free coating on model substrates (glass, silicon, metal) over a large area.

P1.00191 Morphology and charge transport in ammonium based polymerized ionic liquids1, MAXIMILIAN HERES, JOSÉP MINUTOLO, JACOB SHAMBLIN, MAIK LONG, Univ of Tennessee, Knoxville, STEFAN BERDZINSKI, VERONIKA STREMEL, Department of Chemistry and Institute for Coatings and Surface Chemistry, Hochschule Niederrhein University of Applied Sciences, Krefeld, Germany, JOSHUA SANGORO, Univ of Tennessee, Knoxville — Ionic conduction, structural dynamics and morphology in a series of ammonium based polymers and anisotropic nanomaterials are investigated using broadband dielectric spectroscopy, temperature-modulated differential scanning calorimetry, and neutron as well as x-ray scattering techniques. The dielectric spectra are dominated on the low frequency regime by electrode polarization while hopping conduction is the underlying mechanism at higher frequencies. At their respective calorimetric glass transition temperatures, a strong correlation between the morphology and ionic conductivity is found. These results are discussed within the recent approaches proposed to explain the decoupling of charge transport from structural dynamics.

P1.00192 Effect of Supercharging on Coacervation Between Proteins and Polyelectrolytes, BRADLEY OLSEN, ALLIE OBERMEYER, CAROLYN MILLS, XUEHUI DONG, MIT — Complex coacervates have attracted a great deal of attention as a method to encapsulate biological molecules including DNA and proteins. However, a large fraction of proteins will not form coacervates with oppositely charged polyelectrolytes. By using mass spectrometry, we are able to quantify the formal charge distribution of proteins after supercharging, and with this knowledge of the chemical state of the protein measure coacervate formation for a panel of proteins as a function of charge. While many of the proteins studied do not form coacervates or coacervate over only a narrow range of composition in their native form, all proteins form coacervates above a critical charge level with increasing range of coacervation as surface charge density increases. The resulting phase change is attributed to the induction of a multilamellar morphology in which selective striping of water occurs in the center of the ion-rich domain. By conducting humidity-resolved quasielastic neutron scattering (QENS) measurements using deuterated water, we are able to isolate differences in the pico- to nanosecond timescale dynamics of the hydrogenated membrane upon hydration. QENS measurements in the presence of a hydrogenated water source subsequently permit deconvolution and isolation of the translational and rotational dynamics of water as a function of relative humidity, revealing spatial and temporal changes in polymer and water motion at high levels of hydration.

P1.00193 RENEWABLE AND SUSTAINABLE POLYMERS —

P1.00194 Synthesis and Characterization of Branched Poly(ester urea)s with Different Branch Density1, JIAYI YU, MATTHEW BECKER, Univ of Akron — A new class of L-phenylalanine-based poly(ester urea)s (PEU) was developed that possess tunable mechanical properties, water uptake ability and degradation rates. Our preliminary data has shown that 1,6-hexanediol L-phenylalanine-based poly(ester urea) possesses an elastic modulus nearly double that of poly(lactic acid). My work details the synthesis of a series of L-phenylalanine-based poly(ester urea)s possessing a variation in diol chain length and in branch density and shows how these subtle structural differences influence the mechanical properties and in vitro biodegradation rates. The elastic moduli span a range of values that overlap with several currently clinically available degradable polymers. Increasingly the diol chain lengths increases the amount of flexible segment in the chemical structure, which results in reduced elastic modulus values and increased values of elongation at break. The amount of branch monomer incorporated into the system reduces the molecular entanglement, which also results in decreased elastic modulus values and increased values of elongation at break. The L-phenylalanine-based poly(ester urea) also exhibited a diol length dependent degradation process that varied between 1.5 ± 0.5% over 16 weeks. Compared with PLLA, PEUs degrade more quickly and the rate can be tuned by changing the diol chain length. PEUs absorb more water and the water uptake ability can be tuned by changing the branch density.

P1.00195 APPLID POLYMER PHYSICS AND ADVANCED MANUFACTURING —

1This work was supported by Akron Functional Materials Center.
P1.00196 Spray Deposition of Multilayer Gas Barrier Thin Films, TARA GIVENS, FANGMING XIANG, JAIME GRUNLAN, Texas A&M Univ — Dip-assisted assembly is the norm for making multilayer thin films (also known as layer-by-layer [LbL] assembly). Spray-based deposition possesses several advantages over dipping, but has not been studied in great detail, especially for gas barrier layers. In this study, polyethyleneimine [PEI]/poly(acrylic acid) [PAA] bilayers were deposited with varying spray parameters. Spraying time was found to be the most influential parameter to control the roughness, thickness, and gas barrier of the PEI/PAA assembly. A spray-coated sample was prepared using optimized parameters and compared to a dip-coated sample using the same deposition time (5s). The sprayed sample was better in terms of thickness, roughness, and gas barrier. This study is the first report showing that a sprayed multilayer assembly has better properties than its dipped counterpart. These findings could revolutionize the multilayer deposition process, making it more commercially-friendly.

P1.00197 Inexpensive Fabrication of Metallic Interconnects on Flexible Substrates1, ADITI NAIK, ROHIT KOTHARI, JAMES WATKINS, University of Massachusetts - Amherst — Sub-micron metallic interconnects on flexible substrates are important to produce inexpensive bendable devices and electronics. The key component hindering high-performance flexible electronics is the lack of high transistor integration density. Previous researchers have created solution-processable semiconductor and dielectric layers; however, sub-micron solution-processable copper electrodes have yet to be developed. Using cost-effective processing techniques, including soft nanolithography and photonic sintering, with a commercial copper oxide ink, we have demonstrated the fabrication of sub-micron copper interconnects on glass and plastic substrates. This inexpensive, solution-processable method is amenable to high-speed printing over large areas by roll-to-roll processing and will lead to the development of low-cost flexible electronics.

1 National Science Foundation

P1.00198 A Molecular Perspective of Inter-filament Bonding in Fused Deposition Modeling 3-D Printing, EDWARD DURANTY, BRANDON SPRADLIN, MARK DADMUN, University of Tennessee — Fused deposition 3D printing is an important tool for low-cost and rapid prototyping of objects with complex geometries. 3D printed materials are composed of many filaments deposited on a heated substrate, requiring the bonding of neighboring filaments during the deposition process. Filament deposition often creates voids between filaments, which requires necking between them to create a robust sample. Therefore the amount of interfacial contact and interdiffusion between filaments become important parameters that control the macroscopic physical properties of the printed prototype. Our research focuses on quantifying the interfacial adhesion between ABS filaments and its impact on structural properties. The time evolution of the temperature profile near the heated substrate demonstrates that the deposited filaments are repeatedly heated above the Tg of ABS allowing interpenetration of the polymer chains between adjacent filaments. Results of DMA experiments on samples of different geometries have been correlated to microphotography that monitors the degree of necking between filaments and the thermal history. Results indicate that interfacial contact area between filaments and increased thermal energy are crucial to their mechanical properties.

P1.00199 THEORY AND SIMULATION OF MACROMOLECULES —

P1.00200 Contrasting Polymer Behavior Under Nanoconfinement using Thermomechanically Consistent Coarse-Grained Models, SINAN KETEN, WENJIE XIA, DAVID HSU, Northwestern University — We present a systematic, two-bead per monomer coarse graining strategy that simulates the thermomechanical behavior of polymers several hundred times faster than all-atom MD (Hsu et al. JCTC, 2014). The predictive capability of the technique is illustrated here for 5 different methacrylate monomers and polystyrene stereoisomers. The approach involves optimization of analytical bonded potentials from atomistic bonded distributions to emulate local structure, as validated by chain end-to-end length and the radius of gyration comparisons with experiments and random coil theory. Nonbonded Lennard-Jones potentials are tuned to reproduce the elastic modulus (E) and glass transition temperature (Tg) at a single thermodynamic state. Density-corrected parameters capture temperature-modulus dependence in the 150-600 K range. Flory-Fox constants of the CG models are commensurate with all atomistic and experimental results, even though all calibrations are done at a single molecular weight. Finally, we further demonstrate the predictive capabilities of the models by examining thin film nanoconfinement effects for different polymers, film thicknesses, interfacial energies, and molecular weights. Our technique, called thermomechanically consistent coarse graining (TCCG), is demonstrated, using polystyrene and poly(methylmethacrylate) as universal benchmarks, to be a robust and effective technique to understand the thermomechanical behavior of polymers thin films and nanocomposites.

P1.00201 ABSTRACT WITHDRAWN —

P1.00202 Coarse-Graining in Simulations of Multicomponent Polymer Systems, VAIDYANATHAN SETHURAMAN, VENKAT GANESAN, Department of Chemical Engineering, University of Texas at Austin, Austin, Texas 78712, USA — We investigate the mapping required between the interaction parameters of two different coarse-grained simulation models to ensure a match of the long-range structural characteristics of multicomponent polymeric system. We investigate the extensibility of mapping functions deduced in the context of symmetric block copolymers by Morse and coworkers to other polymeric systems by studying a variety of systems, including, asymmetric diblock copolymers, symmetric triblock copolymers and diblock copolymer-solvent mixtures. We observe excellent agreement for peak in the inverse structure between two popular coarse grained models for all sets of polymeric melt systems investigated, thus proving that the mapping function proposed for diblock copolymer melts is transferable to other polymer melts irrespective of the blockiness or overall composition. We use our findings to propose a methodology to create ordered morphologies in simulations involving hard repulsive potentials in a computationally efficient manner.

P1.00203 Structural analysis of liquid crystalline order in polymer melts and blends, KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, The University of Akron — Blends of liquid crystalline and flexible polymers have interesting physical behaviors and important applications in organic electronics. We investigate the liquid crystalline transition in melts and blends of semiflexible polymers with Monte Carlo simulations of a bond fluctuation lattice model. For polymer melts we study the influence of attractive interactions on the isotropic to nematic phase transition for different polymer concentrations. We observe that the structure of the ordered phase is different for melts with and without attractive interactions. We construct the phase diagram and find the transition temperature increases with increasing strength of the attractive interaction. To analyze the structure of ordered and disordered regions in polymer melts and blends, we calculate a set of pair distribution functions. We also investigate the effect of an ordering field on the liquid crystalline order in polymer melts and blends.

P1.00204 Size and Shape Descriptors of Two Dimensional Polymer Sheets in Solution near the Crossover Concentration, SALOMON TURGMAN COHEN, JACOBI TANNER, Kettering Univ — We investigate the size and shape of two dimensional polymer sheets near the crossover concentration as a function of sheet size and concentration. Specifically, fully flexible sheets with local square connectivity in implicit, athermal solvent are investigated by molecular dynamics simulations in the NVT ensemble with a Langevin thermostat. Sheet sizes of $N = 100, 400$, and $1600$ are explored. We monitor the average radius of gyration ($R_g$) tensor and the relative shape anisotropy around the cross-over concentration. Opposite to linear, one dimensional polymers, preliminary results show that the size of the sheets as measured by the average radius of gyration increases as the cross-over concentration is approached. The trends in the relative shape anisotropy suggest that the increasing overlap between the sheets at high concentrations leads to the sheets favoring flatter conformations, explaining the larger values of $R_g$ observed.
P1.00205 The effect of copolymers on the interfaces in incompatible homopolymers blend: Molecular dynamics study

JIHO RUY, WON BO LEE, Sogang Univ — Using molecular dynamics simulations the effect of copolymers as compatibilizer for reducing interfacial tension and enhancement of interfacial adhesion at the interface of thermodynamic unfavorable homopolymers blend is studied with block- and graft-copolymers. We have calculated local pressure tensor of system along the axis perpendicular to interface, varying bending potential energy of one part, which consist of just one kind of beads, of copolymer chain to examine the effect of stiffness of surfactin molecules. Here we consider symmetric diblock copolymer (f = 1/2) having 1/2 N make of beads of type A and the other part made of beads of type B, and graft copolymer having backbone linear chain consist of 1/2 N beads of type A and branched with two side-chain consist of 1/4 N beads of type B. All simulations were performed under the constant NPT ensemble at T* ∼ 0.9, ρ* ∼ 0.85. Also we studied changes of effect of copolymers with increasing pairwise repulsive interaction potential between two beads of types A and B while homopolymers chain length are fixed, N=30.

1 Chemical and Biomolecular Engineering, Sogang University, Seoul, South Korea

P1.00206 Monte Carlo Simulations on Phase Transitions and Conformational Properties of Catenated Double-ring Copolymers

DACHUAN SUN, JUNHAN CHO, Dankook Univ — The thermodynamic and conformational properties of catenated double-ring A/B copolymer melts are investigated through lattice Monte Carlo simulations. The topological constraint on the catenated copolymers is shown to suppress demixing of A and B monomers. This action results in their order-to-disorder transition (ODT) at an increased segregation level and the lamellae below ODT with reduced order, when compared to diblock copolymers of linear or single-ring topology. The A and B rings are pulled closer by catenation in the copolymer, which leads to its smaller gyration radius, lamellar domain spacing, and distance between mass centers of the two rings than for the diblock copolymers. With increasing segregation tendencies, the gyration radii of the A rings of the catenated copolymers stretch along the direction normal to lamellae, while the A-block conformations of the single-ring copolymers change their shapes from ellipsoid to sphere.

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P1.00207 Using graphs to interrogate the atomic structure of polymer blends

OLGA WODO, State Univ of NY - Buffalo, BASKAR CANAPATHYSUBRAMANIAN, Iowa State University — The nanomorphology of polymer blend thin films critically affects performance especially in electronic devices. However, many aspects of the underlying physics linking morphology to performance are still poorly understood. Furthermore, there is increasing evidence that atomic organization can hold the key to efficient charge transport within organic electronic devices. In this work, we take advantage of recent advances in molecular dynamic simulations and quantify atomic-scale morphological aspects of the thin films. Specifically, we present a graph-based technique that allows quantifying the point-cloud data. In our approach, we first convert the point cloud data from atomic simulation into a labelled, weighted, undirected graph and then use standard graph-based algorithms to calculate and quantify morphology features. The conversion of the CGMD-data into a graph preserves all the topological and geometric information about the internal structure, and local connectivity between individual atoms/beads (along and across the polymer chains). Our method provides hierarchical information about the charge paths that a hole/electron needs to take to reach the electrode (path length, fraction of intra-molecular hops, path balance). We showcase capabilities of our approach by analyzing coarse grained molecular simulations, and quantifying effect of various thermal treatment as well as electrode materials on the P3HT:PCBM blend.

P1.00208 An atomistic model for cross-linked HNBR elastomers used in seals

NICOLA MOLINARI, ADRIAN SUTTON, Imperial College London, Department of Physics, London SW7 2AZ, UK; JOHN STEVENS, Baker Hughes, Materials Centre of Excellence, Houston, Texas 77019-2118, USA; ARASH MOSTOFI, Imperial College London, Departments of Materials and Physics, London SW7 2AZ and the Thomas Young Centre for Theory and Simulation of Materials, UK — Hydrogenated nitrile butadiene rubber (HNBR) is one of the most common elastomeric materials used for seals in the oil and gas industry. These seals sometimes suffer “explosive decompression,” a costly problem in which gases permeate a seal at the elevated temperatures and pressures pertaining in oil and gas wells, leading to rupture when the seal is brought back to the surface. The experimental evidence that HNBR and its unsaturated parent NBR have markedly different swelling properties suggests that cross-linking may occur during hydrogenation of NBR to produce HNBR. We have developed a code compatible with the LAMMPS molecular dynamics package to generate fully atomistic HNBR configurations by hydrogenating initial NBR structures. This can be done with any desired degree of cross-linking. The code uses a model of atomic interactions based on the OPLS-AA force-field. We present calculations of the dependence of a number of bulk properties on the degree of cross-linking. Using our atomistic representations of HNBR and NBR, we hope to develop a better molecular understanding of the mechanisms that result in explosive decompression.

P1.00209 Pattern Recognition of Adsorbing HP Lattice Proteins

MATTHEW S. WILSON, GUANGJIE SHI, Center for Simulational Physics, University of Georgia, THOMAS WUST, Scientific IT Services, ETH Zurich, DAVID P. LANDAU, Center for Simulational Physics, University of Georgia, FRIEDERIKE SCHMID, Institute of Physics, Johannes Gutenberg University — Protein adsorption is relevant in fields ranging from medicine to industry, and the qualitative behavior exhibited by coarse-grained models could shed insight for further research in such fields. Our study on the selective adsorption of lattice proteins utilizes the Wang-Landau algorithm to simulate the Hydrophobic-Polar (H-P) model with an efficient set of Monte Carlo move Each substrate is modeled as a square pattern of 9 lattice sites which attract either H or P monomers, and are located on an otherwise neutral surface. The fully enumerated set of 102 unique surfaces is simulated with each protein sequence. A collection of 27-monomer sequences is used— each of which is non-degenerate and protein-like. Thermodynamic quantities such as the specific heat and free energy are calculated from the density of states, and are used to investigate the adsorption of lattice proteins on patterned substrates.

1 Research supported by NSF.

P1.00210 Calculating Pressure and Surface Tension of Lattice Polymers

QIANG WANG, PENGFEI ZHANG, Department of Chemical and Biological Engineering, Colorado State University — Calculating pressure and related surface tension of polymeric systems in lattice Monte Carlo simulations is an important but nontrivial subject. Here we propose several novel, efficient, and accurate methods. In the first method, we combine chain insertion/deletion with the Wang-Landau — Optimized Ensemble (WL-OE) simulation, which is very efficient at low to intermediate polymer volume fractions . In the second method, we introduce a repulsive wall with bridging bonds, which is similar to the repulsive wall method but eliminates its confinement effects. This method works especially well at high where all the methods using chain insertion/deletion fail. Finally, we combine the above two methods, which gives complete thermodynamics over the entire range of continuous and exact —values with negligible finite-size effects. To demonstrate our methods, we apply them to calculate the bulk pressure and surface tension of nano-confined homopolymers.
P1.00211 Protein-like folding and other phase transitions of a single polymer chain\textsuperscript{1}, MARK TAYLOR, Dept. of Physics, Hiram College. WOLFGANG PAUL, Martin-Luther-Universit\"{a}t, Halle, Germany. KURT BINDER, Johannes-Gutenberg-Universit\"{a}t, Mainz, Germany. — A single polymer chain can undergo a series of conformational transitions analogous to the phase transitions exhibited by bulk materials. We have recently studied the conformational transitions of a flexible square-well polymer chain using a Wang-Landau simulation approach in which we directly compute the single-chain partition function \cite{1}. For the case of a tangent-sphere chain, the temperature-interaction range phase diagram includes both a coil-globule and globule-crystal transition as well as an “all-or-none” coil-crystal transition. Despite the non-unique homopolymer ground state, the thermodynamics of this direct freezing transition is identical to the thermodynamics of two-state protein folding. Two-dimensional configurational and free energy landscapes reveal both a dominant “folding” pathway and a “dead-end” pathway resulting in a bimodal distribution of structures at the top of the free energy barrier. A simple AB-heteropolymer variant of this model leads to both rod-like and disk-like ground state structures while a fused sphere version of the model produces helical folded structures.

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P1.00212 Simulation of dynamics of disordered diblock copolymers near the order-disorder transition, PAVANI MEDAPURAM, DAVID MORSE, Univ of Minnesota - Twin Cities. — We present a simulation study of the dynamics of composition fluctuations, chain conformations and stress for diblock copolymers near the order-disorder transition. Specifically, we study the behavior of the van Hove function $S(q,t)$, which is a measure of structural relaxation, the linear response of the bond orientation tensor, which is closely related to optical birefringence, and the linear viscoelastic stress relaxation modulus $G(t)$. We show how a slowly decaying mode associated with slow relaxation of composition fluctuations emerges as the degree of segregation is increased.

P1.00213 Conformation of Single Polymer Chains, HOWARD WANG, Binghamton Univ. XIAORONG WANG, Tongji University. — Large biological molecules such as proteins and DNAs can be packed into condensed forms through hydrogen bonding and specific interactions; the conformation of an ultra-long single chain with no specific intra-chain interactions is considered here. We discuss three possible states, (1) uniformly compressed Gaussian, (2) totally irregular aggregates, and (3) long Gaussian sections separated by segments of frustrated local conformation, or “kinks.” Those states could be related to the methods of preparing the condensed form of the single chain globule. We argue that the Gaussian-Kink conformation is preferred and the segregation of kinks to the surface of globules would significantly alter the chain dynamics.

P1.00214 BIOPOLYMERS AND BIOHYBRID POLYMERS —

P1.00215 Binding Affinity Effects on Physical Characteristics of a Model Phase-Separated Protein Droplet, SARA CHUANG, Princeton University. SALMAN BANANI, UT Southwestern Medical Center, MICHAEL ROSEN, UT Southwestern Medical Center, HHH, CLIFFORD BRANGWYNNE, Princeton University. — Non-membrane bound organelles are associated with a range of biological functions. Several of these structures exhibit liquid-like properties, and may represent droplets of phase-separated RNA and/or proteins. These structures are often enriched in multi-valent molecules, however little is known about the interactions driving the assembly, properties, and function. Here, we address this question using a model multi-valent protein system consisting of repeats of Small Ubiquitin-like Modifier (SUMO) protein and a SUMO-interacting motif (SIM). These proteins undergo phase separation into liquid-like droplets. We combine micro rheology and quantitative microscopy to determine affect of binding affinity on the viscosity, density and surface tension of these droplets. We also use fluorescence recovery after photobleaching (FRAP), fluorescence correlation spectroscopy (FCS) and partitioning experiments to probe the structure and dynamics within these droplets. Our results shed light on how inter-molecular interactions manifests in droplet properties, and lay the groundwork for a comprehensive biophysical picture of intracellular RNA/protein organelles.

P1.00216 Fluorescence microscopy techniques for characterizing the microscale mechanical response of entangled actin networks, SAVANNA BLAIR, TOBIAS FALZONE, RAE ROBERTSON-ANDERSON, University of San Diego. — Actin filaments are semiflexible polymers that display complex viscoelastic properties when entangled in networks. In order to characterize the molecular-level physical and mechanical properties of entangled actin networks it is important to know the in-network length distribution and the response of entangled filaments to local forcing. Here we describe two single-molecule microscopy protocols developed to investigate these properties. Using confocal fluorescence microscopy and ImageJ single-filament analysis we develop a protocol to accurately measure the in-network actin length distribution. To characterize the deformation of actin filaments in response to perturbation, we trap micron size beads embedded in the network with optical tweezers and propagate the beads through the entangled filaments while simultaneously recording images of fluorescent-labeled filaments in the network. A sparse number of labeled filaments dispersed throughout the network allow us to visualize the movement of individual filaments during perturbation. Analysis of images taken during forcing is carried out using a combination of vector mapping and skeletonization techniques to directly reveal the deformation and subsequent relaxation modes induced in entangled actin filaments by microscopic strains. We also determine the dependence of deformation modes on the relative filament position relative to the strain.

P1.00217 Assembly, Properties and Function of Synthetic Phase-Separated RNA/Protein Organelles, NICO TAYLOR, SHANA ELBAUM, HOWARD STONE, CLIFFORD BRANGWYNNE, Princeton Univ. — Non-membrane bound RNA/protein (RNP) bodies play a core role in cellular RNA processing steps. Many RNA helicases, required for RNA processing, are key components of RNPs. Consistent with this, a purified RNA helicase, Laf-1, exhibits a salt and protein concentration dependent phase separation in vitro, resulting in liquid-like droplets. We use such synthetic RNPs to study the biophysics of RNP assembly, and to elucidate the link between their physical properties and function. To accomplish this, we are developing custom microfluidic devices to measure biophysical properties, nucleation and growth kinetics, and RNA processing function of droplets. We measure droplet viscosity by applying a shear stress to protein droplets that adhere to the channel wall; measurements are consistent with those taken using a particle micro rheology approach. We also monitor and control protein droplet nucleation using oil/water emulsions. Our results provide a new platform for addressing how the cell regulates organelle assembly and properties through protein, RNA, and ATP concentration. We anticipate that these findings will offer insight into the contribution of RNPs in key RNA processing functions in the cell.

P1.00218 POLYMERS FOR SOLAR ENERGY —
P1.00219 Design of block and graft copolymers for use as compatibilizers in organic solar cell active layers. DYLAN KIPP, VENKAT GANESAN, University of Texas at Austin — Recent experiments have suggested that the use of block and graft copolymer compatibilizers in polymer-based donor-acceptor materials can improve polymer phase separation and improve photovoltaic active layer properties. Inspired by these successes, we use the framework of self consistent field theory to study the influence of copolymer compatibilizers on the interfacial properties of donor-acceptor blends. First, we calculate the reduction in the interfacial tension (and hence the driving force towards macrophase segregation) brought on by the copolymer compatibilizer as a function of the copolymer architecture. Second, we calculate the effective interaction between two copolymer monolayers at the interfaces between the donor and acceptor domains. The results of this second study allow us to comment on the expected ability of the copolymer compatibilizer to reduce the coalescence of domains. Overall, our results suggest important rules for designing copolymer compatibilizers to influence both kinetically-trapped and equilibrium morphologies of donor-acceptor blends.

P1.00220 Self-Assembly of Carotenoids During Solution Casting of Solar Devices. DUSANTHA ALWIS, DILRU RATNAWEERA, University of Sri Jayewardenepura, Sri Lanka, THUSITHA ETAMPAWALA, MARK DADMUN, University of Tennessee, Knoxville, UDUMALAGALA CHANDRIKA, PRADEEP JAYAWEERA, University of Sri Jayewardenepura, Sri Lanka — Self assembly of carotenoids is a common phenomenon in nature and seems to be closely related to the functions of these natural dyes in solar devices. The large absorption coefficients in the visible region of carotenoids make them a well suited natural resource for dye-sensitized solar cells (DSSC). The performance of carotenoid based solar devices mainly depends on the photo-electrochemical properties of the active material (carotenoids) and their self-assembled morphology within solar devices. These associations of molecules will affect the light absorption, emission and energy harvesting abilities of these solar devices. Two types of highly conjugated natural carotenoids having mono and dicarboxy terminal groups, namely bixin and norbixin, were extracted from annatto seeds. In the current study, small angle neutron scattering experiments were carried out to examine the modes of assemblies of bixin and norbixin during solution processing of DSSCs. Spherical shape aggregates with slightly elongated shape at high volume fractions of carotenoids. Bixin and norbixin show different association behaviors as a function of their concentration.

P1.00221 Hydrogen Bonding-mediated Conjugated Polymers for Bulk-Heterojunction Organic Photovoltaics. YEN-HAO LIN, Rice University, WANYI NIE, ADITYA MOHITE, GAUTAM GUPTA, Los Alamos National Laboratory, RAFAEL VERDUZCO, Rice University — We use hydrogen bonding interactions to prevent large scale phase separation and improve polymer blend morphology. Poly(3-hexylthiophene) (P3HT) donor polymer and poly[2,7-(9′-ethyl-carbazole)/2,5-benzothiadiazole] (PCDTBT) acceptor polymer with self-associating, quadruple hydrogen bonding side groups (4)-[1H]-pyrimidinyl, UPy) are used to explore the role of hydrogen bonding associations on blend morphology and photovoltaic performance. We study three systems: P3HT/PCBM, PFTBT/PCBM and P3HT/PFTBT and analyze by AFM, impedance, and device performance. In P3HT/PCBM, the performance is improved from 1.21% to 2.0% using UPy-terminated P3HT due to the enhanced long range order of semi-crystalline P3HT. In PFTBT/PCBM, the performance is decreased from 1.64% to 1.08% using UPy-terminated PFTBT due to entanglement of non-crystalline PFTBT chains. In P3HT/PFTBT system, the performance is improved from 0.43% to 0.77% with the use UPy-terminated P3HT and PFTBT because of suppressed macro-phase separation with maintained long range order of P3HT under annealing temperature. The impedance analysis under short circuit and illumination conditions indicates the faster charge transport and reduced charge recombination within the better performed devices. This study shows that the hydrogen bonding interactions can reduce phase separation but not produce better BHJ devices in all cases perhaps because some phase separation in blends is still required.

P1.00222 Side Chain Engineering of Naphthalenediimide-Based N-type Polymer for High-Performance All-Polymer Solar Cell near 6% Efficiency. CHANGYEON LEE, HYUNBUM KANG, WONHO LEE, TAESU KIM, KI-HYUN KIM, KAISt, HAN YOUNG WOO, PNU, CHENG WANG, Lawrence Berkeley National Laboratory, BUMJOON KIM, KAISt, PUSAN NATIONAL UNIVERSITY (PNU) COLLABORATION, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION — Despite the attractive features of all-polymer solar cells (all-PSCs), i.e., enhanced absorption coefficients, the tunability of their energetic and chemical properties and their thermal and mechanical stabilities, they still face the great challenge of having significantly low power conversion efficiency (PCE) values of only 3-5%. The prominent origins of the poor efficiency of all-PSCs are the undesirable features of the bulk-heterojunction (BHJ) blend morphology including the phase-separated large-scale domain size, reduced ordering of the polymer chains. Tuning side alkyl chains of conjugated polymers is an effective route for manipulating the blend morphology in BHJ type solar cells. However, the role of side chains in all-PSCs is poorly understood. Herein, we report high-performing all-PSCs with 5.96% efficiency by developing a series of naphthalenediimide (NDI)-based copolymers with different alkyl side chains. We demonstrated that the use of the NDI with hexadecyl side chains produced highly-ordered polymer stackings with strong face-on geometry and at the same time, forming the optimal BHJ morphology with finely separated phase domains, all of which contributed together to induce well-balanced µe/µh ratio and generate efficient all-PSCs with PCEs near 6%.

P1.00223 Fabrication of Organic Bulk Heterojunction Solar Cells on Flexible Substrates. GABRIEL CALDERON, MILZAIDA MERCED-SANABRIA, CAROLYN CARRADERO-SANTIAGO, JOSEE VEDRINE-PAULÉUS, University of Puerto Rico-Humacao — The active layer for the organic solar cells fabricated is composed of P3HT:PCBM, poly(3-hexylthiophene) (P3HT) as electron donor and phenyl-C61-butyric acid methyl ester(PCBM) as electron acceptor. These polymers were used due to their promising characteristics for devices such as bulk heterojunction solar cells. We used polyethylene terephthalate (PET) substrates, a highly flexible plastic, with indium tin oxide (ITO) as the transparent conducting anode for the device, and UV lithography technique to pattern the ITO; this is to facilitate their promising characteristics for devices such as bulk heterojunction solar cells. We used polyethylene terephthalate (PET) substrates, a highly flexible plastic, with indium tin oxide (ITO) as the transparent conducting anode for the device, and UV lithography technique to pattern the ITO; this is to facilitate multipurpose devices on a single substrate. The fabrication process for pattern transfer incorporates developing and etching processes. We diluted the HCI and DI water to etch out the ITO. PEDOT:PSS and active layer of P3HT:PCBM were deposited on (3.0 sq-cm) patterned of ITO/PET by spin coating method. The cathode was thermally evaporated with Al. We characterized the device using a sourcemeter. We also simulated portions of the device using PET on graphene as the substrate.

P1.00224 ORGANIC ELECTRONICS AND PHOTONICS —

P1.00225 Electrocataluminescent Ion Gels for DC-Driven, Sub-2V Solid-State Emissive Devices by Incorporating Redox Coreactants. HONG CHUL MOON, TIMOTHY P. LODGE, C. DANIEL FRISBIE, University of Minnesota — We have demonstrated a solid-state DC-driven electrocataluminescent (ECL) device using a solution processable, emissive ECL gel based on polystyrene-block-polymyristylmaleimide (PS-b-PMMI) and Pt(II) complex (1,1′-bipyridyl)tri(2,3-dimethylmalonato)platinum(II) (Pt-bdt-MA). This ECL gel incorporates butyrammonium oxalate (TBAOX) was incorporated into the ECL gel for a coreactant strategy. Oxalate can be viewed as a consumable fuel for the device providing reducing power and cutting the overall operating voltage. The device was fabricated by a simple two-step solution process. Application of 1.6 V DC bias across the device resulted in the onset of light emission. The maximum luminance was achieved at 1.5 mole ratio of ECL luminophore (Ru(bpy)3)2+(PF6)2− and TBAOX, and the turn-on voltage was independent of the composition. The simplicity of the ECL device and its low voltage operation characteristics make it potentially attractive as a display element for printed electronics.

3TPL and CDF acknowledge financial support from the Air Force Office of Scientific Research under FA9550-12-1-0067.
P1.00226 Ferroelectric switching behavior in morphology controlled ferroelectric-semiconductor polymer blends for organic memory, EUNHEE LIM, GREGORY SU, EDWARD KRAMER, MICHAEL CHABINYC, University of California, Santa Barbara — Memory is a fundamental component of all modern electronic systems. Organic ferroelectric memories are advantageous because they are thin and lightweight devices that can be made printable, foldable, and stretchable. Organic ferroelectric memories comprise a physical blend of an organic semiconducting polymer and an insulating ferroelectric polymer as the active layer in a thin film diode. Controlling the thin film morphology in these blends is important for electrical properties of the resulting device. We have found that when a semiconducting thiopeptide polymer with polar alkanoate side chains (P3EPT) is blended with well-studied ferroelectric polymer poly-[vinylidenefluoride-co-trifluoroethylene] P (VDF-TrFE), the resulting film has low surface roughness and more controllable domain sizes compared to the widely used poly (3-hexylthiophene). This difference allows more reliable study of the ferroelectric switching behavior in devices with domain size of about 100nm. The influence of the 3D composition measured by a combination of methods, including soft x-ray microscopy, on the electrical characteristics will be presented.

P1.00227 Microscopic simulations of electronic excitations in donor-acceptor heterojunctions of small-molecule based solar cells, BJÖRN BAUMEIER, Max Planck Institute for Polymer Research — Fundamental processes involving electronic excitations govern the functionality of molecular materials in which the dynamics of excitons and charges is determined by an interplay of molecular electronic structure and morphological order. To understand, e.g., charge separation and recombination at donor-acceptor heterojunctions in organic solar cells, knowledge about the microscopic details influencing these dynamics in the bulk and across the interface is required. For a set of prototypical heterojunctions of small-molecule donor materials with C60, we employ a hybrid QM/MM approach linking density-functional and many-body Green’s functions theory (DFT/GW-BSE) to polarizable force fields, and analyze the charged and neutral electronic excitations therein. We pay special attention the spatially-resolved electron/hole transport levels, as well as the relative energies of Frenkel and charge-transfer excitations at the interface. Finally, we link the molecular architecture of the donor material, its orientation on the fullerene substrate as well as mesoscale order to the solar cell performance.

P1.00228 Enhancing the Thermoelectric Characteristics of PEDOT:PSS Through the Incorporation of a Redox-Active Small Molecule, EDWARD TOMLINSON, MATTHEW WILLMORE, XIAOQIN ZHU, BRYAN BOUDOURIS, Purdue University — The polymer composed of poly(3,4-ethylene dioxythiophene) and poly(styrene sulfonate) (PEDOT:PSS) is a leading organic thermoelectric material due to its high-performing properties. Here, we establish the effect of incorporating the redox-active small molecule 4-hydroxy-2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO-OH) on the structural and thermoelectric properties of PEDOT:PSS. Specifically, the thermoelectric power factor (PF) was monitored as a function of TEMPO-OH loading, elucidating a clear trend in the PF. Importantly, at loadings as low as 5% TEMPO-OH, by mass, the thermopower of the sample was increased by a factor of two. Furthermore, the role of the TEMPO-OH on the thin film morphology of the composite material is examined through the use of grazing incidence-wide angle x-ray scattering (GI-WAXS) and atomic force microscopy (AFM). Despite the acidic conditions associated with the presence of PSS, the existence of radical functionality is confirmed through electron paramagnetic resonance (EPR) spectroscopy. Through careful tuning, the optimized conditions outlined within this work results in PF gains in excess of 40%.

P1.00229 Morphology optimization for enhanced performance in organic photovoltaics, OLGA WODO, JAROSŁAW ZOLÁ, State Univ of NY - Buffalo, BASKAR GANAPATHYSUBRAMANIAN, Iowa State University — Organic solar cells have the potential for widespread usage due to their low cost-per-watt and mechanical flexibility. Their widespread use, however, is bottlenecked primarily by their low solar efficiencies. Experimental evidence suggests that a key property determining the solar efficiency of such devices is the final morphological distribution of the electron-donor and electron-acceptor constituents. By carefully designing the morphology of the device, one could potentially significantly enhance their performance. This is an area of intense experimental effort that is mostly trial-and-error based, and serves as a fertile area for introducing mechanics and computational thinking. In this work, we use optimization techniques coupled with computational modeling to identify the optimal structures for high efficiency solar cells. In particular, we use adaptive population-based incremental learning method linked to graph-based surrogate model to evaluate properties for given structure. We study several different criterions and find optimal structure that that improve the performance of currently hypothesized optimal structures by 29%.

P1.00230 Facile Control of a Wide Range of Regioregularity: Significant Influence on Mechanical and Electrical Properties of Conjugated Polymers, JIN-SEONG KIM, JAE-HAN KIM, WONHO LEE, KAIST, HOJEONG YU, POSTECH, HYEONG JUN KIM, KAIST, INHO SONG, JOON HAK OH, POSTECH, TAEG-SOO KIM, BUMJOON KIM, KAIST, POSTECH COLLABORATION — While regioregularity (RR) has been known to have a strong influence on inherent properties of conjugated polymer, systematic study of RR has been limited due to the lack of synthetic methodology. Herein, we prepared a series of poly(3-hexylthiophenes) (P3HTs) having a wide range of RR from 64 to 98% by the modified Grignard metathesis method that utilizes the dimer moiety. We observed that the RR determines crystalline behavior, mechanical and electrical properties of P3HT. Although higher RR P3HT had higher hole mobility, its increased degree of crystallinity induced fragile nature of polymers (elongation break <1%). In contrast, lower RR had lower elastic modulus and thereby leading to significant reduction of fragility. Therefore, our finding suggested that the control of RR is critical to regulate the properties of conjugated polymers between electrical performance and mechanical resilience as depending on the purpose of the applications. (i.e flexible portable devices vs high performance panel)

P1.00231 Using COMSOL Multiphysics Software to Analyze the Thin Film Resistance Model of a Conductor on PET, CAROLYN CARRADERO-SANTIAGO, MILZAIDA MERCED-SANABRIA, JOSEE VEDRINE-PAULÉUS, University of Puerto Rico-Humacao — In this research work, we will develop a virtual model to analyze the electrical conductivity of a thin film with three layers, one of graphene or conducting metal film, polyethylene terephthalate (PET) and Poly(3,4-ethylenedioxythiophene) Polystyrene sulfonate (PEDOT-PSS). COMSOL Multiphysics will be the software used to develop the virtual model to analyze the thin-film layers. COMSOL software allows simulation and modeling of physical phenomena represented by differential equations such as that of heat transfer, fluid movement, electromagnetism and structural mechanics. In the work, we will define the geometry of the model; in this case we want three layers-PET, the conducting layer and PEDOT-PSS. We will then add the materials and assign PET as the lower layer, the above conductor as the middle layer and the PEDOT-PSS as the upper layer. We will analyze the model with varying thickness of the top conducting layer. This simulation will allow us to analyze the electrical conductivity, and visualize the model with varying voltage potential, or bias across the plates.
**P1.00232 Study of biodegradable polymers for “green” devices**, CARLOS PEREZ, XIAOMEI JIANG, University of South Florida, JIANG GROUP TEAM — II— conjugated polymers such as polythiophenes are conventional picks for cost-effective organic solar cells. However, these organic semiconductors are not environment-friendly since the polymer backbones require temperature higher than 300°C to be decomposed, thus will cause potential environment problems upon disposal. In this work, the optical and electronic properties of biodegradable polymers, conjugated poly(disulfidediamine), were examined via continuous wave laser spectroscopy, FTIR spectroscopy and conductivity measurement. We found that the attachment of a side chain to aromatic ring increases both photo and thermal stability, as well as higher conductivity. Thermal annealing improved the film morphological, photophysical and electronic properties. Photo-Induced Absorption (PIA) reveals different features comparing with conventional pi-conjugated polymers. No observation of long-lived photoexcitations such as polarons or triplets which are common with pi-conjugated polymers. Instead, we found the formation of low energy species upon thermal annealing in these biodegradable polymers.

**P1.00233 Electron transport and light absorption/emission in molecular complexes**, MIGUEL MARTINEZ, Bronx High School of Science, LEV MOUROKH, Physics Department, Queens College of CUNY — In this work, we address photon-assisted electron transport in molecular triads and tetrads connected to the leads. Donor-bridge-acceptor triads are promising candidates for efficient organic solar cells, as the photon absorption makes it possible to transfer electrons against the applied voltage. Deriving and solving numerically the equations of motion for electron creation/annihilation operators, we obtain the parameters of molecular complexes which are optimal for a maximal efficiency of the light harvesting. For donor-bridge-acceptor tetrads, we determine the conditions for another phenomenon, optical up-conversion. Electron transport along the applied voltage and the photon absorption at one of the bridges facilitates the photon emission at another bridge with higher frequency. Using the same equations of motion approach, we obtain the emitted electromagnetic energy and its dependence on the system parameters.

**P1.00234 Nanostructural Patterning Improves the Performance of Non-volatile Polymer Memory Devices**, SEUNG HYUN SUNG, BRYAN W. BOUDOURIS, Purdue University — Organic nonvolatile memory devices based on polymer ferrocene materials are a promising approach toward the development of low-cost memory due to the ease of processing and flexibility associated with the device. Here, we focus on a memory device with a two-component active layer and a diode structure. This ferrocene diode (FeD) has a nanosstructured active layer, composed of ferroelectric and semiconducting polymers, and it can provide easy access to high-performance polymer-based memory devices. In order to create these nanostructured active layers, we have utilized electron beam (e-beam) lithography for the simple fabrication of a desired pattern on the ferroelectric polymer layer. Then, a semiconducting polymer was deposited into the nanosporous ferroelectric layer to complete the ordered heterojunction. By optimizing the nanostructure, the memory retention and ON/OFF current density ratio performance of FeD is greatly enhanced (e.g., the ON/OFF ratio is a factor of 3 greater) over a traditional blended diode. This ability to control the ferroelectric polymer morphology will open new fields of evaluating the relationships between structure and performance in organic memory devices.

**P1.00235 Cross-linking high-k fluoropolymer gate dielectrics enhances the charge mobility in rubrene field effect transistors**1, JWALA ADHIKARI, MATTHEW GADINSKI, QING WANG, ENRIQUE GOMEZ, Penn State University — Polymer dielectrics are promising materials where the chemical flexibility enables gate insulators with desired properties. For example, polar groups can be introduced to enhance the dielectric constant, although fluctuations in chain conformations at the semiconductor-dielectric interface can introduce energetic disorder and limit charge mobilities in thin-film transistors. Here, we demonstrate a photopatternable high-K fluoropolymer, poly(vinylidene fluoride-bromotrifluoroethylene) P(VDF-BTFE), with a dielectric constant between 8 and 11. The bromotrifluoroethylene moiety enables photo-crosslinking and stabilization of gate insulator films while also significantly enhancing the population of trans torsional conformations of the chains. Using rubrene single crystals as the active layer, charge mobilities exceeding 10 cm2/Vs are achieved in thin film transistors with cross-linked P(VDF-BTFE) gate dielectrics. We hypothesize that crosslinking reduces energetic disorder at the dielectric-semiconductor interface by suppressing segmental motion and controlling chain conformations of P(VDF-BTFE), thereby leading to approximately a three-fold enhancement in the charge mobility of rubrene thin-film transistors over devices incorporating uncross-linked dielectrics or silicon oxide.

1Center for Flexible Electronic, Penn State; The Dow Chemical Company

**P1.00236 Monte Carlo simulations of charge transport in heterogeneous organic semiconductors**, PYIE PHYO AUNG, KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, Departments of Physics and Chemistry, The University of Akron, Akron, OH 44325-4001 — The efficiency of organic solar cells depends on the morphology and electronic properties of the active layer. Research teams have been experimenting with different conducting materials to achieve more efficient solar panels. In this work, we perform Monte Carlo simulations to study charge transport in heterogeneous materials. We have developed a coarse-grained lattice model of polymeric photovoltaics and use it to generate active layers with ordered and disordered regions. We determine carrier mobilities for a range of conditions to investigate the effect of the morphology on charge transport.

**P1.00237 ABSTRACT WITHDRAWN**

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**P1.00239 ABSTRACT WITHDRAWN**

**P1.00240 The impact of P3HT molecular weight and solvent composition on P3HT films processed from binary solvent mixtures**, LAWSON LLOYD, MADELEINE GORDON, DAVID BOUCHER, College of Charleston — Recent experimental endeavors have shown that well-ordered P3HT assemblies formed in solution can improve the crystallinity and morphological uniformity of thin films and composites, thereby providing a promising new route to more efficient polymeric optoelectronic materials. We have studied the assembly and crystallinity of two regioregular poly(3-hexylthiophene) (P3HT) samples, M∞ = 28 kDa and M∞ ≈ 65 kDa, in several different binary mixtures of organic solvents. We use an excitonic coupling analysis of the UV/Vis absorbance spectra to assess the impact that the solvent and the molecular weight of P3HT have on the relative structural order of the polymer assemblies. In addition, we investigate the influence that the solvent composition and the structural order of P3HT aggregates have on the assembly and organization of P3HT films. We use optical and atomic force microscopy techniques to study thin films of P3HT processed from different solvent mixtures. Our results show that relatively small variations to the P3HT solutions can produce significant changes in the morphology and macromolecular structures of the P3HT films.

**P1.00241 POLYMERS IN BATTERIES AND ELECTROCHEMICAL CAPACITORS**

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P1.00242 In situ Mechanistic Investigation of an Organic Radical Polymer Cathode on Interfacial Charge Transport and Cycling Stability, FEI LI, JODIE LUTKENHAUS, Artie McGinnis, Department of Chemical Engineering, Texas A&M University — Organic radical polymers have gained increased attention as cathodes for organic radical batteries due to their fast charge transport and high cycling stability. These features make them a promising alternative to conventional lithium-ion batteries. One polymer of interest is a nitroxide radical polymer, poly(2,2,6,6-tetramethylpiperidinylxomethacrylate) (PTMA), which is capable of a two-electron transfer process. The specific capacity of PTMA as cathode has a reported value between 77 to 220 mAh/g, depending on the charge/discharge conditions. Most work with PTMA has largely emphasized electrode optimization to improve its capacity by adding highly conductive materials or by designing new forms of radical polymers. There is little molecular level detail on the charge storage process and electrode/electrolyte interfacial activities in such systems. Here, we present the application of in situ characterization techniques towards the charge storage process in PTMA. Electrochemical quartz crystal microbalance with dissipation monitoring (EQCM-D) monitors various electrode physical properties (e.g. mass, shear viscosity) during controlled electrochemical interrogation (cyclic voltammetry, charge discharge). Electrochemical impedance spectroscopy probes various charge storage and transport events at a range of frequencies and potentials. With this information attained, a clearer picture of charge storage in organic radical cathode batteries can be formed.

P1.00243 Flexible Hybrid Electrodes Containing Vanadium Pentoxide (V$_2$O$_5$) and an Electron- and Ion-Conducting Diblock Copolymer for Energy Storage, HYOSUNG AN, JARED MIKE, Texas A&M University, Chemical Engineering, KENDALL SMITH, LISA SWANK, YEN-HAO LIN, STACY PESEK, RAFAEL VERDUCZO, Rice University, Chemical and Biomolecular Engineering, JODIE LUTKENHAUS, Texas A&M University, Chemical Engineering — Vanadium pentoxide (V$_2$O$_5$) is a promising cathode material for Lithium-ion batteries due to its high capacity, high energy density, and cost-effectiveness. However, its low lithium-ion diffusion coefficient ($10^{-12}$ - $10^{-13}$ cm$^2$/s), low electronic conductivity ($10^{-2}$ - $10^{-3}$ S/cm), and severe volumetric changes during cycling have hindered its application in practical devices. One way to address these issues is to use hybrid electrodes that incorporate a second active material. For this purpose, poly(3-hexylthiophene)-block-poly(ethylene oxide) (P3HT-b-PEO) block copolymer containing electron- and ion-conducting polymer blocks was introduced to a V$_2$O$_5$ electrode system. Cathodes are prepared by mixing aqueous dispersions of block copolymer, V$_2$O$_5$, and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) and drop casting. The V$_2$O$_5$ and P3HT-b-PEO hybrid electrode showed synergistic results, having improved electrochemical storage performance and mechanical property. We also demonstrated a flexible battery prototype using the P3HT-b-PEO/V$_2$O$_5$ cathode.

P1.00244 Phase Behavior and Electrochemical Performance of Solid-State Magnesium Ion Electrolytes from Diblock Copolymers, JACOB THELEN, University of California Berkeley; Lawrence Berkeley National Laboratory, SEBNEM INCEOGLU, Lawrence Berkeley National Laboratory, NITASH BALSARA, University of California Berkeley; Lawrence Berkeley National Laboratory — Batteries utilizing magnesium metal anodes are considered a promising candidate for the next generation of energy storage with performance beyond lithium ion technology. The development of a safe, stable magnesium ion-conducting electrolyte represents one of the major barriers to the advancement of magnesium battery technology. One approach to increasing the safety and stability of electrolytes is to replace flammable organic solvents with more stable polymeric electrolytes. We report on the phase behavior and electrochemical performance of solid-state magnesium ion electrolytes derived from diblock copolymers.

P1.00245 Polyhedral Oligomeric Silsesquioxanes – Based Hybrid Electrolytes with Controlled Network Structure, QIWEI PAN, South China University of Technology; Drexel University, CHRISTOPHER LI, Drexel University, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, SOUTH CHINA UNIVERSITY OF TECHNOLOGY TEAM, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, DREXEL UNIVERSITY TEAM — High ion conductivity and mechanical integrity are the most important properties in the application of solid polymer electrolytes (SPEs). We herein report synthesis and characterization of hybrid electrolytes with inorganic polyhedral oligomeric silsesquioxanes (POSS) as the crosslinker. The SPEs were prepared by a facile one-pot reactions between octakis[3-(glycidyloxy)propyl] trimethoxysilane and bis(3-aminopropyl) terminated poly(ethylene glycol) (PEG) in the present of bis(trifluoromethanesulfonamide) lithium salt (LiTFSI). Uniform distribution of POSS and LiTFSI in the SPEs were confirmed by SEM-BSD and SEM-EDX. We show that both ionic conductivity and mechanical properties of the SPE can be easily tuned by varying POSS contents. Correlation between the SPE network structure and the ionic conductivity and mechanical properties will be discussed.

P1.00246 HIERARCHICAL ASSEMBLY OF BLOCK COPOLYMERS AND SOFT NANOPARTICLES IN SOLUTIONS. –

P1.00247 Structure and Ionic Conductivity Evolution of a Block Copolymer Electrolyte during Thermal Annealing, MAHATI CHINTAPALLI, NITASH BALSARA, Univ of California - Berkeley — Mixtures of block copolymers (BCPs) and lithium salts are promising materials for battery electrolytes because they exhibit high ionic conductivity and high modulus. However, since most polymer electrolytes show high conductivities only at temperatures above ambient, it is important to understand how the structure and ionic conductivity of BCP electrolytes evolve during thermal annealing. In situ small angle X-ray scattering and ac impedance spectroscopy were used to characterize a BCP electrolyte, lamellar polystyrene-block-poly(ethylene oxide) mixed with lithium bis(trifluoromethanesulfonylimide) (LiTFSI), during thermal annealing. As annealing progressed, long range lamellar order and domain spacing increased, and scattering contrast between the two BCP phases decreased. A concomitant decrease in ionic conductivity was observed.

P1.00248 β−NMR Measurements of Lithium Ion Transport in Thin Films of Pure and Lithium-Salt-Doped Poly(ethylene oxide), IAIN MCKENZIE, TRIUMF, MASASHI HARADA, University of British Columbia, C.D. PHILLIP LEVY, TRIUMF, W. ANDREW MACFARLANE, RYAN M.L. MCFADDEN, University of British Columbia, GERALD D. MORRIS, TRIUMF, SHIN-ICHI OGATA, Toyota Central Research and Development Laboratories, Inc., MATTHEW R. PEARSON, TRIUMF, JUN SUGIYAMA, Toyota Central Research and Development Laboratories, Inc. — β−Detected nuclear spin relaxation of $^6$Li$^+$ has been used to study the microscopic diffusion of lithium ions in thin films of poly(ethylene oxide) (PEO), PEO with lithium bis(trifluoromethanesulfonylimide) (LiTFSI), PEO with lithium triflate (LiTf) and PEO with lithium trifluoroacetate (LiTfA) with monomer-to-salt ratios of 8:3:1. Hopping of Li$^+$~ above ~ 250 K follows an Arrhenius law in all of the films. Diffusion of Li$^+$ is fastest in pure PEO and decreases in order LiTFSI > LiTF > LiTfA. We observed the activation energy for hopping ($E_A$) and the intrinsic hop rate ($r_0$) both increasing in order LiTfA < LiTF < LiTFSI < PEO but the larger $r_0$ outweighs the larger $E_A$ and results in Li$^+$ motion being fastest in the pure polymer. The results will be discussed in terms of the ionicity of the salt.
P1.00249 Increase of the Effective Dispersity in ARB-Type Triblock Copolymer  
SANGHOON WOO, HYUNJUNG JUNG, JUNE HUH, Department of Chemical and Biological Eng., Korea University, Seoul 136-713, Korea, JOONA BANG, Department of Chemical and Biological Eng., Korea University, Seoul 136-713, Korea — The domain spacing of block copolymer (BCP) has been mainly controlled by molecular weight and block immiscibility. Instead of these traditional variables, we designed a new type of BCP, namely ARB type triBCP, where the R represents the short middle block composed of A and B random copolymers. It was expected that the R block provide the effect of increasing “effective” dispersity via compositional distribution leading to an increased domain size compared to the AB diBCP with same MW and dispersity. We prepared various ARB type triBCPs and AB diBCPs having the similar dispersity via living-radical polymerization, and their morphologies were characterized by TEM, SAXS, and GIXSAXS. As a result, it was shown that the ARB-type triBCP exhibited a significant increase in the domain spacing compared to the AB diBCPs with same MW and dispersity. These results were also compared with theoretical viewpoint.

P1.00250 Control Large Nanoparticle Assemblies in Supramolecular Nanoparticle Thin Films  
JINGYU HUANG, TING XU, University of California, Berkeley — Nanocomposites can generate new properties beyond those offered by organic and inorganic building blocks. Nanospheres assembled by self-assembly are often very uniform in size and spatial arrangements. With the recent development, colloidal synthesis and surface modification methods provide inorganic nanoparticles (NPs) with various sizes, compositions, and properties in a facile manner. Block copolymer-based supramolecules further provide more versatile routes to control spatial arrangement of the nanoparticles over multiple length scales. Nanoparticle size is a critical parameter determining the optical and electronic properties. However, most of studies to date focused on nanoparticle smaller than 10 nm in size. Here, our recent studies showed that the assembly of nanoparticles with size larger than 10 nm can be achieved in the supramolecular nanocomposite thin films by finely tuning the ligand-polymer interactions and the sample treatment conditions. Both the overall morphology of the nanoparticle assemblies and inter-particle distances can be readily tailored. These new results opened a viable approach to construct functional materials using nanoparticles with different quantum confinement effects.

P1.00251 Crystallization Driven Responsive Janus Assembly  
HAO QI, SHAN MEI, CHRISTOPHER LI, Drexel university, SOFT MATERIALS LAB TEAM — Responsive and dynamic nanostructures are ubiquitous in Nature, and they are also utter importance for applications such as sensing and drug delivery. Herein we report a series of hierarchical block copolymer nanostructure that is able to undergo 2D (sheet-like) to 3D (bowl-like) shape changing upon specific external stimuli. Freestanding Janus nanosheets were prepared via crystallization-driven self-assembly of poly(ε-caprolactone)-b-poly(acrylic acid) (PCL-b-PAA) and subsequent crosslinking and disassembly process. Due to the mechanical contrast between the two layers, and the chemical responsiveness of the PAA layer, such Janus nanosheets transform a mechanically stable nanobowl upon pH change. Atomic force microscopy and transmission electron microscopy results confirmed the Janus structure and bending behavior. Detailed structural characterization and shape changing mechanisms will be discussed.

P1.00252 Meso-scale Modeling of Self-assembly of Polymer-Grafted Nanoparticles  
DERRICK MANCINI, Illinois Inst of Tech, SANKET DESHMUKH, SUBRAMANIAN SANKARANARAYANAN, Argonne National Laboratory — We develop meso-scale models to explore the self-assembly behavior of polymer-grafted nanoparticles. Specifically, we study nanoparticles with grafts of the thermo-sensitive polymer poly(N-isopropylacrylamide) (PNIPAM), which undergoes a coil-to-globule transition across the LCST at around 305 K. The atomic-scale mechanism of the coil-to-globule transition of polymers grafted nanoparticles and their interactions (agglomeration, assembly behavior) with other particles that are in its vicinity is poorly understood, yet knowledge about these interactions would enable designing novel self-assembled materials with well-defined structural and dynamical properties. Additionally, the effects of chemical nature, geometry, and morphology of the nanoparticle surface on the conformational transition of thermo-sensitive polymers is also unknown. We report on 1) development of all-atom models of polymer-grafted nanoparticles to conduct MD simulations at atomic-levels and 2) perform mesoscopic scaling of the conformational dynamics resulting from the atomistic simulations with the aid of coarse-grained or meso-scale models of PNIPAM and its composites. Coarse-grained simulations allow modeling of larger assemblies of polymer-grafted nanoparticles over longer time scales.

P1.00253 Mesoscale Polymer Assemblies  
SATYAN CHOUDHARY, JONATHAN PHAM, ALFRED CROSBY, University of Massachusetts Amherst — Materials encompassing structural hierarchy and multi-functionality allow for remarkable physical properties across different length scales. Mesoscale Polymer (MSP) assemblies provide a critical link, from nanometer to centimeter scales, in the definition of such hierarchical structures. Recent focus has been on exploiting these MSP assemblies for optical, electronic, photonics and biological applications. We demonstrate a novel fabrication method for MSP assemblies. An important innovation in this method is the length scale and volume of such assemblies. A new methodology developed uses a simple piezo-actuated motion for de-pinning of a polymer solution trapped by capillary forces between a flexible blade and a rigid substrate. The advantages of new method include ability to make MSP of monodisperse length and to fabricate sufficient volumes of MSP to study their physical properties and functionality in liquid dispersions. We demonstrate the application of MSP as filler for soft materials, providing rheological studies of the MSP with surrounding matrices.

P1.00254 SURFACES INTERFACES AND POLYMERIC THIN FILMS –

P1.00255 Structure of polymer brushes on flat substrates and its dependence on the conditions of the surface-initiated polymerization  
ROHAN PATIL, JIRI SROGL, North Carolina State Univ, DOUGLAS KISEROW, US Army Research Office, JAN GENZER, North Carolina State Univ — We demonstrate an efficient method of degrafting surface anchored poly(methyl methacrylate) (PMMA) brushes using tetra butyl ammonium fluoride (TBAF). The grafted polymers are grown using standard atom transfer radical polymerization method which provides good control by varying the catalyst ratio (Cu(II):Cu(I)). The sample surface has been characterized before and after degrading by means of X-ray photoelectron spectroscopy, ellipsometry, and time-of-flight secondary ion mass spectrometry. The degraded polymer has been characterized using highly sensitive size exclusion chromatography, which provided information about the complete molecular weight distribution. The grafting density of PMMA chains is calculated as 0.517 chains/μm². The study of the dependence of the grafting density on the ATRP inhibitor/catalyst ratio evidences to an effect of early termination of the growing chains when a lower control on the polymerization step is exercised. Control of the degrading process is provided by tuning time, temperature, concentration of the TBAF, which - in conjunction with spatial control - allows for the creation of polymer brush patterns and surface gradients.

P1.00256 Tribological properties of adsorbed PEO nanolayers on planar solids  
WENDUO ZENG, NAISHENG JIANG, JAKE LINDBERG, MAYA K. ENDOH, TADANORI KOGA, State University of New York at Stony Brook — We report tribological properties of irreversibly adsorbed poly(ethylene-oxide) (PEO) nanolayers onto planar Si substrates. The adsorbed nanolayers (~ 3 nm in thickness) were derived from spin-coating polymer thin films (~ 50 nm in thickness) via thermal annealing and subsequent solvent leaching with water. We characterized the formation process of the adsorbed nanolayers and the detailed surface/film structures by using x-ray reflectivity, grazing incidence x-ray diffraction, and atomic force microscopy. In addition, the contact angle and adhesive property of the adsorbed layers were characterized. We will discuss the structure-property relationship of the adsorbed nanolayers.

1T. K. acknowledges the partial financial support from NSF Grant No. CMMI-1332499.
P1.00257 Effects of the Adsorbed Polymer Nanolayers on the Dewetting of Polystyrene Thin Films

1. JUSTIN CHEUNG, JIAJUN WANG, NAISHENG JIANG, MAYA ENDOH, TADANORI KOGA, Stony Brook University — It was previously reported that irreversibly adsorbed polymer nanolayers can be produced on solid substrates by thermal annealing. This study sought to determine the impact of the adsorbed nanolayers on film stability of ultrathin polystyrene (PS) films. A series of bilayers composed of the bottom PS adsorbed nanolayers and PS overlayers with different molecular weights were prepared as model systems. The surface structures of the bilayer films annealed above the bulk glass transition temperature were analyzed by using optical and atomic force microscopes. We will discuss the unique roles of the adsorbed polymer chains in the stability of the liquid thin films.

T. K. acknowledges the partial financial support from NSF Grant No. CMMI-1332499.

P1.00258 Coatings with Thermally Switchable Surface Energy Produced From Block Copolymer Films

1. RAEL DAVIS, RICHARD REGISTER, Princeton University — Polymer-based coatings are employed across a wide array of sectors. One application of such coatings is to impart a prescribed surface energy, i.e. hydrophilic or hydrophobic character. The present work explores an approach to create surfaces with thermally switchable wetting behavior by employing coatings based on block copolymers which possess both hydrophilic and hydrophobic segments. The amphiphilic block copolymers were synthesized by coupling allyl-ended poly(ethylene oxide) (PEO) and hydride-ended poly(dimethylsiloxane) (PDMS) oligomers via a Pt catalyst. One PEO-PDMS diblock possessed an order-disorder-transition-temperature (TODT) of 64°C as characterized by small angle x-ray scattering. Above the TODT the polymer is a disordered melt, but below this temperature it self-assembles into alternating lamellae with a repeat spacing of 7.7 nm. When cooled through the TODT in vacuum or dry air, the PDMS-enriched domains wet the film’s surface, producing a hydrophobic surface with a contact angle (CA) ≈ 90° as measured from CA goniometry. However, when cooled under water or in humid air, a PEO-rich hydrophilic surface is produced, yielding CAs ranging from 20-40°. The coatings can then be reversibly switched between the two states by reheating above the TODT, exposing to the appropriate environment, and re-cooling, ideally “locking in” the structure until the next processing cycle. The TODT, and thus the switching temperature, can be continuously tuned by blending with PEO-PDMS diblocks of different molecular weights.

P1.00259 Potential Energy Calculations for Water Adsorption on Poly (methyl methacrylate) Films

1. MATEUSZ J. ZUBA, PATRICK HOWARD, BRIAN FAMILIO, THORIN KANE, ROSS L. NETUSIL, CAROLINA C. ILIE, State University of New York at Oswego — The generosity of the NOYCE Research Grant enabled me to focus on the study of various polymers. The main goal was to study the molecular orbitals of poly (methyl methacrylate) (PMMA) and calculate the energy band gap. We also performed the potential energy calculations for our system: two polymer chains and water molecules. We obtained the activation energy from thermal desorption spectra of water on poly (methyl methacrylate) by employing Arrhenius analysis.
P1.00264 Effect of Interfaces on Self-diffusion and Glass Transition Temperature of Poly(isobutyl methacrylate) Thin Films, REIKA KATSUMATA, AUSTIN DULANEY, CHRISTOPHER ELLISON, University of Texas at Austin - McKetta Department of Chemical Engineering — In thin films, physical properties such as the glass transition temperature (Tg), modulus, and viscosity, are different compared to that in thick films due to higher interfacial area to volume ratio. However, the effects of film thickness and associated interfaces on self-diffusion are not well understood, partly because only a few techniques are available for such studies. In this study, we employed fluorescence recovery after patterned photobleaching to evaluate the self-diffusion coefficient (D) of fluorescently labeled poly(isobutyl methacrylate) (PiBMA, Mn = 11 kg/mol, PDI = 1.2). Films 16 - 300 nm in thickness were spin coated onto two substrates then D and Tg were examined: one set of films possessing attractive polymer/substrate interactions on silica substrates, and the other set possessing repulsive polymer/substrate interactions using poly(cyclohexylethylene) substrates. D was measured in the melt state (Tg = 48 K) and the D of thick films were identical to the bulk value regardless of the substrate type. The D of a ~19 nm thick film on a repulsive substrate was four times larger than its bulk value while Tg was increased by about 10-15 K. In contrast, attractive substrates typically do not affect D or Tg of PiBMA.

P1.00265 Programming Surface Energy Driven Marangoni Convection in Polymer Thin Films to Generate Topographic Patterns, CHAE BIN KIM, DUSTIN JANES, TALHA ARSHAD, JOSHUA KATZENSTEIN, NATHAN PRISCO, DANA MCGUFFIN, ROGER BONNÉCAZE, CHRISTOPHER ELLISON, University of Texas at Austin - McKetta Department of Chemical Engineering — The Marangoni effect describes how fluid flows in response to gradients in surface energy. We recently developed a method for photochemically preprogramming spatial surface energy patterns in glassy polystyrene (PS) thin films. UV irradiation through a mask selectively dehydrogenates the PS, thus increasing surface energy in the UV exposed regions compared to the unexposed regions. After heating the film to the liquid state, transport of polymer occurs from regions of low surface energy to regions of high surface energy. This method can be harnessed to rapidly manufacture polymer films possessing prescribed three-dimensional topographies reflective of the original light exposure pattern. To quantify and verify this phenomenon, a theoretical model that gives a more thorough understanding of the physics of this process, its limits and ways to apply it efficiently for various target metrics will also be presented along with comparisons between theoretical predictions and experimental observations. Finally, while PS dehydrogenation can be used to produce a variety of topographical patterns, judicious selection of the photosensitizing compounds in an otherwise transparent polymer expands the use of this method to more readily available light sources.

P1.00266 Work of adhesion and separation between soft elastomers1, NANSHU LU, University of Texas at Austin — The JKR (Johnson-Kendall-Roberts) method is widely used to measure the work of adhesion between soft materials. In this paper, the JKR theory is summarized and three dimensionless parameters are proposed to design a proper JKR experiment. The work of adhesion and the work of separation between two commonly used soft elastomers PDMS (Sylgard 184) and Ecoflex 0300 are obtained with the measured pull-in and pull-off forces using a dynamical mechanical analyzer (DMA). The effect of crosslinking density and solvent extraction are examined. It is found that the pull-in adhesion stays more or less constant for all contact pairs we measured. While the effect of crosslinking density is not significant for pristine PDMS, it is very obvious that the higher self-adhesion can be found in less crosslinked PDMS after solvent extraction. Such an effect is even more drastic for PDMS-to-Ecoflex adhesion. A unified adhesion mechanism is proposed to explain these complex adhesion behaviors. It is concluded that the chain-matrix interaction is the most effective adhesion mechanism compared to chain-chain or matrix-matrix interactions and the three interactions are exclusive to each other.

P1.00267 BLOCK COPOLYMER THIN FILMS —

P1.00268 The Effect of Hydrogen Bonding on the interfacial width of PS-b-PMMa Block Copolymer Microdomains, KYUSEONG LEE, SUNGYUN HAN, SANGSHIN JANG, JICHEOL PARK, JONGHEON KWAK, JIN KON KIM1, Pohang Univ of Sci & Tech — Sharp interface between two blocks in block copolymer nano pattern is one of the important issues because of strong demand in industrial applications to nano-patterning. We utilized hydrogen bonding between N-(4-aminomethyl-benzyl)-4-hydroxymethyl-bezamide (BA) and urea (U) at the interface of polystyrene-block-poly(methyl methacrylate) copolymer (PS-PMMa). For this purpose, we first synthesized PS by ATRP method, then the end group was converted to amino group. Next, it was reacted with BA, followed by reaction with 4-pentynoic acid, resulting in alkény-lined terminated group. In this study, azide-alkyne click reaction between PS-U-BA-alkyne and PMMA-azide, PS-U-BA-PMMa was synthesized. We investigated, via small angle X-ray scattering and transmission electron microscopy, phase behavior of PS-U-BA-PMMa.

P1.00269 Long-Range Ordering of Block Copolymers on Well-Controlled Patterned Substrates, DONG-EUN LEE, NAM-KYUN KIM, JINA PARK, DONGHYUN LEE, Dankook University — In this study, we achieved long-range ordering of block copolymers (BCPs) by combining solvent-annealing process and well-controlled patterned substrates. Nano-lines of poly(tetrafluoro ethylene) (PTFE) were firstly fabricated in large area as a PTFE bar was rubbed on Si substrates at 340 °C. The amplitude and pitch distance of PTFE nanolines were around 17 nm and 150 nm, respectively. Then, asymmetric polystyrene-block-poly(2-vinylpyridine) copolymers (PS-b-P2VP) were subsequently spin-coated on the patterned substrates after a thin layer of poly(vinyl alcohol) (PVA) was prepared on the PTFE patterned substrates to enhance the wettabillity of BCP thin films. As BCP thin films were solvent-annealed in vapor of organic solvents, highly ordered BCP nanostructures oriented either parallel or perpendicular to the surface were generated in large area. In addition, the nanopatterns were successfully transferred to the underlying PVA layer or Si substrate by dry etching. Thus, the resulting nanopatterns were utilized as templates to synthesize inorganic nanofeatures. The ordering behavior of BCP thin films on the patterned substrates was characterized by using AFM, SEM and GI-SAXS.

P1.00270 Macroscopic Alignment of Cylindrical Block Polymer Thin Film via Raster Solvent Vapor Annealing with Soft Shear, MING LUO, DOUGLAS SCOTT, THOMAS EPPS, University of Delaware — One challenge associated with the utilization of block polymer thin films in nanotechnology is the difficulty of orienting and aligning the self-assembled nanostructure on macroscopic length scales, as block polymers typically self-assemble in an isotropic manner in the absence of surface forces and external fields. In this work, macroscopic alignment of block polymer cylinders was achieved through raster solvent vapor annealing with soft shear. Spatial control over nanoscale structures was accomplished through the application of a solvent vapor delivery nozzle, poly(dimethylsiloxane) shearing pad, and motorized stage. Complex patterns such as dashes, cross-shapes, and curved structures were demonstrated along with the possibility of scale-up for industry production. The simplicity of instrumentation and the versatility of patterns possess advantages over other directed self-assembly methods that are currently available.
P1.00271 Tracking Solvent Uptake in Block Polymer Thin Films during Solvent Vapor Annealing. CAMERON SHELTON, University of Delaware, RONALD JONES, JOSEPH DURA, National Institute of Standards and Technology, THOMAS EPPS, University of Delaware — A key goal in the block polymer (BP) thin films community is the design of a template-free, universal annealing method to control nanoscale self-assembly over large length scales. Solvent vapor annealing (SVA) offers a unique solution to this challenge with its ability to tune substrate surface, free surface, and polymer-polymer interactions by exposing films to appropriate solvents. However, there is little understanding of how the solvent behaves during the SVA process. In this work, we utilized the combination of deuterated solvents with small-angle neutron scattering (SANS) and neutron reflectometry to track solvent uptake in poly(styrene-b-isoprene-b-styrene) thin films. Two solvents were chosen for this analysis: d-hexane (isoprene selective) and d-benzene (styrene selective). Our work has shown that solvent choice and partial pressure have a significant impact on how solvent segregates within individual polymer domains and the film as a whole, directly impacting the restructuring of polymer domains. This work provides further understanding of the mechanism behind SVA, thereby making it easier to select appropriate conditions for desired self-assembly control.

P1.00272 ABSTRACT WITHDRAWN —

P1.00273 Optimization and Characterization of Self-assembled Triblock Polymer Membranes with Chemically-Tunable Pore Wells for Nanofiltration Applications. JESSICA SARGENT, RYAN MULVENNA, RAFAEL PRATO, Purdue University, JACOB WEIDMAN, WILLIAM PHILLIP, University of Notre Dame, BRYAN BOUDOURIS, Purdue University — The ability to control nanoscale self-assembly over large length scales and the field of block polymer-based membranes for separation applications has grown considerably in the past several years. However, decreasing the domain sizes of these membranes to below 5 nm has proven to be a challenge in many instances. Here, we demonstrate that a triblock polymer, polyisoprene-b-polystyrene-b-poly(tet-butyl methacrylate) (PI-PS-PtBMA), can be utilized to form nanoporous membranes capable of high flux and high selectivity based on both size and chemical composition. By controlling the synthesis, solution self-assembly, and non-solvent induced phase separation of these polymers, a scalable fabrication process can produce thin-film membranes that feature monodisperse pores approaching 1 nm in diameter, tunable pore-wall chemistry, good mechanical stability, and chlorine degradation resistance. The PtBMA functionality can further be converted to a number of side chain functionalities through simple coupling chemistry to produce membranes with specific chemical and structural characteristics tailored to meet the needs of various applications. In particular, these membranes provide a promising, inexpensive platform for chlorine degradation and fouling-resistant membranes for water purification that can be produced on an industrial scale.

P1.00274 Thin Films of Bottlebrush Block Copolymers with Homopolymer. GAJIN JEONG, Univ of Mass - Amherst, BENJAMIN R. SVEINBJORNSSON, ROBERT HOWARD GRUBBS, California Institute of Technology, THOMAS P. RUSSELL, Univ of Mass - Amherst, POLYMER SCIENCE AND ENGINEERING DEPARTMENT, UNIVERSITY OF MASSACHUSETTS AMHERST TEAM, CHEMISTRY DEPARTMENT, CALIFORNIA INSTITUTE OF TECHNOLOGY TEAM — We have investigated the self assembled structures of bottlebrush block copolymers (BrBCPs) in thin films by blending deuterated homopolymer. By use of neutron reflectivity (NR), the assemblies with microdomain oriented parallel to the substrate, the distribution of the homopolymer in the bottlebrush block copolymer was obtained. Polynorbornene-backbone-based bottlebrush BCPS with polylactide (PLA) and polystyrene (PS) side chains of different molecular weights were investigated. Small angle x-ray scattering was used to complement the NR studies.

P1.00275 Investigation of solvent annealing time dependence on morphology formation in polystyrene–block–polylactide thin films. RYAN GNABASIK, GUNNAR NELSON, ANDREW BARUTH, Creighton Univ — Solvent vapor annealing exposes a block polymer film to the vapors of one or more solvents, swelling the film. This process increases polymer mobility and can direct a self-assembly process by tuning the surface energy. Despite its efficacy to produce well-ordered, periodic nanostructures, no standardized production scheme exists. This is primarily due to a lack of understanding the intricate role multiple, incommensurate parameters play. By analogy to thermal annealing of elemental solids, the time a thin film spends in an equilibrium solvent concentration is one factor that will dictate the degree of ordering. To elucidate, optimized annealing conditions for perpendicular cylinder forming polystyrene-block-polylactide exist at solvent concentrations just below the order-disorder transition, where the kinetic and thermal processes required for recrystallization and crystal growth are optimally fast (similar to thermal annealing). By use of a purpose-built, climate-controlled solvent annealing chamber, we map out the annealing time dependence for non-optimized solvent concentrations. Namely, at lower solvent concentrations, where mobility is limited, longer times are required for large lateral correlation lengths. In situ spectral reflectance monitors solvent concentration, regulated via a mass-flow controlled solvent inlet, offering precision control over annealing. Atomic force microscopy, in conjunction with O2 plasma etching, provides 3-dimensional imaging of the nanoscale morphology. This work was funded by NASA Nebraska Space Grant.

P1.00276 Controlling Structure in Sulfonated Block Copolymer Membranes. PHUC TRUONG, GILA STEIN, Univ of Houston, JOE STRZALKA, Argonne National Lab — In many ionic block copolymer systems, the strong incompatibility between ionic and non-ionic segments will trap non-equilibrium structures in the film, making it difficult to engineer the optimal domain sizes and transport pathways. The goal of this work is to establish a framework for controlling the solid-state structure of sulfonated pentablock copolymer membranes. They have ABCBA block sequence, where A is poly(t-butyl styrene), B is poly(hydrogenated isoprene), and C is poly(styrene sulfonate). To process into films, the polymer is dissolved in toluene/n-propanol solvent mixtures, where the solvent proportions and the polymer loading were both varied. Solution-state structure was measured with small angle X-ray scattering (SAXS). We detected micelles with radii that depend on the solvent composition and polymer loading. Film structure was measured with grazing-incidence SAXS, which shows (i) domain periodicity is constant throughout film thickness; (ii) domain periodicity depends on solvent composition and polymer loading, and approximately matches the micelle radii in solutions. The solid-state packing is consistent with a hard sphere structure factor. Results suggest that solid-state structure can be tuned by manipulating the solution-state self-assembly.

P1.00277 Capillary forces induced wrinkling onto ultrathin single and bilayer polymer films. JOOYOUNG CHANG, JOSEPH PAULSEN, KAMIL TOGA, NARAYANAN MENON, THOMAS RUSSELL, Univ of Mass - Amherst — We have studied wrinkling phenomena on ultrathin polymer sheets floated onto the aqueous media. As previously studied (Science, 2007, 317(5838), 650–653, and Soft Matter, 2013, 9, 8293–8296), the capillary forces of a water droplet placed on a floating sheet generate compressive hoop stresses, causing the sheet to wrinkle. In our current work, we investigate this phenomenon over a broader range of film thicknesses (7 nm to 950 nm) of Polystyrene (PS), Poly(methyl methacrylate) (PMMA), as well as with PS/PMMA bilayers. We report that the Young’s modulus of PS (Mw: 97K) inferred from the wrinkle pattern is not significantly affected even if the thickness of PS is less than 10 nm. Furthermore, we also show that the type of the polymer (i.e. PS or PMMA) of the bottom layer of the bilayer system affects the length of the wrinkles.

1 Keck Foundation
2Kamil Bugra Toga is currently working at Eastman Chemical Company.

P1.00278 POLYMER COMPOSITES —
P1.00279 Electrical Properties of PVDF Based Nanocomposites. JERRY CONTRERAS, HEINRICH D. FOLTZ, The University of Texas Pan American, YUPING DUAN, Dalian University of Technology, China, HASINA F. HHUQ, STEVEN C. TIDROW, MIRCEA CHIPARA, The University of Texas Pan American — Nanocomposites based on polyvinylidene fluoride (PVDF) have been obtained by melt mixing, loading the polymeric matrix with various weight fraction (between 0 % to 40 %) of different fillers (multiwalled carbon nanotubes, carbon nanofibers, and barium titanate). Pellets of nanocomposites have been obtained by hot pressing at about 175 °C. Copper contacts have been deposited on the as-obtained pellets and the electrical features have been measured by using the two point technique. PVDF is a semicrystalline ferroelectric and piezoelectric polymer with a glass transition temperature of -35 °C and a melting temperature of about 175 °C. Electrical measurements have been performed in a wide range of frequencies starting from dc to ac (up to about 250 MHz). The dependence of the resistivity and dielectric constant on frequency and temperature (between -50 °C to 150 °C) was investigated in detail. Supplementary DSC, WAXS, and Raman data provided detailed information regarding the effect of fillers on phase transitions (glass, crystallization, and melting) and crystalline composition/structure of these nanocomposites.

P1.00280 Additive-Driven Assembly of Block Copolymer and Nanoparticles: Influence of Nanoparticle Size and Loading1, YUE GAI, Univ of Mass - Amherst, YING LIN2, 3M, JAMES WATKINS3, Univ of Mass - Amherst — Additive-driven assembly of block copolymer (BCP)/nanoparticle (NP) composites in which functionalized NPs exhibiting strong hydrogen bond interactions with one domain of the BCP has been shown to strengthen phase segregation and yield well-ordered materials at high NP loadings. Here we report a systemic study of how phase behavior and NP distribution in BCP/ Au NP composites are influenced by the NP size, NP loading and block copolymer domain size. 2nm, 5nm, 9nm and 15nm diameter Au nanoparticles at loadings ranging from 10% to 50% weight percent, in polystyrene-block-poly (2-vinyl pyridine) block copolymers with domain spacing ranging from 14 nm to 75 nm were used in the investigation. We find that strong interactions enable the incorporation of larger diameter NPs with respect to domain size as compared to systems in which interactions between the NP and BCP are weak or enthalpically neutral.

P1.00281 Mechanically Robust Polymer-Graphene Aerogels, HEONJOO HA, University of Texas at Austin - McKetta Department of Chemical Engineering, KADHIRAVAN SHANMUGANATHAN, National Chemical Laboratory, Pune, Maharashtra, India, CHRISTOPHER ELLISON, University of Texas at Austin - McKetta Department of Chemical Engineering — Graphene has been intensely studied for the past several years due to its many attractive properties. Graphene oxide (GO) aerogels are particularly interesting due to their light weight and excellent performance in various applications, such as environmental remediation, super-hydrophobic and super-oleophilic materials, energy storage, etc. However, GO aerogels are generally weak and delicate which complicates their handling and potentially limits their application outside the research lab. The focus of this work is to synthesize mechanically stable aerogels that are robust and easy to handle without substantially sacrificing their low density. To overcome this challenge, we found that by intermixing a small amount of readily available and thermally crosslinkable polymer can enhance the mechanical properties without disrupting other characteristic intrinsic properties of the aerogel itself. This method is a simple straight-forward procedure that does not include any tedious chemical reactions or harsh chemicals. Furthermore, we will demonstrate the performance of these materials as a super-absorbent and pressure sensor.

P1.00282 Life-time of the bound layer in nanocomposites, DAN ZHAO, JACQUES JESTIN, SANAT K. KUMAR, Columbia University — It is now well accepted that an effectively irreversibly adsorbed monolayer of polymer forms when a polymer melt is intimately mixed with nanoparticles, in the limit where their enthalpic interactions are favorable. This bound layer has been postulated as being a central player in many of the highly favorable properties that result from polymer based nanocomposite materials. We investigated well-defined nanocomposites formed with different combinations of deuterated and hydrogenated polymers (P2VP and PMMA) and silica nanoparticles. SANS, in conjunction with contrast variation, then provides a direct means of probing the structure of the bound layer as a core-shell and its exchange kinetics with bulk (unbound) chains with annealing time and temperature. SANS directly provides information on the particle-particle partial structure factor and particle dispersion. Thermodynamic equilibrium of the bound layer is reached one day at 150 °C while its exchange life time is ~ one hour at 180 °C.

P1.00283 POLYMER NANOCOMPOSITES: ACTIVE PARTICLES AND DYNAMICS —

P1.00284 Unusual dielectric loss properties of carbon nanotube - polyvinylidene fluoride composites in low frequency region (100 Hz < f <1 MHz)1, GUANG-LIN ZHAO, YI ZHEN, JUAN ARREDONDO, Physics Department, Southern University and A&M College — Systematic investigations on the dielectric properties of multi-walled carbon nanotubes (MWCNTs)-polyvinylidene fluoride (PVDF) composites with a wide MWCNT concentration range (2-9wt%) have been carried out. It was revealed that the dielectric constant are increased by the addition of an appropriate amount of MWCNTs at room temperature. However, when the concentration of MWCNTs in the composites reaches above 5wt%, negative dielectric constants and large dielectric loss in the composites are observed in the low frequency range. The ferroelectric CNT-PVDF polymer composites containing more than 5 wt% MWCNTs have a strong dielectric absorption, which has the potential for acoustic applications.

P1.00285 Dispersion of bimodal polymer brushes functionalized anisotropic gold nanoparticles in polymer nanocomposites1, LILI ZHU. Peking University Shenzhen Graduate School, GI XUE, Nanjing University, LINDA REVEN, McGill University — Polymer nanocomposites (PNCs), which are composed of the nanofiller component and polymer matrix, have attracted growing interests due to their fascinating properties. Great efforts have been made to achieve high compatibility between the nanofillers and the polymer matrix. The dispersion of spherical gold nanoparticles (GNPs) in the matrix have been extensively studied, while there are few studies using anisotropic GNPs. The goal of this work is to produce homogeneous PNCs of anisotropic NPs in stimuli responsive polymer matrix. We compared the dispersion of gold nanoparticles (GNPs) with single and bimodal poly(2-vinylpyridine) P2VP brushes. Bimodal brushes consist of mixture of low and high molecular weight (Mw) polymers. GNPs with P2VP were dispersed into polymer matrix and the Mw of the matrix was systematically varied to investigate the Mw effect. UV-Visible-Near Infrared spectroscopy was utilized to monitor the special plasmonic properties and architectures of GNPs. The dispersion and morphology of PNCs were characterized by electron microscopy. This work will help to establish the correlations between the properties of anisotropic NPs (shape and protecting ligands) and the miscibility of corresponding PNCs.

1We gratefully acknowledge the National Science Foundation of China (nos.21404002)
P1.00286 Time-resolved WAXD studies on the crystallization of isotactic polypropylene/graphene nanocomposites, SHOTARO NISHITSUJI, MAYA ENDOH, YICHEN GUO, MIRIAM RAFAILOVICH, TADANORI KOGA, Department of Materials Science and Engineering, Stony Brook University — Graphene is one layer of carbon atoms, which has good electronic, thermal conductivity and mechanical properties. By adding graphene to isotactic polypropylene (iPP), the mechanical and electrical properties of the polymer are significantly improved. To further achieve high performance of iPP/graphene nanocomposites ("NCs"), it is important to investigate the relationship between the crystalline structure of iPP and the mechanical property of the iPP/graphene NCs. In this study, the effect of the graphene on the crystallization behavior of the polymer was investigated by using time-resolved wide angle X-ray diffraction (WAXD). The iPP/graphene NCs with different weight ratios of graphene were prepared by using a twin screw extruder. After temperature jump from 210 °C (>Tm) to 170 °C, the melt-crystallization process was observed by in situ WAXD. The results showed that the crystalline structure of all the samples was still α-form that is the same as the neat PP, while the ratios of the diffraction peaks are quite different from those of the neat PP. We will discuss the detailed structure in this presentation.

P1.00287 Rheology and Phase Transitions in Highly Filled Additive/Block Copolymer Composites, BENJAMIN M. YAVITI1, ROHIT KOTHARI2, H. HENNING WINTER3, JAMES J. WATKINS4, University of Massachusetts Amherst — We have recently demonstrated that strong, segment-specific interactions between multi-functional additives (organics, nanoparticles and nanotubes) and one segment of a block copolymer can yield highly filled, well-ordered composites. In this study we used rheology to determine phase transitions and materials properties in systems containing high volume fractions of nanoparticles that are not accessible in by other means. We utilized well-defined surface functionalized nanoparticle systems by which we can assess the role of the number, strength, and surface density of functional groups on the phase behavior and mechanical properties of the composites. From this study, we developed an understanding of the interactions and structure between nanoparticles and block copolymer, and the mechanisms by which these characteristics are affected by temperature.

P1.00288 PEO-MWCNTs Nanocomposites: The Effect of the Nature of Solvent on the Morphology and Physical Properties of Nanocomposites, ALFONSO SALINAS, CHARLES CARTWRIGHT, KEVIN L. NEWCOMBE, MIRCEA CHIPARA, IBRAHIM ELMAM, JAMES HINTHORNE, DORINA M. CHIPARA, KAREN LOZANO, The University of Texas at Pan American — PEO-MWCNTs nanocomposites have been obtained by dissolving the polymer within selected solvents (water, ethanol, toluene, and chloroform), addition of the nanofiller (Multiwalled Carbon Nanotubes: MWCNTs), dispersion of the as obtained mixture by stirring at 500 rotation per minute for 1 h followed by a sonication for 30 minutes using a high power sonicator (500 W), and solvent evaporation in an oven at 110 °C, for 10 h. Nanocomposites containing 0 to 40 wt % MWCNTs have been obtained and investigated. Scanning Electron Microscopy was used to assess the dispersion of MWCNTs within the polymeric matrix. Wide Angle X-Ray Scattering, Raman, FTIR, and UV-VIS were used to characterize the crystalline structure and molecular/atomic motions in the as obtained samples. Differential Scanning Calorimetry was used to estimate the glass, crystallization, and melting temperatures. Thermal stability will be questioned by thermogravimetric analysis. The effect of the nature of the solvent on the dispersion of nanotubes and on the physical properties of the as obtained nanocomposites will be analyzed in detail.

P1.00289 Photo-actuating waveguiding fibers based on light responsive hydrogels, YING ZHOU, ADAM HAUSER, Univer of Mass - Amherst, NATHAN RASMUSSEN, MARK KUYZYK, Washington State University, RYAN HAYWARD, Univ of Mass - Amherst — The combination of light-absorbing nanoparticles with thermally sensitive hydrogels has been widely explored as a strategy for photo-thermal actuation. Here, we employ a system of photo-crosslinkable copolymers containing pendant benzenophene units to prepare planar waveguiding polymethylmethacrylate(PMMA) fibers patterned with poly(N-isopropyl acrylamide) (PNIPAM) copolymer hydrogels containing Au nanoparticles. These structures show both thermally- and photo-actuated bending behavior due to swelling stresses developed in the PNIPAM gel layer. Further, we establish that light can be successfully guided into micro-patterned fibers, yielding a route to remotely controlled micro-actuators.

P1.00290 Polymer Grafted Nanoparticle-based Oil Dispersants, DAEHAK KIM, RAMANAN KRISHNAMOORTI, Univ of Houston — Particle-based oil dispersants mainly composed of inorganic nanoparticles such as silica nanoparticles are considered as environmentally friendly oil dispersants due to their biocompatibility and relatively low toxicity. The oil-water interfacial tension is reduced when nanoparticles segregate to the oil-water interface and this segregation is improved by grafting interfacially active polymer brushes. In this study, surfactant-like amphiphilic block copolymers were grafted from silica nanoparticles using an atom transfer radical polymerization (ATRP) method in order to increase their interfacial activity. We have studied the interfacial activity of such hybrid nanoparticles using pendant drop interfacial tension measurements, and their structure using small angle X-ray scattering. Amphiphilic grafted nanoparticle based significantly reduced oil-water interfacial tension compared to the interfacial tension reduction induced by homopolymer grafted nanoparticles or the corresponding free ungrafted copolymer. Moreover, hard and stable oil-water emulsions were formed by applying the block copolymer grafted nanoparticles due to the formation of interparticle network structures, which were observed by cryo-scanning electron microscopy (SEM) and small angle neutron scattering (SANS).

P1.00291 PNIPAM grafting on the surface of zirconium phosphate, HAI LI, XUEZHEN WANG, ZHENGDONG CHENG, Texas A&M Univ, DR.CHENG'S GROUP TEAM — We are reporting for the first time the grafting of the thermoresponsive polymer PNIPAM (poly N-isopropylacrylamide) on the surface of inorganic nanopolates zirconium phosphate. Particularly, the grafting on inorganic nanopolates using gamma rays has never scarcely been reported and yet proved to be successful in our synthesis. We proved that by gamma ray irradiation, the peroxide groups has been produced on the ZrP particles since that peroxide groups, on the surface of the hexagonal nanoplates, which upon heating initiated the free radical polymerization and subsequent attachment of PNIPAM. The presence of covalent band between ZrP and PNIPAM were observed and characterized by TGA, FTIR and solid state NMR respectively. The attachment of a thermoresponsive polymer to ZrP nanocrystals brings thus remarkable possibilities for their employment in the fields of medicine, oil industry, as well as physics.

P1.00292 Toward Designer Nanoparticle Assemblies: Supramolecular Nanocomposites on Patterned Surfaces, KATHERINE EVANS, JOSEPH KAO, TING XU, Univ of California - Berkeley — Nanoparticles have unique properties due to the quantum confinement effect. Controlled assemblies of nanoparticles of different sizes and chemical composition are predicted to have new optoelectronic properties. Supramolecules are ideal structural framework to guide nanoparticle assemblies in thin films without modifying the particle ligand chemistry. We recently showed that optically patterned trench patterns can effectively guide the assembly of supramolecular nanocomposites over micrometer to form aligned nanoparticle lines. I will report our recent investigation on more complex patterns to evaluate how the curvature of the pattern affects the nanoparticle assembly. Preliminary studies show potential for controlling and tailoring nanoparticle assemblies, and in turn, the optical properties of such assemblies.
P1.00293 Fluorescence in nanocomposites based on polyethylene oxides and block copolymers of polyethylene oxide-polypropylene oxide loaded with rare earth doped fluorides. BRIAN YUST, Univ of Texas, Pan American, FRANCISCO PEDRAZA, DHIRAJ SARDAR, University of Texas at San Antonio, AARON SAENZ, MIRCEA CHIPARA, Univ of Texas, Pan American — Rare earth doped fluoride nanoparticles with a size of about 25 nm have been synthesized by a solvothermal process. Polymer-based nanocomposites, containing various weight fraction of nanofillers, have been obtained by dissolving the polymeric matrix (polyethylene oxide) within a solvent (deionized water), adding the nanoparticles, sonicing the mixture, and finally removing the solvent. The complete removal of the solvent has been confirmed by Thermogravimetric Analysis. Additional information about the thermal features have been obtained by Differential Scanning Calorimetry, Wide Angle X-Ray Scattering, FTIR, UV-Visible, and Raman. The effect of the loading with nanoparticles on the glass, crystallization, and melting transition temperatures of the polymeric matrix are reported. Fluorescence of rare earth doped nanoparticles dispersed within the polymeric matrix has been tested by laser spectroscopy. The dependence of fluorescence intensity on the concentration of nanofillers and on temperature in the range 300 to 400 K is analyzed.

P1.00294 Anisotropic Polymer Conformations in Aligned SWCNT/PS Nanocomposites1, WEI-SHAO TUNG, RUSSELL COMPOSTO, University of Pennsylvania, NIGEL CLARKE, University of Sheffield, KAREN WINEY, University of Pennsylvania — In our previous study of isotropic SWCNT/polystyrene (PS) nanocomposites, we found that the polymer radius of gyration (Rg) increases and the SWCNT mesh size decreases with increasing SWCNT concentration. Here, we investigate the effect of aligning SWCNTs on Rg and the SWCNT mesh. SWCNT alignment was accomplished by melt fiber spinning or extrusion, and small angle neutron scattering was used to probe the structure. As expected, SWCNT alignment produces anisotropic meshes. Below 2 wt% SWCNT, no significant change in Rg is observed and Rg parallel and perpendicular to the direction of SWCNT alignment are comparable. More interestingly, at higher wt% SWCNT the polymer conformations are anisotropic with a larger Rg perpendicular to the SWCNT than along the SWCNT. For example, with 6 wt% SWCNT, the Rg perpendicular to the SWCNT is ~15% larger than parallel to the SWCNT. This anisotropy in the polymer conformation becomes more prominent at higher SWCNT concentrations, perhaps because at higher SWCNT concentrations the distribution of mesh shifts to smaller meshes (<2Rg) so that a single polymer chain interacts with multiple SWCNTs. Implications of this finding will be discussed.

1National Science Foundation DMR-12-10379

P1.00295 THE PHYSICS OF CONFINED FLUIDS –

P1.00296 Capillary instability of periodic polymer structures: Influence of viscosity, substrate confinement and local curvature, ZHENG ZHANG, YIFU DING, Univ of Colorado - Boulder — We investigate the simultaneous capillary instability among periodic polymer lithographic structures suspended on an immiscible viscous medium. The first system we studied was straight polystyrene (PS) stripes arranged in parallel in PMMA medium. When annealed at a temperature above the glass transition temperature of both polymers, the stripes undulated and then ruptured via capillary instability. We found that the PS-to-PMMA viscosity ratio strongly affected the rupture kinetics, while it had little influence on the rupture wavelength. The rupture behavior of those stripes could be drastically altered due to initial spacing and substrate confinement. For closely-neighboring stripes that were confined on a rigid substrate, the capillary waves became correlated in-phase among neighbors. Under strong confinement, the capillary rupture was always correlated, irrespective of the viscosity ratio. In addition, we examined the influence of in-plane curvature on capillary instability in concentrically arranged PS rings. When the rings were relatively far apart, their rupture behaviors were independent from each other; when they were close to each other, the primary mode in the capillary breakup became strongly correlated from the center towards the peripheral.

P1.00297 Static and Dynamic Capillary Forces in Pollen Adhesion and Detachment. CARSON MEREDITH, DONGLEE SHIN, HAISHENG LIN, Georgia Tech — Nature provides remarkable examples of adhesive bioparticles including diatoms, pollens, and fungal spores, which are robust examples of nature’s solutions to particle adhesion. These particle’s interactions are often mediated by liquid films at micro- and nanometer length scales, and their study can lead to new physical insights into confined fluids. This talk will detail recent discoveries of the wet adhesive mechanisms of pollen, which provide useful insights into the role of capillary forces and confined fluids in nature. In particular, we describe how pollenkitt, a viscous fluid coating many pollen particles, forms nanoscale capillary bridges that mediate the adhesion and detachment of pollen from surfaces of insects and plants. We will present experimentally observed static and dynamic regimes of pollenkitt capillary forces. Models are utilized to understand the role of rheological properties of pollenkitt in creating these forces. Importantly, the forces generated by pollenkitt give pollen attachment and release from surfaces a sensitive dependence on humidity, rate, and surface morphology. This talk will explore how the physics of these forces contributes to pollenation in nature and how they might be harnessed to engineer new materials.

P1.00298 EXTREME MECHANICS: CONTORTION OF RILAMENTS, RIBBONS AND BUNDLES –

P1.00299 EXTREME MECHANICS OF ORIGAMI: FOLDING, MECHANISMS AND MECHANICS –

P1.00300 Hysteretic self-folding of micro-scale polymer origami films. JUN-HEE NA, University of Massachusetts Amherst, JESSE SILVERBERG, Cornell University, ARTHUR EVANS, CHRISTIAN SANTANGELO, University of Massachusetts Amherst, THOMAS HULL, Western New England University, ITAI COHEN, Cornell University, RYAN HAYWARD, University of Massachusetts Amherst — Origami-inspired self-folding materials have attracted interest for the design of actuators and remotely deployable devices. While well-established geometric rules have been used to create rigidly self-foldable origami structures, the behavior of non-rigidly foldable crease patterns remains incompletely understood. In particular, understanding the relationship between crease geometry and the resulting elastic energy barrier remains a central challenge. Here, we describe a simple model system based on the well-known square twist folding pattern to explore how self-folding structures overcome such energy barriers, and the resulting hysteresis in the folding/unfolding behavior. We show that the magnitude of the hysteresis can be tuned by variations in the plane angle characterizing the crease pattern, as well as by selectively weakening the panel diagonals to reduce the energy cost of bending. These results provide insights into geometrically-controlled energy barriers in non-rigidly foldable origami and design rules for the construction of bistable self-folding systems.

P1.00301 CONFORMATIONS AND DYNAMICS OF BIOPOLYMERS –
P1.00302 Conformations and dynamics of a translocating semi-flexible chain through a Nanopore facilitated by chaperones1, RAMESH ADHIKARI, ANIKET BHATTACHARYA, University of Central Florida — We have studied the translocation dynamics of a semi-flexible polymer through a nanopore from a to a compartment containing binding particles (chaperones) which introduce a bias for the translocating chain. We have used a model semi-flexible polymer using excluded volume (Lennard-Jones), anharmonic spring (elastcicity), and three-body bond bending (chain stiffness) potentials, and applied Langevin dynamics simulation to study various aspects of conformations and dynamics of the translocating chain. In particular, we have investigated the conditions for the most efficient translocation as a function of the chain stiffness, strength of the attractive interaction, and the density of the binding particles, reflected in the mean first passage time (MFPT) of translocating chain through the pore. We have observed that for certain binding strengths and concentrations of the chaperons, the translocation is faster than the ideal Brownian ratchet (BR) process [Simon et al., Proc. Natl. Acad. Sci. U.S.A. 89, 3770 (1992)].

1Partially supported by UCF Office of Research and Commercialization & College of Science SEED grant

P1.00303 Uncovering the effect of DNA topology on the mobility and conformational dynamics of crowded DNA molecules1, STEPHANIE GORZCZYZA, University of San Diego, COLE E. CHAPMAN, University of California, San Diego, RAE M. ROBERTSON-ANDERSON, University of San Diego — Using single molecule fluorescence microscopy and particle-tracking, we examine the effects of crowding on the diffusion and conformation of large, double-stranded circular DNA molecules. To determine diffusion, we track the mean-squared-displacement of single fluorescent-labeled DNA molecules embedded in solutions of different crowding agents. Using image analysis techniques, we also characterize the conformational change (from random coil configuration) induced in DNA by crowding. Our previous studies with linear DNA crowded by dextran reveal crowding-induced mobility reduction of DNA, dependent on crowder size, and elongation of DNA random coils, dependent on DNA size. Here, we compare our previous results to those for circular DNA crowded by varying crowding agents including dextran, Ficoll and Polyethylene Glycol. We determine the dependence of circular DNA mobility and conformation on the level of crowding, molecular weight of the crowding agent, structure of the crowder, and DNA length (11-115 kilobases). Thus, this research uncovers the underlying mechanisms responsible for observed DNA dynamics in crowded environments and biological cells.

1Funded by AFSOR YIP Grant No. FA9550-12-1-0315

P1.00304 DYNAMICS OF GLASSY POLYMERS UNDER CONFINEMENT —

P1.00305 Glass transition cooperativity from broad band heat capacity spectroscopy , YEONG ZEN CHUA, GUNNAR SCHULZ, EVGENI SHOIFET, HEIKO HUTH, University of Rostock, REINER ZORN, Juelich Centre for Neutron Science, JUERN W.P. SCHMELZER, CHRISTOPH SCHICK, University of Rostock — Molecular dynamics is often studied by broad band dielectric spectroscopy (BDS) because of the wide dynamic range available and the large number of processes resulting in electrical dipole fluctuation and with that in a dielectrically detectable relaxation process. Calorimetry on the other hand is an effective analytical tool to characterize phase and glass transitions by its signatures in heat capacity. In the linear response scheme, heat capacity is considered as entropy compliance. Consequently, only processes significantly contributing to entropy fluctuations appear in calorimetric curves. The glass relaxation is prominent example for such a process. Here we present complex heat capacity at the dynamic glass transition (segmental relaxation) of polystyrene (PS) and poly(methyl methacrylate) (PMMA) in a dynamic range of 11 orders of magnitude, which is comparable to BDS [1]. As one of the results, we determine the temperature dependence of the characteristic length of the corresponding fluctuations. The characteristic length decreases from about 4 nm to about 0.7 nm in the temperature range from 370 K to 500 K. This proves an estimate for possible confinement effects on the segmental relaxation, which is different from vitrification as discussed by Cangialosi et al. [2]. [1] Y. Z. Chua et al., Col & Poly Sci 292, 2014. [2] D. Cangialosi, J of Phys. Cond Matt 26 (15), 2014.

P1.00306 STABLE GLASSES, PROPERTIES AND ORIGINS —

P1.00307 Thermal Stability of Vapor-Deposited Stable Glasses of an Organic Semiconductor, DIANE WALTERS, University of Wisconsin-Madison, RANKO RICHERT, Arizona State University, MARK EDGER, University of Wisconsin-Madison — Organic glasses prepared by physical vapor deposition can be highly stable and resistant to transformation upon heating. Unlike ordinary glasses, transformation to the supercooled liquid state is a first order transition which can be determined using calorimetry. We have prepared organic glasses using a simple co-evaporation process through a material with a constant velocity front. In this work, we show that an organic semiconductor commonly used as an active layer in organic electronics, TPD, transforms via propagating fronts when heated above the glass transition temperature. We measure transformation front velocities using spectroscopic ellipsometry. Using high-throughput preparation and annealing techniques, we find that front velocity can vary by over an order of magnitude depending upon the substrate temperature during the deposition of the glass. Transformation front velocity is also influenced by the mobility of the supercooled liquid at the annealing temperatures and, consistent with this view, transformation fronts have the same activation energy for stable glasses prepared with a wide range of the substrate temperatures. These results may aid in designing organic electronic devices with improved lifetimes.

P1.00308 Effect of absorbed water on the thermodynamic and kinetic properties of vapor-deposited organic glasses , MARTA GONZALEZ-SILVEIRA, CRISTIAN RODRIGUEZ-TINOCO, JOAN RAFOLS-RIBE, AIITOR F. LOPEANDIA, JAVIER RODRIGUEZ-VIEJO, Physics Dept. - Universitat Autonoma de Barcelona — Most organic glasses absorb water when exposed to ambient conditions. As a consequence, the glass can experiment changes in its physicochemical properties, being the triggering of crystallization one of the most inconvenient drawbacks. The amount of absorbed water depends on the partial pressure but also on the stability of the glass. Previous studies have shown that ultrastable indomethacin glasses absorb less water than the conventional counterpart. We show here how water absorption modifies the kinetic properties of the glass while, unexpectedly, the thermodynamic stability remains unaltered. By means of ex-situ and in-situ calorimetry, we analyze the relationship between water absorption and kinetic properties for glasses that are vapor-deposited at different temperatures around 0,85 Tg. Moreover, glasses exposed to water vapor exhibit a double glass transition, a clear indication of the presence in the glass of regions with different kinetic stability.

P1.00309 Surface Self-diffusion of Organic Glasses and Low Molecular Weight Polystyrene, WEI ZHANG, CALEB BRIAN1, LIAN YU, Univ of Wisconsin, Madison — The study of surface self-diffusion of organic glasses and low molecular weight polystyrene help understand the formation of stable glasses by vapor deposition, the nature of surface mobility on polymer glasses and the fast surface crystal growth. Surface self-diffusion was measured via surface grating decay. Corrugated patterns were embossed on sample surfaces with master gratings at elevated temperatures. The smoothing of surface gratings was monitored with Atomic Force Microscopy or light diffraction. It was identified by Müllins’ model that viscous flow dominates grating decay at high temperatures, but surface diffusion is the leading mechanism upon cooling. Surface diffusion coefficients were measured for organic glasses and polystyrenes with different glass transition temperatures and intermolecular forces. Surface diffusion is at least 105 times faster than bulk diffusion at Tg, and unlike bulk diffusion, surface diffusion exhibits strong material dependence. The fast surface diffusion implies fast rearrangement of molecules on surface during vapor deposition and helps the formation of stable glasses.

1Now at 3 M Inc.
**P1.00301 Infrared spectroscopic investigation of stable glasses of indomethacin** JING JIANG, MARK EDIGER, University of Wisconsin- Madison — Glasses with high density and kinetic stability can be prepared by physical vapor deposition. By varying the substrate temperature, stable glasses can be produced with an anisotropic distribution of molecular orientations. We use infrared transmission spectroscopy to investigate the effect of substrate temperature on the structure of indomethacin stable glasses. At normal incidence, height of peaks which are assigned to asymmetric hydrogen-bonded acid C=O stretching vary systematically with the substrate temperature. This indicates either more hydrogen-bonded acid carbonyl groups in the most stable glass or a dependence of molecular orientation upon substrate temperature can be shown by IR.

**P1.00311 MANIPULATING GLASSES —**

**P1.00312 Non-affine reorganizations in glassy polymers under applied strain in the plastic regime** DIDIER LONG, LUCA CONCA, CNRS/Solvay, ALAIN DEQUIDT, Université de Clermont-Ferrand, JEAN-YVES DELANNOY, PAUL SOTTA, CNRS/Solvay, FRANÇOIS LEQUEUX, CNRS/ESPCI — A model for the dynamics of non-polar polymers, based on percolation of slow subunits, has been proposed and developed over the past ten years. This model has been extended for describing plastic deformation of glassy polymers. It has been proposed that the applied stress results in an acceleration of the dynamics of the subunits. At deformation amplitudes of a few percent, we can observe plastic yield. The onset of plasticity is accompanied by an increase of the non-affine nature of the deformation at microscopic scales. Localization phenomena are observed in the plastic regime. We present here a detailed study of the complex reorganization which takes place on a scale of a few nanometers. We show that the correlation length of non-affine deformation increases at yield, but remains finite, with typical value 10-20 nm, corresponding to typical distance between shear bands. We compare in detail the microscopic mechanisms at play during shear deformation, uni-axial extension and compression.

**P1.00313 POLYMERIC GLASSES —**

**P1.00314 Volume Recovery of Polymeric Glasses**, N. SAKIB, S.L. SIMON, Texas Tech University — Following the seminal work of Kovacs, capillary dilatometry has been used for the last fifty years to study volume recovery of polymeric glass formers. Our capillary dilometer, which previously used a Linear Variable Differential Transducer (LVDT) to measure the height of the Hg column in the capillary, has been modified following the work of Richter. The current study demonstrates the use of a capacitance bridge as the transducer. A metallic layer of silver sputtered on the exterior of the dilometer serves as the outer electrode, mercury (the confining fluid) serves as the inner electrode, and the glass in between serves as the dielectric of the capacitor. The Andeen-Hagerling 2550A 1kHz ultraprecision capacitance bridge is used for the measurements. Volume recovery of various glass formers will be used to test the new design; new measurements are planned to test models of structural recovery.

**P1.00315 Cure Kinetics of the Hydroxyl-Epoxide Reaction in DGEBA Epoxy Hardened with Diethanolamine** LELELO HAILEISLASSIE, NARJES FREJDI, CAITLYN M. CLARKSON, JOHN D. MCCOY, New Mexico Tech, MATHEW C. CELINA, JAMIE M. KROPKA, Sandia National Laboratories — The curing of a diglycidyl ether of bisphenol-A Epoxy (Epon 828) with diethanolamine (DEA) involves a fast amine-epoxide reaction followed by a slower hydroxyl-epoxide reaction. At curing temperatures below 70°C, the time scales of these two reactions are well separated. This permits the study of the hydroxyl addition as an “isolated” reaction. The reaction is strongly auto-catalyzed and is well fit to a modified form of the Kamal equation. Here we study the temperature dependence of the Kamal parameters with modulated differential scanning calorimetry and infrared spectroscopy.

**P1.00316 Liquid Substrate Effects on the Glass Transition Temperature of Nanoscopically Confined Polystyrene Spheres**, DANE CHRISTIE, Princeton University, CHUAN ZHANG, Sphera Materials, RODNEY PRIESTLEY, Princeton University — The effect of the liquid-polymer interface on the glass transition temperature (Tg) of polystyrene (PS) was investigated using differential scanning calorimetry. Polystyrene nanoparticles of different radii were suspended in either water, glycerol or an ionic liquid. Particles suspended in water (or cast into a film in air) exhibited a Tg-confinement effect consistent with that of freestanding films of PS. Particles suspended in an ionic liquid exhibited an invariance in Tg with confinement while those suspended in glycerol exhibited a modest, depression in Tg with confinement. Upon re-suspension in water, particles formerly suspended in glycerol showed a partial recovery of their Tg in water. However, particles re-suspended in water from an ionic liquid showed no recovery of their Tg in water. These results are explained in the context of chain mobility and interfacial energy, and provide insight and a probable resolution to contradictory observations in the literature.

**P1.00317 POSTDEADLINE ABSTRACTS —**

**P1.00318 Chirality Induced Spin Selectivity for Memory Applications**, RAHAMIM GULIAMOV, SHINTO MATHEW, KIRAN VANKAYALA, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel, HAGAY MOSHE, YITZHAK MASTAI, Department of Chemistry, Bar-Ilan University, Ramat-Gan Israel, RON NAAMAN, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel, PROF. RON NAAMAN GROUP COLLABORATION1, PROF. YITZHAK MASTAI GROUP COLLABORATION2 — Creation and manipulation of spin current is one of major aspects of memory devices. In conventional devices spin-polarized current is created by permanent magnetic layer. Further miniaturization of the memory is limited by super-paramagnetic behavior of layer. Hence, high density memory requires out-of-plane geometry with perpendicular magnetic anisotropy. Achieving this goal with inorganic magnetic layers is a challenge. We present a new approach in which the permanent magnetic layer has been replaced with inorganic chiral film producing spin polarized current due to Chirality Induced Spin Selectivity (CISS) effect. Chiral Al2O3 film grown by ALD on self-assembled monolayer of chiral molecules acts as a spin filter. Spin polarization is parallel/antiparallel to the electron velocity depending on chirality. Devices show asymmetric magneto-resistance and slopes with opposite sign for left/right handed chirality. Hence, CISS-effect based device shows, for first time, an asymmetric magneto-resistance, which has potential application in magnetic memory and magnetic field sensors. Reference: Shinto P. Mathew et al., Appl. Phys. Lett. 105, 242408 (2014)

1Weizmann Institute of Science, Rehovot, Israel
2Bar-Ilan University, Ramat-Gan Israel
P1.00319 Proving grain boundaries and transport study of graphene grown on liquid Cu, SEONG-YONG CHO, MIN-SIK KIM, KI-JU KIM, MIN-SU KIM, HYUN-MI KIM, SANG-HOON LEE, KI-BUM KIM, Seoul Natl Univ, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING TEAM — We revealed grain boundaries of graphene grown on liquid Cu via hydrogen etching and Cu oxidation, and found out that small gap and voids exist between graphene islands on liquid Cu due to small supersaturation ratio which was required for self-assembly to occur. Modified two-step growth was applied in order to fill the gap between graphene islands and continuous graphene was synthesized on liquid Cu. The continuity of the film was verified through hydrogen etching and NaCl assisted oxidation. Electrical resistance of graphene grown on liquid Cu was lower than graphene grown on solid Cu if there is no crack damage which might be resulted from thermal stress related solidification of Cu and wet-transfer. Also, Hall mobility of graphene grown on liquid Cu was twice higher value compared to that of graphene grown on solid Cu. In order to verify the aligned grain boundary of graphene on liquid Cu, direct patterning enabled electrode deposition on two neighboring graphene single crystal which aligns in the same orientation. Grain boundary resistance was negligible based on our electrical measurement results which has a great potential impact on graphene growth on liquid Cu.

P1.00320 Enhancement of Electromagnetically Induced Transparency Cooling by an Optical Cavity1, WEI WU, JIE ZHANG, SHUO ZHANG, BAO-QUAN OU, PING-XING CHEN, National University of Defense Technology — One of the most popular methods for cooling trapped ions to ground state cooling, however, carrier and blue sideband still exist, which are the obstacles for reaching lower phonon number. EIT cooling cancels the carrier transition and suppressed blue sideband transition to some extent, blue sideband transition still exists. To further suppress the blue sideband transition and improve EIT cooling, Introducing an optical cavity provides us a promising way to enhance the EIT cooling and reach lower phonon number for a trapped ion. A λ-configuration ion with mass \( M \) is trapped in a Paul trap, we consider the situation that the radial confinement is much stronger than that of the axial direction, only one dimensional movement along the axis should be concerned. If we set the dutuning properly, EIT effect occurs, canceling the carrier transition, while the heating effect from blue sideband transition can be suppressed by quantum interference between the laser and cavity. Analytical calculation shows that cooling limit of this new scheme is

\[
\langle n \rangle_{st} = \frac{1}{C},
\]

Numerical simulation shows that the standard EIT cooling is enhanced with the help of the high finesse cavity.

1 National Natural Science Foundation of China (Grant Nos 11304387 and 61205108)

P1.00321 Properties of Transparent Conducting Oxides from First Principles: In-O, In-Zn-O, In-Sn-O, and Zn-In-Sn-O, RABI KHANAL, JULIA MEDVEDEVA, Missouri University of Science and Technology — Systematic investigations of amorphous In-based oxides, In-X-O with X=Zn and/or Sn, obtained via ab-initio molecular dynamics liquid-quench simulations, are performed to understand the role of composition in the structural, optical, transport, and mechanical properties of these oxides. First, the structural characteristics of the first, second, and third shells are compared between amorphous In-O, In-Zn-O, In-Sn-O, and Zn-In-Sn-O. The results reveal that the local Metal-Oxygen structure for both In and X cations — and hence, optical band gap and electron effective mass governed by the metal-oxygen interactions — remains nearly intact upon the transition to amorphous state. In all amorphous oxides considered, Indium is undercoordinated with little dependence on X, whereas the X cations reach their natural coordination. This finding suggests that the carrier generation is primarily governed by In atoms, in agreement with transport measurements in the amorphous oxides. In contrast to the first shell, the composition affects the Metal-Metal distances, coordination, and oxygen sharing. The interconnectivity and spatial distribution of In6 and OX polyhedra limits the charge transport via scattering and ultimately determines the formation of the amorphous oxides and their properties.

P1.00322 Perovskite Structured Oxide Thin Film as Photocapacitor, JOYPROKASH CHAKRABARTTY, RIAD NACHACHE, FEDERICO ROSEI, INRS - Energie et Materiaux — Photocapacitor is a device that converts solar energy through photovoltaic effect, and stores the converted energy by maintaining the charge concentration difference across a membrane upon light irradiation. It eliminates additional storage devices, for example, extra battery towards device miniaturization by enabling generated charge storage facilities in the same system. Till to date published reports show those devices that used artificial layer within single structure to make storage facility. Here we show some preliminary results on Bi-Mn-O thin film systems that differ from others in such a way that it will employ self-assembled system to convert and to store solar energy.

P1.00323 Development of Magnetization Detecting Electron Spin Resonance Method, SATOSHI MATSUZAWA, HIROYUKI NOJIRI, Institute for Materials Research, Tohoku University, NOJIRI LAB TEAM — Electron spin resonance: ESR is a spectroscopy by using electromagnetic wave absorption in Zeeman split multiplet of spins. The split energy is determined by the resonance field and the line width is governed by relaxation and anisotropies. The absorption intensity is proportional to the population difference between the initial and the final states. These populations also determine the total z-component of magnetization of the system. It means that ESR absorption can be measured by magnetization under electromagnetic wave irradiation. This type of ESR is called magnetization detecting ESR: MDES. We have developed two types MDES, namely, SQUID-ESR and XMCD-ESR. XMCD is the abbreviation of X-ray Magnetic circular dichroism and is the method to measure magnetization in element and orbital selective manner. SQUID-ESR is easy to conduct by attaching radiation source to a conventional MPMS-SQUID machine. The advantage of SQUID-ESR is the evaluation of absolute value of ESR intensity. While, XMCD-ESR is very sensitive and can detect the magnetization of a few atomic layers. Details of the experimental systems and the test results will be presented.

P1.00324 Application of Scanning Probe Nanolithography to fabrication and study of large area graphene and Transition Metal Dichalcogenides heterostructures1, RUI DONG, LOGAN MOORE, IRMA KULJANSIHVILI, Saint Louis University — Two-dimensional atomic crystals, such as graphene and layered transition metal dichalcogenides (TMDs), have drawn significant attention because of the unique physical and chemical properties. Recently developed graphene/TMDs stacking structures provide an area graphene and Transition Metal Dichalcogenides heterostructures. Raman spectroscopy and AFM characterization demonstrates high quality of as-prepared Graphene/TMDs nanostructures. Mask free approach significantly reduces contamination of the graphene surface during patterning and demonstrates a promising unconventional technology for fabricating high quality Graphene/TMDs or other layered nanostructures in a convenient and economical manner with the nanoscale precision.

1 IK acknowledges support from Saint Louis Univeristy's President's Research Fund
P1.00325 Geometric and Electromagnetic Field Effects on the Excitonic Properties of Core-multishell Semiconductor Quantum Wires

The effect of eccentricity distortions in the otherwise circular geometry of core-multishell quantum wires on their excitonic transitions is theoretically investigated. Within the effective mass approximation, the Schrödinger equation is numerically solved for electrons and holes in systems with single and double radial heterostructures, whereas the resulting exciton binding energy is calculated by means of a variational approach. Our results demonstrate that for a single shell heterostructure, in-plane electric fields applied in different directions produce qualitatively different energy spectra, which can be used to identify the eccentricity of the system. For a double heterostructure, the eccentricities of the inner and outer shells play an important role on the excitonic binding energy and on the oscillator strength. Our results also show that for a single shell heterostructure with a type-II confinement, i.e. with spatially separated electrons and holes, one of the carriers exhibits either a ring-like or a dot-like energy spectrum, depending on the radius of the system. In this case, a shell-to-core confinement transition for the electron can be induced also by an external magnetic field.

1 Fundao de Apoio a Pesquisa do Rio Grande do Norte e UFERSA
2 Universidade Federal Rural do Semi-rio
3 Universidade Federal do Ceará
4 Universidade Federal do Ceará
5 Universidade Federal Rural do Semi-rio

P1.00326 Final state lifetime effects in spectroscopic studies of iridium oxide

The effect of eccentricity distortions in the otherwise circular geometry of core-multishell quantum wires on their excitonic transitions is theoretically investigated. Within the effective mass approximation, the Schrödinger equation is numerically solved for electrons and holes in systems with single and double radial heterostructures, whereas the resulting exciton binding energy is calculated by means of a variational approach. Our results demonstrate that for a single shell heterostructure, in-plane electric fields applied in different directions produce qualitatively different energy spectra, which can be used to identify the eccentricity of the system. For a double heterostructure, the eccentricities of the inner and outer shells play an important role on the excitonic binding energy and on the oscillator strength. Our results also show that for a single shell heterostructure with a type-II confinement, i.e. with spatially separated electrons and holes, one of the carriers exhibits either a ring-like or a dot-like energy spectrum, depending on the radius of the system. In this case, a shell-to-core confinement transition for the electron can be induced also by an external magnetic field.

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5 Universidade Federal Rural do Semi-rio

P1.00327 Giant Spin Hall Effect in Perpendicularly Magnetized Ta/CoFeB/MgO Structure and Temperature Dependence

The Giant Spin Hall Effect (GSHE) in non-magnetic metals with strong spin-orbit coupling (SOC) has been found in various solids like Pt, beta-Ta, and beta-W. The spin current from GSHE solids yields a spin-transfer torque (STT) inside an adjacent ferromagnetic layer with perpendicular magnetic anisotropy (PMA) to effect a magnetization switching. The combination of PMA with STT-induced switching has the advantage of low power consumption, high reliability and durability and data non-volatility over earlier generations of MRAM. Here we first studied the post-annealing effect on achieving PMA in Ta/CoFeB/MgO multilayers. We achieved so far the lowest critical current density of 2.3 MA/cm² for the STT-induced switching in the presence of 5mT magnetic field as compared to earlier PMA structures. Using a macrospin model, we are able to obtain the Spin Hall Angle of 0.11 in Ta and anisotropy field of 260mT at room temperature, and both values increase with reducing temperature. We also found a scaling law between Ta resistivity and Spin Hall angle in a quadratic relation. Our results are important for magnetic memory and spin-logic applications through optimizing the engineering of such multilayer structures with PMA.

1 This work was supported by Nanoelectronics Research Initiative (NRI) through the Institute for Nanoelectronics Discovery and Exploration (INDEX) and by National Science Foundation through Grant No. DMR-1307056.

P1.00328 Transition to Metallic Phase of Fluid Hydrogen at High Pressure and High Temperature

The transition to the metallic phase of fluid hydrogen under high pressure and high temperature by the laser heated diamond-anvil cell (LHDAC) up to 100 GPa and 2500 K. Compressed hydrogen was heated by IR laser with a thin gold foil, acts as the laser absorber. The temperature of hydrogen was determined by National Science Foundation through Grant No. DMR-1307056.

P1.00329 Spin Correlations in Quantum Wires

We consider theoretically spin correlations in an 1D quantum wire with Rashba-Dresselhaus spin-orbit interaction (RDI). The correlations of non-interacting electrons display electron-spin resonance at a frequency proportional to the RDI coupling. Interacting electrons on varying the direction of external magnetic field transit from the state of Luttinger liquid (LL) to the spin density wave (SDW) state. We show that the two-time total spin correlations of these states are significantly different. In the LL the projection of total spin to the direction of the RDI induced field is conserved and the corresponding correlator is equal to zero. The correlators of two components perpendicular to the RDI field display a sharp ESR driven by RDI induced intrinsic field. In contrast, in the SDW state the longitudinal projection of spin dominates, whereas the transverse components are suppressed. This prediction indicates a simple way for experimental diagnostic of the SDW in a quantum wire.
Our study reveals that m-xylene plays an important role in both the structure and property of the formed novel phase [MG. Yao et al, App Phys Lett 103, 2013]. This work was supported by Grant-in-aid for Young Scientists A (No. 25708002), Scientific Research on Innovative Areas (No. 25107002), and Scientific Research S (No. 22250001) from MEXT, Japan, and the Global COE Program in Chemistry, Nagoya University.

1 Corresponding author


1 This work was supported by the Institute for Basic Science (IBS) and the National Research Foundation (RF) funded by the Ministry of Education, Science, and Technology (Grant No. 2010-0008341) in Korea. The work at
P1.00335 Selective formation of zigzag-edges in graphene cracks, MIHO FUJIHARA, Nagoya University, RYOSUKE INOUE, YUTAKA MANIWA, Tokyo Metropolitan University, HISANORI SHINOHARA, Nagoya University, YASUMITSU MIYATA, Tokyo Metropolitan University — Graphene edges have attracted much attention due to their unique electrical and magnetic properties. To understand these properties, it is highly desired to prepare clean, smooth, and structure-controlled edges. However, structure selective preparation of zigzag or armchair edges has not been achieved yet. Here, we report the selective formation of graphene edges aligned in the zigzag orientation by cleavage with thermally-assisted tensile stress. Graphene flakes were grown from methane on copper foil by using chemical vapor deposition. After cooling to room temperature, we occasionally observed zigzag-shaped cracks in graphene. Considering the grain edges which have the zigzag face, these cracks are found to propagate parallel to the zigzag edges. The origin of tension is probably due to the non-uniform lattice strain of graphene induced by thermal shrinking of Cu substrates as supported by Raman strain mapping. Furthermore, we demonstrate the carrier tuning around graphene edges by applying the electric field to the cracks. Our findings pave the way for the fabrication and applications of smooth, long zigzag edges of graphene and other two dimensional materials.

P1.00336 Thrust generation of thickness-varying flexible fins, YAUNLI DA, PETER YEH, ALEXANDER ALEXEEV, Georgia Institute of Technology — We use three dimensional computer simulations to probe the hydrodynamics and thrust generation of an oscillating flexible fin with varying thickness. The fin is modeled as an elastic rectangular plate that plunges at its leading edge and is submerged in a viscous fluid. Since we assume that the thickest part of the fin is very small compared to its length and width, the plate is modeled as infinitely thin. We introduce an appropriate mass gradient and stiffness gradient in the plate to simulate the effects of the thickness gradient. As the fin flaps, fluid is displaced backwards and a net thrust is generated. We characterize this thrust generation as a function of driving frequency and find optimal conditions for largest propulsion. These findings are useful for designing biomimetic underwater propulsion devices.

P1.00337 Precise Analysis of Perfect Zero-Birefringence Polymer, YUKI KADA, OSAMU URAKAWA, TADASHI INOUE, Osaka Univ — Control of strain-induced birefringence of amorphous polymers is an important issue for their optical applications. It is widely accepted that strain-induced birefringence of amorphous polymers has two origins, segment orientation and glassy deformation. The intrinsic birefringence, $\Delta n_{0}$, and the photoelastic coefficient, $C_{ij}$, are indexes of the two origins, respectively. $\Delta n_{0} - C_{ij}$ map help us to predict strain-induced birefringence of copolymers. Perfect zero-birefringence polymers, PZP, means $\Delta n_{0} = 0$ and $C_{ij} = 0$. One of the method to obtain the PZP is random copolymerization of three kinds of monomers. In a three components system, the birefringence of copolymers can be characterized by a point inside of the triangle region formed by three points for homopolymers of the three monomers in $\Delta n_{0} - C_{ij}$ map. In this study, PZP of MMA (Methyl methacrylate), TFEMA (Trifluoroethoxy methacrylate) and BzMA (Benzyl methacrylate) was synthesized and its birefringence behavior was analyzed. Following the reported composition, we synthesized PZP and conducted dynamic birefringence measurement. $\Delta n_{0}$ value of the synthesized PZP was unexpectedly large at high temperatures because $\Delta n_{0}$ of PMMA and PBzMA showed temperature dependence. More importantly, we found that zero birefringence of PZP is achieved only at a certain temperature. We will also discuss effect of sub relaxations in the talk.

P1.00338 Chaos and Big-bang singularity in Bianchi type-IX universe for the Einstein equation, YUYA TAKEUCHI, Osaka Prefecture University, TOMIO PETROSKY, LINDA REICHL, The University of Texas at Austin, SATOSHI TANAKA, Osaka Prefecture University — Chaotic dynamics of a spatially homogenous and anisotropic case in the Bianchi type-IX universe model for the Einstein equation has been studied for the vacuum case. There is a hyperbolic fixed point and a separatrix only for the type-IX model with positive cosmological constant. A difficulty in numerical analysis due to the Big-Bang singularity is avoided by constructing an analytical solution near the singular point. Thanks to the local analytic solution and by combining it with global numerical solution, we are able to construct Poincarés surface of a section near the separatrix. A new type of chaotic motion characteristics to the Einstein equation will be discussed.

P1.00339 NMR Spin-Lattice Relaxation Time $T_1$ of Thin Films Obtained by Magnetic Resonance Force Microscopy, SUNGSIN Kwon, SEUNG-BO SauN, SOONCHIL Lee, KAIST, SOONHO WON, Advanced Metallic Materials Division, Korea Institute of Materials Science — NMR spectrum and spin-lattice relaxation time($T_1$) of CaF$_2$ thin film samples deposited on a silicon cantilever tip were obtained by magnetic resonance force microscopy(MRFM). Thickness of the thin films were 50nm and 150nm. In order to measure $T_1$, a cyclic adiabatic inversion method was used with periodic phase inversion. A comparison of the bulk and two thin films showed that $T_1$ becomes shorter as the film thickness decreases. To make the comparison as accurate as possible, all three samples were loaded onto different beams of a multi-cantilever array and measured in the same experimental conditions such as temperature and magnetic field.

P1.00400 Computational and Physical Analysis of Catalytic Compounds, RICHARD WU, JUNG JAE SOHN, RICHARD KYUNG, Choice Research Group — Nanoparticles exhibit unique physical and chemical properties depending on their geometrical properties. For this reason, synthesis of nanoparticles with controlled shape and size is important to use their unique properties. Catalyst supports are usually made of high-surface-area porous oxides or carbon nanomaterials. These support materials stabilize metal catalysts against sintering at high reaction temperatures. Many studies have demonstrated large enhancements of catalytic behavior due to the role of the oxide-metal interface. In this paper, the catalyzing ability of supported nano metal oxides, such as silicon oxide and titanium oxide compounds as catalysts have been analyzed using computational chemistry method. Computational studies have demonstrated large enhancements of catalytic behavior due to the role of the oxide-metal interface. In this paper, the catalyzing ability of supported nano metal oxides, such as silicon oxide and titanium oxide compounds as catalysts have been analyzed using computational chemistry method. Computational programs such as Games and Chemcraft have been used in an effort to compute the efficiencies of catalytic compounds, and bonding energy changes during the optimization convergence. The result illustrates how the metal oxides stabilize and the steps that it takes. The graph of the energy computation step(N) versus energy(kcal/mol) curve shows that the energy of the titania converges faster at the 7th iteration calculation, whereas the silica converges at the 9th iteration calculation.

P1.00401 Superconductivity in Opal-based superconducting nanocomposites, M.K. LEE, MOST Instrument Center At NCKU, Tainan 70101, Taiwan, E.V CHARNAY, Institute of Physics, St. Petersburg State University, St. Petersburg, Petrodvorets 198504 Russia, L.J. CHANG, Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan, YU. A. KUMZEROV, A. F. Ioffe Physico-Technical Institute RAS, St. Petersburg 194021, Russia, M.F. LIN, Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — In this study, we investigate superconducting nanocomposites (SCNCs) to elucidate superconductivity in nanostructured type I superconductor. In, Sn and Hg are loaded into opal matrices by high pressure up to 10kbar, in which introducing superconducting metals into templates preserves their own 3D nanostructures. The opal matrices is adopted because it is a well-developed nanoconfinement and widely used in the studies of photonic crystal due to its periodically-superlatticed nanogometry. Exotic phase diagrams in the opal SCNC studies reveal an enhanced upper critical field ($H_{c2}(0)$) and curvature crossover of upper critical field line. Additionally, according to the field dependence of $U_{a}(H)$, curvature crossover of the upper critical field line can occur, owing to vortex phase transition.

P1.00402 The physics of a cell doublet: a minimal system to study early embryo morphogenesis, HERVE TURLIER, JEAN-LEON MAITRE, TAKASHI HIIRAGI, FRANCOIS NEDELEC, European Molecular Biology Laboratory — In early embryos, the shape of cells is determined in part by the actomyosin cortex and in part by interactions with the surrounding environment. Cell-cell adhesion, in particular, is determinant for the overall embryo organization. This complex interplay between cell autonomous mechanical properties and cell-cell interactions can advantageously be analyzed in pairs of isolated cells. We study theoretically and experimentally shape changes in doublets of mouse embryo blastomeres. Simple scaling analysis and numerical simulations can predict the various configurations adopted by blastomere doublets over different stages of embryo development. Our study provides a simple and robust physical framework to understand and characterize quantitatively diverse morphogenetic events such as compaction, entosis and cell internalization.
P1.00343 Calculation of modal contributions to thermal transport across Si/Ge and In$_{0.53}$Ga$_{0.47}$As/InP interfaces , KIARASH GORDIZ, ASEGUN HENRY, Georgia Institute of Technology — Reliable and quantitative calculation of the conductance of different phonons across an interface can have a significant impact on the applications where thermal interface resistance is limiting and can aid in the rational design of thermal interface materials. A new formalism for extracting the modal contributions to thermal interface conductance with full inclusion of temperature dependent anharmonicity and all of the atom level topography is presented. Application of the formalism to Si/Ge and In$_{0.53}$Ga$_{0.47}$As/InP interfaces reveals fundamental information on the nature of the vibrational modes involved in heat transfer and the interactions/correlations among them. Four distinct classes of vibrational modes are detected for the two interfaces. For Si/Ge interface, the density of states for these vibrational classes are completely mixed, while surprisingly for In$_{0.53}$Ga$_{0.47}$As/InP interface they are completely segregated. For Si/Ge interface, interfacial modes, located around 12THz, contribute near 20% to the total conductance, while for In$_{0.53}$Ga$_{0.47}$As/InP interface, low frequency extended modes contribute more than 50% to the total conductance. The high frequency extended modes have a temperature dependent anharmonicity analysis shows that increasing temperature decreases the contribution by extended modes and increases the contribution by partially extended modes. In both of the interfaces, Interfacial modes exhibit the maximum per mode contribution.

P1.00344 Coherence lengths in attractively interacting Fermi gases with spin-orbit coupling , YU XIXIANG, JINWU YE, Mississippi State Univ, WUMING LIU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences — Extensive research has been lavished on the effects of spin-orbit couplings (SOCs) in attractively interacting Fermi systems in both neutral cold-atom systems and condensed-matter systems. Recently, it was suggested that a SOC drives a class of BCS to Bose-Einstein condensate (BEC) crossover that is different from the bulk cases. Beside the strong hybridization of $s$-electrons of the impurity center with the confined electrons, the Coulomb and exchange interaction of the d-electrons of the impurity centers with the extra electron and the states of the impurity ion together with the confinement effect mix the wave functions, split the impurity energy levels at three dimensions (3D) (the bound-state energy at 2D) for three attractively interacting Fermi gases with 3D Rashba, 3D Weyl, and 2D Rashba SOC, respectively. We show that only the coherence length can be used to characterize this BCS to BEC crossover. Furthermore, it is the only length which can be directly measured by radio-frequency dissociation spectra type of experiments. We stress crucial differences among the coherence length, Cooper-pair size, and the two-body bound-state size. Our results provide the fundamental and global picture of the BCS to BEC crossover and its experimental detections in various cold-atom and condensed-matter systems.

P1.00345 Theory of Luminescent Emission in a Nanocrystal Doped by Co$^{2+}$ , GEORGE CHAPPELL, QUE HUONG NGUYEN, Marshall University — We theoretically study the effect on the electronic structures and optical properties of a Co-doped semiconductor nanocrystal (NC) of the interaction between the impurity atom and an electron existing inside the NC. The optical properties of impurity centers in NCs are very different from the bulk cases. Beside the strong hybridization of $s$-electrons of the semiconductor host and $d$-electrons of the impurity due to confinement and the modification of the crystal field near the surface of the NCs, the Coulomb and exchange interaction of the $d$-electrons of the impurity centers with the extra electron and the states of the impurity ion together with the confinement effect mix the wave functions, split the impurity energy levels, break the previous selection rules, and change the transition probabilities. Energy, wave functions, luminescence efficiency, and transition lifetime have been calculated. The results imply that the PL intensity increases and the lifetime is shortened inside the NC.

P1.00346 Role of precursor crystal structure on electrochemical performance of carbo-derived carbon electrodes , BENJAMIN PALAZZO, ZACH NORRIS, GREG TAYLOR, Department of Physics and Astronomy, Rowan University, LEI YU, Department of Chemistry and Biochemistry, Rowan University, SAMUEL LOFLAND, JEFFREY HETTINGER, Department of Physics and Astronomy, Rowan University — Binary carbides with hexagonal and cubic crystal structures have been synthesized by reactive magnetron sputtering of vanadium and other transition metals in acetylene or methane gas mixed with argon. The binary carbides are converted to carbide-derived carbon (CDC) films using chlorine gas in a post-deposition process in an external vacuum reaction furnace. Residual chlorine has been removed using an annealing step in a hydrogen atmosphere. The CDC materials have been characterized by x-ray diffraction, x-ray fluorescence, and scanning electron microscopy. The performance of the CDC materials in electrochemical device applications has been measured with the hexagonal phase precursor demonstrating a significantly higher specific capacitance in comparison to that of the cubic phase. We report these results and pore-size distributions of these and similar materials.

P1.00347 Stabilizing the false vacuum: Mott skyrmions$^1$, MÁRTON KANÁSZ-NAGY, Harvard University and Budapest University of Technology and Economics, BALÁZS DÓRA, Budapest University of Technology and Economics, EUGENEM DEMLÉR, Harvard University, GERGELY ZARAND, Budapest University of Technology and Economics — Topological excitations keep fascinating physicists since many decades. While individual vortices and solitons have been observed in many areas of physics, their intriguing higher dimensional topological relatives, skyrmions remained mostly elusive. In particular, earlier attempts to create stable individual skyrmions in ultracold atomic experiments suffered from important instabilities: skyrmions have a tendency to shrink or expand, and to slip away from the atomic trap. In this work, we propose that loading a three-component nematic superfluid, such as $^2$Na, into a deep optical lattice and thereby creating an insulating core, one can create topologically stable individual skyrmions, and investigate their properties in detail. Furthermore, the spectrum of the excitations of the superfluid and their quantum numbers change dramatically in the presence of the skyrmion, and they reflect the presence of a trapped monopole, as imposed by the skyrmion’s topology.


$^1$Acknowledgements: Hungarian Scientific Research Funds (K101244, K105149, CNKS0991), the Bolyai Program of the Hungarian Academy of Sciences. E. A. D. acknowledges support through the DOE (FG02-97ER25308), the Harvard-MIT CUA, the ARO-MURI on Atomtronics, and the ARO MURI Quism program.

P1.00348 In Silico Discovery of High Deliverable Capacity Metal-Organic Frameworks$^1$, YI BAO, Rice Univ, RICHARD MARTIN, Lawrence Berkeley National Lab, CORY SIMON, UC Berkeley, MACIEJ HARANCZYK, Lawrence Berkeley National Lab, BEREND SMIT, UC Berkeley, MICHAEL DEEM, Rice Univ, MICHAEL W. DEEM TEAM, MACIEJ HARANCZYK TEAM, BEREND SMIT TEAM — Metal organic frameworks (MOFs) are actively being explored as potential adsorbed natural gas storage materials for small vehicles. Experimental exploration of potential materials is limited by the throughput of synthetic chemistry. We here describe a computational methodology to complement and guide these experimental efforts. The method uses known chemical transformations in silico to identify MOFs with high methane deliverable capacity. The procedure explicitly considers synthesesizability with geometric requirements on organic linkers. We efficiently search the composition and conformation space of organic linkers for nine MOF networks, finding 48 materials with higher predicted deliverable capacity (at 65 bar storage, 5.8 bar depletion, and 298 K) than MOF-5 in four of the nine networks. The best material has a predicted deliverable capacity 8% higher than that of MOF-5.

$^1$US Department of Energy.
P1.00349 Many-body calculation for charge transport through triangular quantum dot molecules

1 CHIH-CHIEH CHEN, YIA-CHUNG CHANG, Department of Physics, University of Illinois Urbana-Champaign, DAVID M.T. KUO, Department of Electrical Engineering and Department of Physics, National Central University — We study the many-body effect of electron tunneling through the coupled quantum dots systems in the Coulomb blockade regime. Using the equation of motion method for the non-equilibrium Green’s function, we calculate the charge current and conductance of junctions consisting of metallic electrodes and a few quantum dots. Many-particle correlation functions are explicitly solved numerically. Quantum phenomena like quantum interference, Coulomb blockade and spin blockade for the triangular quantum dot molecules are discussed. Our work suggests a new method for the modeling of the mesoscopic transport.

2 This work was supported in part by the Ministry of Science and Technology, Taiwan under Contract Nos. NSC 101-2112-M-001-024-MY3 and NSC 103-2112-M-008-009-MY3.

2 Research Center for Applied Sciences, Academia Sinica, and Department of Physics, National Cheng-Kung University

P1.00350 Confinement of metal nanoparticles with various sizes in silica matrices

JEEUN LEE, SHIN-HYUN KANG, SUNG-MIN CHOI, KAIST — Many studies have been focused on metal nanoparticles since they have interesting properties due to their high surface area to volume ratio. While bulk metals have constant properties regardless of their sizes, the noble properties of metal nanoparticles such as catalytic activity, magnetic, and electronic properties dramatically change depending on their sizes. Here, metal nanoparticles with various sizes are synthesized, functionalized, then confined in stable silica matrices and their physical and chemical properties are investigated. The structure of each system is characterized by transmission electron microscopy (TEM) and scanning electron microscopy (SEM).

P1.00351 Fitness, environmental changes and the growth of modularity - a quasispecies theory for the evolutionary dynamics of modularity

LIANG NIESTEMSKI, Western New England University, JEONG-MAN PARK, The Catholic University of Korea, MICHAEL DEEM, Rice University — Although the modularity of a biological system is demonstrated and recognized, the evolution of modularity is not well understood. We here present a quasispecies theory for the evolutionary dynamics of modularity. Complemented with numerical models, this analytical theory shows the calculation of the steady-state fitness in a randomly changing environment, the relationship between rate of environmental changes and rate of growth of modularity, as well as a principle of least action for the evolved modularity at steady state.

P1.00352 Pressure dependence of the nematic spin correlations in detwinned BaFe$_{1.97}$Ni$_{0.03}$As$_2$

1 WENLIANG ZHANG, XINGYE LU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, JITAÉ PARK, Heinz Maier-Leibniz Zentrum, Technische Universität München, Garching, Germany, PENGCHENG DAI, Department of Physics and Astronomy, Rice University, Houston — In the paramagnetic tetragonal phase of BaFe$_{2-x}$Ni$_x$As$_2$, inelastic neutron scattering shows a spin excitation anisotropy emerges at a temperature well above the structure transition temperature ($T_c$) [1], consistent with the onset of in-plane resistivity anisotropy [2]. However, how the applied uniaxial strain, which artificially breaks the four-fold symmetry, influences the observed anisotropy is still unclear. Here we studied the pressure dependence of the nematic spin correlations in detwinned BaFe$_{1.97}$Ni$_{0.03}$As$_2$. We find that the spin excitation anisotropy temperature ($T^*$) is largely enhanced when changing the pressure from a medium level ($\sim$8MPa) to a high level ($\sim$15MPa) [3]. Our results suggest the $T^*$ may be not a characteristic temperature where the system transit to a nematic phase, but a temperature the nematic fluctuations can reach under a uniaxial stress.


1 Supported by MOST(973 programs), NSFC, CAS and CAEP.

P1.00353 Evolution of sparsity and modularity in a model of living matter

MATHIEU HEMERY, Laboratoire Interdisciplinaire de Physique (Grenoble), OLVIER RIVOIRE, CNRS & Université Grenoble Alpes — How much of the sequence of a protein accounts for its current function and how much is the result of its past evolutionary history? Being the product of a long evolutionary process in an ever changing environment, the sequence of current natural proteins may retain the trace of prior selected functions. Or more simply, it may contain elements that are not – or no more – subject to selection. Using a simple physical model previously analysed to study the folding problem, we probe the influence of past evolutionary environments on protein sequences. Simulations of evolutionary dynamics generically lead to non-trivial correlations between temporal fluctuations and geometrical structure, illuminating the link between history, geometry and function.

P1.00354 Supramolecular Polymer Nanocomposites – Improvement of Mechanical Properties

JESSE HINRICH, South Dakota Sch Mines & Tech, COLIN NEIKIRK, RODNEY PRIESTLEY, Princeton University — Supramolecular polymers differ from traditional polymers in that their repeat units are connected by hydrogen bonds that can reversibly break and form under various stimuli. They can be more easily recycled than conventional materials, and their highly temperature dependent viscosities result in reduced energy consumption and processing costs. Furthermore, judicious selection of supramolecular polymer architecture and functionality allows the design of advanced materials including shape memory and self-healing materials. Supramolecular polymers have yet to see widespread use because they can’t support much weight due to their inherent mechanical weakness. In order to address this issue, the mechanical strength of supramolecular polymer nanocomposites based on ureidopyrimidinone (UPy) telechelic poly(caprolactone) doped with surface activated silica nanoparticles was investigated by tensile testing and dynamic mechanical analysis. The effects of varying amounts and types of nanofiller surface functionality were investigated to glean insight into the contributions of filler-filler and filler-matrix interactions to mechanical reinforcement in supramolecular polymer nanocomposites.

1 MRSEC NSF DMR 0819860 (PI: Prof. N. Phuan Ong) REU Site Grant: NSF DMR-1156422 (PI: Prof. Mikko Haataja)

P1.00355 Slip and flow dynamics of polydisperse thin polystyrene films

SEYED MOSTAFA SABZEVARI, Concordia university, JOSHUA D. MCGRAW, KARIN JACOBS, Saarland University, PAULA M. WOOD-ADAMS, Concordia university — We investigate the slip of binary and ternary mixtures of nearly monodisperse polystyrene samples on Teflon-coated (AF2400) silicon wafers using dewetting experiments. Binary mixtures of long and short chains along with ternary mixtures with a fixed weight-average molecular weight Mn but different number-average molecular weight Mn were prepared. Thin films of ca. 200 nm were spin coated on mica from polymer solutions and transferred to Teflon substrates. Above the glass transition temperature $T_g$ the films break up via nucleation and growth of holes. The hole growth rate and rim morphology are monitored as a function of Mn and annealing protocol of the films before transfer to Teflon substrates. Slip properties, accessed using hydrodynamic models, and flow dynamics are then examined and compared. We found that the rim morphology and slip of polystyrene blends on Teflon depends on the molecular weight distribution. Similarly, flow dynamics is affected by the presence of short chains in mixture. Moreover, we can provoke differences in slip by choosing appropriate annealing and film transfer protocols for PS films that have first been spin cast on mica surfaces.
State Univ, JIE XU, University of Illinois at Chicago — Little interest has been paid to the final stage of a Leidenfrost droplet until a recent study by Celestini et al [Phys. Rev. Lett. 109, 034501 (2012)] reporting an unexpected take-off phenomenon of micrometer sized pure liquid droplets \( R_l < R < R_t \), where \( R_t \) is the take-off radius, and \( R_l \) is the critical radius above which droplets start to lose sphericity. In our study, we first report an unexpected observation on millimeter sized water Leidenfrost droplets \( R > R_l \), which behave quite differently from the previous study. While an originally micrometer sized Leidenfrost droplet takes off due to breakdown of lubrication regime, and hovers above its vapor layer until disappearing in the final stage of evaporation, an originally millimetric Leidenfrost droop is observed to hover and oscillate, taking off and falling back consecutively. We further report another interesting observation on water droplets containing micrometric glass beads. These droplets spontaneously organize and buckle together during evaporation. In addition to oscillation just like pure droplets, these particle-laden drops create an unexpected explosive shoot-up at the end of evaporation.

P1.00357 Carbon Nanotubes Synthesis Through Gamma Radiation, PABLO TIRADO, RAFAEL GARCIA, Center of Research in Physics, University of Sonora, JORGE MONTES, Department of Nanotechnology, University of Sonora, RODRIGO MELENDREZ, MARCELINO BARBOZA, Center of Research in Physics, University of Sonora, OSCAR CONTRERAS, Center of Nano science and Nanotechnology, UNAM — Carbon nanotubes show a great potential of applications since their discovery by Iijima in 1991 due to their numerous physical-chemical properties such as their high weight to strength relationship, which make them ideal to use in high resistance compound materials, and in many other applications. In this work, a novel method for the synthesis of carbon nanotubes is presented, starting from an ultra-thin sheet of graphite synthesized by the chemical vapor decomposition technique (CVD), using ultra high purity methane and hydrogen at 1200°C in a horizontal quartz reactor. For the synthesis of carbon nanotubes, the graphite sheets were exposed to different doses of radiation, with the objective of breaking the graphite bonds and form carbon nanotubes; a Gammacell equipment model 220 Excel was used for the purpose, which counts with a radiation source of cobalt 60, and a current radiation rate of 0.9 Gy/seconds. The time of exposure to radiation was varied in each sample, according to the desired dose of radiation in each case, afterwards the samples were characterized using the Raman spectroscopy and TEM microscopy techniques with the objective of observing the kind of nanotubes formed, their morphology and their number of defects. Results will be shown during the poster session.

P1.00358 Hydration Layer of Enzymes Partially Controls Conformational Dynamics, ZAHRA ALAVI, Student at UCLA, ZOCCHI TEAM — For a typical (20 kDa, 4 nm size) monomeric enzyme, more than 50% of the residues are at the surface. The mechanics of these soft, heterogeneous nanoparticles was recently shown to be viscoelastic. Here we explore the contribution of the enzyme’s surface to the mechanics of the molecule. Nano-rheology provides sub-angstrom resolution measurements of the reversible deformation of the enzyme subject to an oscillatory mechanical stress. We perturb the surface of the enzyme by adding small amounts of DMSO, believed to affect ordering of the enzyme - water interface. We observe a dramatic though reversible change in the mechanics of the enzyme, which becomes more viscous. On the other hand, the catalytic speed is unaffected, while at higher DMSO concentrations (>1%) it even increases. Our measurements show that small (<1%) bulk concentrations of DMSO, which have negligible effect on the physico-chemical properties of bulk water, including the viscosity and dielectric constant, have nonetheless dramatic effect on the dynamics of the hydration layer of the enzyme, and ultimately on the enzyme’s mechanics. DMSO accumulates in the hydration layer (“binds to the surface of the enzyme”). Apparently the order - inducing (“kosmotropic”) quality of DMSO leads to a hardening of the enzyme - water interface.

1 US-Israel Bina tional Science Foundation

P1.00359 Effect of monomer sequence distribution in poly(vinyl alcohol-co-vinyl acetate) on the hydrogen bonding structure and physical properties, SHUN TASAKA, OSAMU URAKAWA, TADASHI INOUE, Department of Macromolecular Science, Graduate School of Science, Osaka University — It has been well known that hydrogen (H-) bonding interaction in polymer materials strongly affects their properties. For example, glass transition temperature \( (T_g) \) and terminal relaxation time increase by introducing H-bonding sites. This is because the molecular motion is restricted due to the formation of inter- and intra-chain H-bonds. For H-bonding copolymers in which H-bonding monomer and non- bonding one are incorporated, the fraction dependence of their properties has been examined so far. However, the influence of sequence distribution on their properties has not been studied in detail. In this work, we investigated the H-bonding structure and physical properties of molten poly(vinyl alcohol-co-vinyl acetate) with different monomer sequences to clarify the effect of the sequence distribution. We found that, with increasing the randomness in monomer sequences, the number of H-bonds between carbonyl group and hydroxyl (OH) group increased. Moreover, OH groups form linearly connected structure (OH-OH-OH) and its number also increases with the sequence randomness. \( T_g \) for the samples with higher sequence randomness are higher than those with lower randomness for high VOH copolymers. These results indicate that formation of larger number of H-bonds makes \( T_g \) higher.

P1.00360 Quantum Behavior of an Autonomous Maxwell Demon, ADRIAN CHAPMAN, AKIMASA MIYAKE, Univ of New Mexico — A Maxwell Demon is an agent that can exploit knowledge of a system’s microstate to perform useful work. The second law of thermodynamics is only recovered upon taking into account the work required to reversibly update the demon’s memory, bringing information theoretic concepts into a thermodynamic framework. Recently, there has been interest in modeling a classical Maxwell demon as an autonomous physical system to study this information-work tradeoff explicitly. Motivated by the idea that states with non-local entanglement structure can be used as a computational resource, we ask whether these states have thermodynamic resource quality as well by generalizing a particular classical autonomous Maxwell demon to the quantum regime. We treat the quantum description using a matrix product operator formalism, which allows us to handle quantum and classical correlations in a unified framework. Applying this, together with techniques from statistical mechanics, we are able to approximate nonlocal quantities such as the erasure performed on the demon’s memory register when correlations are present. Finally, we examine how the demon may use these correlations as a resource to outperform its classical counterpart.

Wednesday, March 4, 2015 2:30PM - 5:30PM –
Session Q0 APS: Kavli Foundation Special Symposium: Frontiers of Light Ballroom A -
2:30PM Q0.00001 The Optical Microscopy Revolution, STEFAN HELL, Max Planck Institute —
3:42PM Q0.00003 Developing Photo Activated Localization Microscopy
HARALD HESS, Janelia Research Campus — Photo Activated Localization Microscopy, PALM, acquires super-resolution images by activating a subset of activatable fluorescent labels and estimating the center of each molecular label to sub-diffractive accuracy. When this process is repeated thousands of times for different subsets of molecules, each image can be rendered from all the center coordinates of the molecules. I will describe the circuitous story of its development that began with another super-resolution technique, NSOM, developed by my colleague Eric Betzig, who imaged single molecules at room temperature, and later we spectrally resolved individual luminescent centers of quantum wells. These two observations inspired a generalized path to localization microscopy, but that path was abandoned because no really useful fluorescent labels were available. After a decade of nonacademic industrial pursuits and the subsequent freedom of unemployment, we came across a class of genetically expressible fluorescent proteins that were switchable or convertible that enabled the concept to be implemented and be biologically promising. The past ten years have been very active with many groups exploring applications and enhancements of this concept. Demonstrating significant biological relevance will be the metric if its success.

4:18PM Q0.00004 History and Future Developments of Blue/Green/White LEDs and Laser Diodes
SHUJI NAKAMURA, University of California, Santa Barbara —

4:54PM Q0.00005 The Light Science of Coherent X-rays: How Quantum Dynamics Solved a 50 Year Challenge
MARGARET MURNANE, University of Colorado, Boulder —

Wednesday, March 4, 2015 5:45PM - 7:00PM
Session R3 APS: The Division of Materials Research at NSF - Mary Galvin-Donahue, Division Director, followed by discussion of Broader Impacts in Research 202AB -

5:45PM R3.00001 The Division of Materials Research at NSF - Mary Galvin-Donahue, Division Director, followed by discussion of Broader Impacts in Research —

Wednesday, March 4, 2015 6:30PM - 8:00PM
Session R20 APS: "App"y Hour Grand Hyatt San Antonio Republic B -

6:30PM R20.00001 “App”-y Hour —

Wednesday, March 4, 2015 5:45PM - 6:45PM
Session R21 APS: Joint Task Force on Undergraduate Physics Programs 201 -

5:45PM R21.00001 Joint Task Force on Undergraduate Physics Programs —

Wednesday, March 4, 2015 6:00PM - 7:00PM
Session R50 APS: NSBP NSHP Receptions Grand Hyatt Travis B Travis C -

6:00PM R50.00001 NSBP/NSHP Reception —

Wednesday, March 4, 2015 6:00PM - 7:00PM
Session R51 APS: LGBT Roundtable Discussion Grand Hyatt San Antonio Bonham B -

6:00PM R51.00001 LGBT Roundtable Discussion —

Wednesday, March 4, 2015 7:30PM - 9:30PM
Session R52 APS: Special Evening Event Hosted by the Editors of Physics Texas DE - Jessica Thomas, Editor, Physics

7:30PM R52.00001 Rise of the Colloidal Machines
SHARON C. GLOTZER, University of Michigan — Digital matter is a new approach in science, engineering, and medicine that uses powerful algorithms and fast computers to discover and design the materials of the future. The idea is to identify and program atoms, molecules, nanoparticles, and microparticles with the optimal shapes and interactions for forming new materials with unprecedented properties. In this talk, I’ll discuss the exciting possibilities of using nano- and micron-sized colloidal particles in the design and fabrication of functional elements for robot-like machines, such as colloidal muscles, digital colloidal bits, bionic colloidal assemblies, and colloidal swarms. These functional colloidal elements could allow researchers to make smart, shape-shifting materials, like those comprising the Terminator T-1000. I’ll also outline the fundamental physics challenges to realizing smart colloidal materials and machines.

Wednesday, March 4, 2015 7:00PM - 8:30PM
Session R53 APS: Diversity Networking Reception Grand Hyatt San Antonio Crockett CD -
for materials design will be discussed. Material are not resolved. We present results from our theoretical investigation of a mechanical model in which the atoms and their bonds are replaced by point

Experiments explain many puzzles. Experimental investigations for further results are important. Electromagnetic energy alone. The discovery of the charge-mass interaction establishes the need for unification of electromagnetism and gravitation and would

faith toward Einstein and accumulated errors. The Einstein equation with an electromagnetic wave source has no valid solution unless a photonic energy-stress for the Einstein equation. Thus, Gullstrand is right and the 1993 Nobel Prize for Physics press release is incorrect. Awards to Christodoulou reflect the blind

connection between the most consistently successful neural network topologies and their relevance to the physics of heat transport in tokamak plasmas. [1] O.

addressed by providing the time-derivative information of the plasma parameters that are input to the neural network. Finally, an attempt is made to draw a

transport data from DIII-D, TFTR, and JET respectively. A comparative analysis shows that previous success of neural networks in predicting heat transport in

SMITH, General Atomics, JAMES PENNA, MIT — Three multi-layer, feed-forward, back-propagation neural networks have been built and trained on heat

investigated.

We show that such obstructions are classified by the cohomology group $H^{d+1}(G, U(1))$, in agreement with the classification of bosonic SPT phases proposed by Chen et al [Science 338, 1604 (2012)]. Our analysis allows for a straightforward calculation of the element of $H^{d+1}(G, U(1))$ corresponding to physically meaningful models such as non-linear sigma models with a theta term in the action. SPT phases outside the classification of Chen et al are those in which the symmetry cannot be represented locally on the edge. With some modifications, our framework can also be applied to fermionic systems in $(2+1)$-D.

Topological phase transition in a bilaer toric code model, HONG-CHEN JIANG, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, YUAN-MING LU, Department of Physics, The Ohio-State University, ASHVIN VISHWANATH, Department of Physics, University of California, Berkeley — We study a bilayer toric-code model in two spatial dimensions by density matrix renormalization group approach. We show that as the interlayer coupling is increased, the system goes through a continuous phase transition from two decoupled copies of $Z_2$ topological orders (bilayer limit) to a single $Z_2$ topological order (monolayer limit). This phase transition is revealed by a jump of topological entanglement entropy. Moreover, the two phases are featured by distinct topological properties: in the bilayer limit the system supports symmetry protected gapless edge states, while the edge states are fully gapped in the monolayer limit. The nature of this continuous topological phase transitions is also investigated.

Predicting Heat Transport across Multiple Tokamaks with Neural Networks, CHRISTOPHER LUNA, Arizona State University, ROBERT BUDNY, Princeton Plasma Physics Laboratory, ORSO MENEGHINI, STERLING SMITH, General Atomics, JAMES PENNA, MIT — Three multi-layer, feed-forward, back-propagation neural networks have been built and trained on heat transport data from DIII-D, TFTR, and JET respectively. A comparative analysis shows that previous success of neural networks in predicting heat transport in DIII-D [1] is reproduced for TFTR and JET. The effect of using different neural network topologies has been investigated across all of the devices. It is found that the neural networks can consistently predict the total species’ heat fluxes for all of the devices, however they have difficulty in predicting the individual components of the heat fluxes in presence of significant transient variations in stored energy (i.e. non-steady-state conditions). Such limitation has been addressed by providing the time-derivative information of the plasma parameters that are input to the neural network. Finally, an attempt is made to draw a connection between the most consistently successful neural network topologies and their relevance to the physics of heat transport in tokamak plasmas. [1] O. Meneghini, et al., Phys. Plasmas 21 (2014) 060702

Classifying symmetry-protected topological phases through the anomalous action of the symmetry on the edge, DOMINIC ELSE, CHETAN NAYAK, Department of Physics, University of California, Santa Barbara, CA — It is well known that $(1+1)$-D bosonic symmetry-protected topological (SPT) phases with symmetry group $G$ can be identified by the projective representation of the symmetry at the edge. Here, we generalize this result to higher dimensions. We assume that the representation of the symmetry on the spatial edge of a $(d + 1)$-D SPT is local but not necessarily on-site, such that there is an obstruction to its implementation on a region with boundary. We show that such obstructions are classified by the cohomology group $H^{d+1}(G, U(1))$, in agreement with the classification of bosonic SPT phases proposed by Chen et al [Science 338, 1604 (2012)]. Our analysis allows for a straightforward calculation of the element of $H^{d+1}(G, U(1))$ corresponding to physically meaningful models such as non-linear sigma models with a theta term in the action. SPT phases outside the classification of Chen et al are those in which the symmetry cannot be represented locally on the edge. With some modifications, our framework can also be applied to fermionic systems in $(2+1)$-D.

This publication is supported by the Chan Foundation, Hong Kong

Mechanical modeling of structures exhibiting negative thermal expansion, JOSEPH SCHICK, Villanova Univ, ANDREW RAPPE, University of Pennsylvania — Materials that exhibit negative thermal expansion (NTE) over a wide range of temperatures are of great technological importance in creating materials that are structurally stable despite being exposed to wide variations in operational temperature. One well-known NTE material, ZrW$_2$O$_8$, has been the subject numerous investigations and yet the details of the underlying causes of NTE in this material are not resolved. We present results from our theoretical investigation of a mechanical model in which the atoms and their bonds are replaced by point masses and anharmonic potentials. We demonstrate that negative thermal expansion can result solely from the differential expansion of the bonds. Implications for materials design will be discussed.
12:39PM Z23.00008 Derivative Structure Enumeration: Trimming a Combinatoric Tree1

WILEY S. MORGAN, Department of Physics and Astronomy Brigham Young University, RODNEY W. FORCADE, Department of Mathematics Brigham Young University, CONRAD W. ROSENBROCK, GUS L.W. HART, Brigham Young University – Provo — A good computational physics course teaches students to say ‘well that’s completely wrong’ anytime the computer gives them a result. Once cast in doubt, it is the scientist’s responsibility to convince themselves that the result is in fact correct. As programs become more complicated, it usually becomes more difficult to guarantee that the final output is right. I will present a new framework that automates the production of robust, high quality Fortran code. The talk will include a brief overview of good coding principles and a demonstration of the most useful features of the framework that help automate implementation of these principles. By providing an XML-based documentation standard and automated unit testing, fortpy helps researchers ensure that their code produces accurate physics and is easier to use by others.

1 WSM, RWD, CW and GLWH acknowledge support from ONR (MURI N00014-13-1-0635)

12:51PM Z23.00009 Robust Computational Physics and Automated Sanity Checks1

CONRAD W. ROSENBROCK, GUS L.W. HART, Brigham Young University – Provo — A good computational physics course teaches students to say ‘well that’s completely wrong’ anytime the computer gives them a result. Once cast in doubt, it is the scientist’s responsibility to convince themselves that the result is in fact correct. As programs become more complicated, it usually becomes more difficult to guarantee that the final output is right. I will present a new framework that automates the production of robust, high quality Fortran code. The talk will include a brief overview of good coding principles and a demonstration of the most useful features of the framework that help automate implementation of these principles. By providing an XML-based documentation standard and automated unit testing, fortpy helps researchers ensure that their code produces accurate physics and is easier to use by others.

1 WSM, RWD, CW and GLWH acknowledge support from ONR (MURI N00014-13-1-0635)

1:03PM Z23.00010 Equilibrium shape of colloidal crystals

DIMITRIOS MAROUDAS, RAY SEHGL, Univ of Mass - Amherst — Clusters of colloidal crystals exhibit a wide range of size dependent properties. Leveraging such properties requires a strong fundamental understanding of the thermodynamics of colloidal clusters. A first step in developing this understanding is to accurately describe the equilibrium structure and morphology of these assemblies. In this presentation, we report the results of a generalized Wulff construction that is able to accurately describe the equilibrium, i.e., of minimum free energy, shape of an assembly of colloidal particles. The colloidal system that we focus on is modeled with an interparticle interaction consisting of two terms, an electrostatic repulsion and an Asakura-Oosawa (AO) depletion attraction. The generalized Wulff construction can account for both surface facet and surface edge effects on the stable colloidal crystalline morphology. This construction results in a configuration of minimum free energy for given crystal volume. We carry out these equilibrium calculations over a range of crystal sizes to examine size dependent effects on the stability of colloidal clusters. These calculations enable the determination of cluster sizes which exhibit improved stability (lower free energy) compared to that of similar-size clusters.


BENJAMIN VOLLMAYR-LEE, Bucknell University — Coarsening dynamics is effectively described by phase field models, which provide nonlinear field equations of motion that can be integrated numerically. However, these simulations are hampered by a numerical instability that imposes a time step restriction, and that has the additional feature of being linear in the implicit fields, allowing for efficient simulation with fast Fourier transforms. Using this method enables simulations to extend decades farther into the coarsening scaling regime. I will report measurements of similarities and agreements obtained with this method.

1:27PM Z23.00012 ABSTRACT WITHDRAWN

1:39PM Z23.00013 Developing Accurate and Transferable Artificial Neural Network Potentials for Li-Si Alloys1

BERK ONAT, EKIN DOGUS CUBUK, BRAD MALONE, EFFTHIMIOS KAXIRAS, Department of Physics and School of Engineering and Applied Sciences, Harvard University — Investigation of the lithiation and delithiation of Si anode in Li-ion batteries using realistic simulations is important and requires large numbers of atoms and long time scales which is generally inaccessible with first-principle approaches. These simulations can be carried out using interatomic potentials that can capture the dependence of structure on chemical composition. Compared with the fixed functional form of empirical potentials, a promising approach to construct the potential energy surface is using artificial neural networks (ANN) that extends the time scales of simulations without sacrificing the accuracy and transferability. Using ab-initio density functional theory data for training, we developed an environment-dependent high-dimensional ANN potential for Li-Si alloys. Our calculations based on the geometry optimizations and molecular dynamic simulations show that the developed potential can accurately predict total energies and equilibrium structures of Li, Si and Li-Si alloys. Using several training databases that include different concentrations of Li in the alloy, we investigated the range of the validity of the ANN potential. Our results show that ANN potentials are widely transferable to Li-Si alloys with various concentrations of Li.

1 This work was supported in part by TUBITAK under post-doctoral research grant no 2219.


DAYONG CAO, Avoid Earth Extinction Association — Massenergy and spacetime build up a balance system of flat universe; massenergy equals negative spacetime. Like mass attract, opposite mass repel; like energy repel, opposite energy attract; like space attract, opposite space repel; like time repel, opposite time attract. In the balance macrosystem: http://meetings.aps.org/link/BAPS.2011.MAR.Y33.9 In the balance macrosystem: E + E′ = mc² + m′c², http://meetings.aps.org/link/BAPS.2011.MAR.K1.68 There is a unified balance between macro-micro system. In cold area of CMB, the dark massenergy, the spacetime particle which has spacetime center, causes an expanding of period-wavelength of light and redshift which equals negative gravitational redshift of massenergy particle; in hot area, the dark massenergy causes more redshift of light. The sun and dark hole are a balance system-SDS which triggered periodic mass extinctions and created new life on our earth. The quantum orbits both of planets and dark comets of dark hole decided the period. Consciousness remotely change output voltages of solar cell and a balance between Electrons and electron holes which is a negative balance of SDS. By the nuclear energy of spacetime, consciousness should change the orbit of the balance of SDS for avoiding impaction.