Monday, March 18, 2013 5:45PM - 6:45PM –
Session D1 APS: APS Prizes and Awards Ceremonial Session  Hilton Baltimore Key Ballroom 8 - Michael Turner, American Physical Society, University of Chicago

5:45PM D1.00001 Award Ceremony –

Monday, March 18, 2013 6:45PM - 8:00PM –
Session E1 APS: Welcome Reception  Exhibit Hall D -

6:45PM E1.00001 WELCOME RECEPTION –

Monday, March 18, 2013 7:30PM - 8:30PM –
Session E11 APS: Special Outreach Session: Meso-Physics 310 - Laura H. Greene, University of Illinois at Urbana-Champaign

7:30PM E11.00001 Meso Scale Science: Challenges and Opportunities  HARRIET KUNG, Basic Energy Sciences, Department of Energy, Office of Science — The Director of DOE’s Office of Science issued a charge to the Basic Energy Sciences Advisory Committee (BESAC) in 2011 to define the research agenda for mesoscale science, the regime where classical, quantum, and nanoscale science meet. The charge builds on over a decade’s strategic planning BESAC has undertaken that establishes the importance of nanoscale science — atomic and molecular scale understanding of how nature works and how this relates to advancing the frontiers of science and innovation. Beyond a new level of science, the opportunity for new, cheaper and more efficient technology and solutions to societal problems is significant and timely. This presentation will discuss the impact of the report and how it has shaped and will continue to inform future research programs in DOE Office of Science.

7:50PM E11.00002 From Quanta to the Continuum: Opportunities for Mesoscale Science, GEORGE CRABTREE1, Materials Science Division, Argonne National Laboratory; Depts of Physics, Electrical and Mechanical Engineering University of Illinois at Chicago — Mesoscale science embraces the regime where atomic granularity and quantization of energy yield to continuous matter and energy, collective behavior reaches its full potential, defects, fluctuations and statistical variation emerge, interacting degrees of freedom create new phenomena, and homogeneous behavior gives way to heterogeneous structure and dynamics. Mesoscale architectures form a hierarchy extending from atoms and molecules through polymers, supramolecular assemblies, periodic lattices, multilayers, nanocrystal arrays and multiphase materials. Mesoscale science builds on the foundation of nanoscale knowledge and tools that the community has developed over the last decade and continues to develop. Mesoscale phenomena offer a new scientific opportunity: designing architectures and interactions among nanoscale units to create new macroscopic behavior and functionality. Examples of mesoscale successes, challenges and opportunities will be described.

A more complete discussion of mesoscale science can be found in the BESAC report, From Quanta to the Continuum: Opportunities for Mesoscale Science, http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/
Innovative community input on opportunities for mesoscale science can be found on the Mesoscopic Materials and Chemistry website, http://www.meso2012.com/

1In collaboration with John Sarrao, Los Alamos National Laboratory

Wednesday, March 20, 2013 8:00AM - 9:30AM –
Session M48 APS: Tutorial for Authors and Referees  Key Ballroom 9-10 -

8:00AM M48.00001 Tutorial for Authors and Referees —Editors from Physical Review Letters and Physical Review will provide information and tips for our less experienced referees and authors. This session is aimed at anyone looking to submit to or review for any of the APS journals, as well as anyone who would like to learn more about the authoring and refereeing processes. Topics for discussion will include advice on how to write good manuscripts, similarities and differences in writing referee reports for PRL and PR, and other ways in which authors, referees, and editors can work together productively. Following a short presentation from the editors, there will be a moderated discussion. A light breakfast of bagels, pastries, coffee and tea will be served.

2:00PM - 2:00PM –
Session Q1 APS: Poster Session II (Polymer Physics Poster 11:15-2:15; all other posters 2:00 - 5:00PM)  Exhibit Hall EF -

Q1.00001 POLYMERS AND SOFT MATTER PHYSICS –

Q1.00002 Phase Behavior of Miscible Block copolymer Blends, YONGHOOON LEE, HYUNJU AHN, HOYEON LEE, DU YEOL RYU, Yonsei University — We have investigated the phase behavior for the binary block copolymer (BCP) blends composed of a weakly interacting (with no specific interaction) polystyrene-b-poly(alkyl methacrylate) (PS-b-PAMA) copolymers using small-angle neutron scattering (SANS), small-angle x-ray scattering (SAXS), and depolarized light scattering (DPLS) experiments. A series of phase behaviors were reproduced from a lower disorder-to-order transition (LDOT) to closed-loop having a LDOT and an upper order-to-disorder transition (UODT), to an UODT type depending on composition in the BCP blends. On the basis of the results and previous observations, we will discuss the phase behavior type of polystyrene-b-poly(alkyl methacrylate) (PS-b-PAMA) copolymers.
Q1.00003 Investigation of Ternary Multiblock Copolymer Melts using Self-consistent Field Theory

DACHUAN SUN, JUNHAN CHO, Department of Polymer Science and Engineering, Dankook University, South Korea — Recently, A-b-(B-b-A)n-b-C multiblock copolymer melts have drawn attention due to their hierarchical nanostructures. Several phase diagrams for these copolymers using an analytical method have been made by G. ten Brinke et al. Here, we performed numerical self-consistent field calculations on the same copolymers to reconstruct the phase diagrams. The perpendicular lamellae phase disappears and is replaced by the parallel lamellae phase in our phase diagrams. For the parallel lamellae phase, there are only two A layers rather than three. Moreover, one B layer is located between the two A layers, with another two thin B layers located near the interface between the A and C blocks. The interfacial energy between the C and A blocks is reduced dramatically due to the existence of the B layers between them. Because thus formed parallel lamellae phase has much lower free energy, the perpendicular lamellae phase is replaced by the parallel ones.

We acknowledge the financial support from NSF through Basic Research Program and also from Center for Photofunctional Energy Materials at Dankook University.

Q1.00004 Self-assembly of polymer systems in the presence of disorder

DAVID TEMPEL, Harvard University — A solid mathematical understanding of how complex polymer systems behave in the presence of disorder is important for understanding a variety of recent experiments on systems that have important applications. Examples include self-assembly on patterned substrates for lithography applications, and adsorption of charged polymers and biopolymers onto patterned substrates. In all these systems, one finds competition between phases exhibiting long-range order driven by the self-assembly properties of the polymers, and phases exhibiting short-range or no order due to the presence of random external forces. In this work we will present a general mathematical description of this competition, using tools from localization theory in solid-state physics. Our results will help guide experimentalists in determining how much external disorder can be tolerated to achieve a given self-assembled phase and conversely, which phases are most robust to external disorder. Results from simple analytical models and self-consistent field theory simulations will be presented.

Q1.00005 Efficient Formation of Multicomponent Ion Gels by Stepwise Self-Assembly of Thermoresponsive ABC Triblock Terpolymers

SCOTT DANIelsen, University of Pennsylvania, CAN ZHOU, TIMOTHY LODGE, University of Minnesota — The gelation behavior of a poly(ethylene-alt-propylene)-b-poly(ethylene oxide)-b-poly(N-isopropyl acrylamide) (PON) triblock terpolymer in room-temperature ionic liquids, 1-butyl-3-methylimidazolium tetrafluoroborate ([BMM][BF4]) and 1-ethyl-3-methylimidazolium bis[trifluoromethylsulfonyl]imide ([EMIM] [TFSI]), has been studied by rheology over the concentration range 1-10 wt%. PON terpolymers have proven better gelation efficiency and mechanical properties (modulus) in hydrogels. Physical ion gels from PON terpolymers in [BMM][BF4] and [EMIM][TFSI] have been studied to determine improvements in gelation efficiency and mechanical properties (modulus) for triblock terpolymers. A two-compartment micellar network is believed to result from the stepwise gelation of PON terpolymers involving micellization at elevated temperatures and gelation at lower temperatures.

Q1.00006 Design of Optimal Surface Topographies for Low Fouling Surfaces by Computer Simulation

PHILLIP SCHOC, JAN GENZER, North Carolina State University — Biofouling is a major problem affecting many industries ranging from shipping to medical implants. Recent work in had pointed towards the importance of surface topography in limiting the adhesion of biofouling agents. Here we report on a Monte Carlo model to simulate the adhesion of spherical particles with sticky polymeric hairs on a variety of surfaces that possess sinuousoidal variation of amplitude and periodicity in an effort to design the optimal set of surface attributes. We explore adhesion of such particles with varying diameter and the number and length of hairs on a range of sinuousoidal periodic surface structures. This approach allows us to establish the optimal surface parameters minimizing the adhesion of particles with varying properties. Specifically, we will report that surfaces with very large or very low periodicity are nearly indistinguishable from flat supports (in some cases they even perform worse). Optimal surfaces are those whose periodicities are comparable to the “hydrodynamic size” of the particle (i.e., particle and hair). Additionally the role of amplitude has been less significant than wavelength as long as the amplitude of the surface corrugation is larger than the size of the particle. We have also developed an order parameter that characterizes how well the particles organize over the periodic structures on the surface.

Q1.00007 Template Polymerization using a controlled reaction scheme

PREETA DATTA, JAN GENZER, North Carolina State University — We employ a Monte Carlo simulation scheme based on the bond fluctuation model to simulate template polymerization via controlled scheme (i.e., termination and chain transfer reactions are neglected) involving co-polymerization of free monomers and monomers bound to a planar template with equidistant sites occupied by bound monomers. A new macromolecule is initiated in bulk by activation of an initiator; any monomer (free or bound) that is within the reaction distance (nearest neighbors) of the initiator can be incorporated into the growing chain. As the chain propagates, it adds new monomers to the macromolecule. Those monomers can either be bulk (i.e., free) monomers or those that are placed on the predefined template. We analyze the effect of the number and the density of monomers bound on the substrate on the composition and monomer distribution in the resultant co-polymers. Our results reveal that a greater number of bound monomers on the planar template promotes polymerization of most/all of the bound monomers to form an array attached to the template. In addition, there exists an optimum density of spacing of bound monomers on the template, at which the likelihood of the bound monomers getting incorporated in the growing chains is maximum. This is in contrast to our earlier findings for linear templates, where a higher density of spacing favors the incorporation of bound monomers in the growing chains.

Q1.00008 The Co-axial Flow of Injectable Solid Hydrogels with Encapsulated Cells

BRANDON STEWART, DARRIN POCHEAN, SAMEER SATHAYE, University of Delaware — Hydrogels are quickly becoming an important biomaterial that can be used for the safe, localized injection of cancer drugs, the injection of stem cells into areas of interest or other biological applications. Our peptides can be self-assembled in a syringe where they form a gel, sheared by injection and, once in the body, immediately reform a localized pocket of stiff gel. My project has been designed around looking at the possibility of having a co-axial strand, in which one gel can surround another. This co-axial flow can be used to change the physical properties of our gel during injection, such as stiffening our gel using hyaluronic acid or encapsulating cells in the gel and surrounding the gel with growth medium or other biological factors. Rheology on hyaluron stiffened gels and cells encapsulated in gels was performed for comparison to the results from co-axial flow. Confocal microscopy was used to examine the coaxial gels after flow and to determine how the co-axial nature of the gels is affected by the concentration of peptide.
Q1.00009 Kinetic control of block copolymer self-assembly into novel multicomponent and multigeometry nanoparticles\(^1\), YINGCHAO CHEN, University of Delaware, SHIYI ZHANG, ANG LI, University of Texas A&M, XIAOJUN WANG, University of Tennessee, JIAHUA ZHU, University of Delaware, KAREN WOOLEY, University of Texas A&M, JIMMY MAYS, University of Tennessee, DARRIN POCHAN, University of Delaware, UNIVERSITY OF DELAWARE TEAM, UNIVERSITY OF TEXAS A&M COLLABORATION — Nanoparticles with the phase separation of unlike hydrophobic blocks trapped in the same core have been produced via blending of two block copolymers in THF/water dilute solution. The dissolution of two amphiphilic block copolymer sharing the same polyacrylic acid PAA block and different hydrophobic block in pure THF undergoes consequent aggregation and phase separation via different kinetic control pathways. Importantly, the polymer is complexed with diamine molecules prior to either slow titration or fast addition of selective solvent which is the key of forming controlled miscible structure. Vesicle-cylinder, nested vesicle MGM and MCM nanoparticles were assembled and characterized via cryogenic TEM and selective staining methods. Small Angle X-ray scattering is applied to track the early-stage phase separation behavior which determines the final MGM/MCM nanoparticle formation.\(^2\) Thanks for NSF funding. We also thank the W. M. Keck College of Engineering electron microscopy laboratory at the University of Delaware, and the nuclear magnetic resonance facilities of the Dept of Chemistry at University of Texas A&M.

Q1.00010 Printing Polymer Semiconductors with Controlled Crystal Orientations, NIHILHA MAHADAVAPURAM, DAVID SHAKARISAZ, SUCHANUN MOUNGTHAI, PAUL RUCHHOEFT, GILA STEIN, University of Houston — Solar energy is considered to be an alternate promising source of clean energy. Polymer-based solar cells have low manufacturing costs and these devices can be fabricated in light weight, flexible and durable modules. The most widely studied active layer in polymer-based solar cells is the bulk heterojunction (BHJ) design. BHJs are formed by arresting the phase separation of a polymer/fullerene blend and producing an interpenetrating network that provides a large interfacial area for charge separation. However, the non-equilibrium BHJ structure makes it difficult to understand the fundamental structure-property relations. We report a simple approach to control the active layer morphology by direct patterning of \(\pi\)-conjugated polymers into nanostructures or microstructures.\(^1\) We studied polymer crystallinity in patterned poly(3-hexylthiophene) (P3HT) films as a function of developing solvent using grazing incidence wide angle X-ray scattering. It was observed that the \(\pi\)-\(\pi\) stacking of patterned P3HT domains can be changed from edge-on to face-on orientation by varying the developing solvent. This change in orientation improves the power-conversion efficiency by nearly a factor 2.

Q1.00011 Investigation of phase coexistence in block copolymer/salt mixtures near order-disorder phase transitions\(^1\), JACOB THELEN, NITASH BALSARA, University of California Berkeley — Mixtures of polystyrene-b-poly(ethylene oxide) (PS-b-PEO) copolymer and lithium bis(trifluoromethanesulfonyl) imide (LiTFSI) salt can microphase separate into ion-conducting (PEO/LiTFSI) and mechanically reinforcing (PS) domains, facilitating their application as solid electrolytes in lithium batteries. PS-b-PEO/LiTFSI mixtures that exhibit thermally accessible order-disorder phase transitions (ODTs) are used to gain thermodynamic insight to the polymer/salt system. The Gibbs phase rule requires a coexistence of phases during a phase transition in binary systems. We use birefringence and SAXS measurements to confirm the presence of coexisting ordered and disordered phases near the ODT and quantify their relative volume fractions throughout the coexistence temperature window.

Q1.00012 Self-assembled nanostructures in cross-linkable block copolymer/homopolymer blends, CHUNLIN HE, IAN CAMPBELL, MARK STOYKOVICH, CU-Boulder — The self-assembly of block copolymers in films that are 50–100 nm thick provides an attractive approach to patterning nanoscale features. Thermal, chemical, and mechanical stability of the nanoscale morphology in thin films is critical for the generation of robust templates for subsequent fabrication processes, and can be improved by cross-linking the copolymer domains. We have used atom transfer radical polymerization to synthesize PS-b-PMMA diblock copolymers with cross-linkable units capable of reacting through a thermally-activated mechanism or by photoinitiation in response to UV exposure. The self-assembly behavior of lamellar-forming block copolymers with or without cross-linkable units will be compared in thin films. We have developed approaches, including solvent-anneling, for processing the cross-linkable materials in thin films that enable the self-assembly behavior to be decoupled from the cross-linking behavior. The cross-linked nanostructures exhibited enhanced solvent and thermal stability, and have been demonstrated for the fabrication of three-dimensional block copolymer nanostructures in thick films using a layer-by-layer approach.

Q1.00013 Adjusting microstructure and properties of polypropylene nanocomposites through \textit{in situ} interfacial reaction\(^1\), TAO TANG, YUJIE WANG, DONG WAN, XIN WEN, Changchun Institute of Applied Chemistry, CAS — In this report, polypropylene (PP) nanocomposites, in which the interfacial reaction between PP and nanoparticles was \textit{in situ} mediated by peroxide, were prepared by melt mixing method. Carbon nanotubes (CNTs) showed a well dispersed state in the resultant nanocomposites. Interestingly, aligned morphology of CNTs appeared in PP/CNTs nanocomposites in the presence of peroxide and tetrabenzylthiuramdisulfide (TBzTD). We found that two kinds of interfacial interaction between PP chains and CNTs, including chemical linking between two components and \(\pi\)-\(\pi\) interaction between the grafted TBzTD to PP chains and CNTs, showed a synergistic effect on enhancing stress sensitivity of CNTs. As a result, the responsive ability of CNTs in PP matrix to external stress field becomes strong. In this case, CNTs can be easily oriented in PP matrix under weak stress field, such as mold-pressing and injection molding. The resultant nanocomposites have shown more than three times impact strength as pristine PP.

Q1.00014 Interfacial assembly of Graphene Oxide at oil/water and polymer/polymer interfaces, ZHIWEI SUN, TAO FENG, THOMAS RUSSELL, University of Massachusetts Amherst — Amphiphilic structure of graphene oxide makes it a candidate “surfactant” to preferentially segregate to the interface between different fluids. The affinity of graphene oxide towards different phases was tuned by grafting with polystyrene (PS-NH\(_2\)) through hydrogen bonding, and its interfacial behavior, both in toluene/water and polystyrene/poly(methyl methacrylate), was studied. The surface tension of the toluene/water interface decreases in the presence of PS-NH\(_2\) grafted graphene oxide, indicating that graphene oxide flakes can be forced to the toluene/water interface when grafted with PS-NH\(_2\). Transmission electron microscopy shows that graphene oxide can even be forced into a “jammed” state at the water/toluene interface. In addition, polystyrene and poly(methyl methacrylate) were blended with graphene oxide, its morphology changes from island type to co-continuous structure, but the mechanism of this behavior is still not clear. These interfacial sheets may provide a model system to study buckling and crumpling behavior at interfaces.
Q1.00015 Designing Reconfigurable Stimuli-Responsive Gel/Nanofibers Composites, XIN YONG, OLGA KUKSENOK, ANNA BALAZS. Chemical Engineering Dept. University of Pittsburgh — Using dissipative particle dynamics (DPD), we model the response of a composite gel, which encompases active nanofibers, to external stimuli, such as light and temperature. The gel is constructed by crosslinking polymer chains in a coarse-grained manner. We probe the volume phase transition and swelling kinetics of the gels in explicit solvents. Our model is validated through qualitative comparisons with Flory-Huggins theory, and the effects of solvent quality, crosslink density and temperature are analyzed. By incorporating nanofibers into the gel matrix, we utilize different responses of the fibers and gel to variations in external stimuli. We focus on the fiber-gel and fiber-fiber interactions and establish routes for modeling composites with multiple types of fibers, which enable greater control of materials functionality. Utilizing the adaptability of gel/nanofiber composites, we design composites that can dynamically reconfigure shape via external stimuli to achieve actuation and locomotion. Our findings provide fundamental insights into the dynamics of gel-based composites, as well as guidelines for designing re-programmable multi-functional materials.

Q1.00016 Interfacial activity of acid functionalized single-walled carbon nanotubes (SWCNTs) at the fluid-fluid interface, TAO FENG, THOMAS RUSSELL, DAVID HOAGLAND. University of Massachusetts at Amherst — Interfacial assembly of acid-functionalized single-walled carbon nanotubes at the oil/water interface is achieved by the addition of low molecular weight (MW) amino-terminated polyurethane in the oil phase. The surface activity of carboxylated SWCNTs is strongly influenced by the end-group chemistry and molecular weight of the polystyrene component, the concentrations of this component and the SWCNTs, along with the degree of functionalization of the SWCNTs. The prerequisites for interfacial trapping are amino termini on chains with MW less than 5k and 6 hours or longer incubation of pristine SWCNTs to achieve their carboxylation. Pluronic in interfacial tension resembling those for surfactants were observed at critical bulk concentrations of both SWCNTs and PS-NH₂. In dried droplets, SWCNTs densely packed with associated PS-NH₂ form a bird nest-like interfacial structure, with the SWCNTs preferentially oriented perpendicular to the original interface.

Q1.00017 Plasmonic Coupling via Au@stimuli-responsive polymer Hybrid Core@shell Nanoparticles Monitored by Surface Plasmon Resonance Spectroscopy, JI-EUN LEE, KYUNGWA CHUNG, DONG HA KIM, Ewha Womans University — Noble metal nanostructures with responsive polymers can be used to probe unique plasmonic properties associated with swelling-shrinking transitions in polymer chains triggered by a specific external stimulus. The phase transition causes changes in the refractive index in the vicinity of the particle surface and induces concurrent changes in the characteristic inter-particle distance. We designed a plasmonic-coupling-based sensing device consisting of Au nanoparticles separated from the Au substrate in Kretschmann configuration SPR spectroscopy through a thermo-responsive polymer linker layer. Concretely, Au NPs having stimuli-responsive polymer chains tethered to the Au surface were first fabricated through SI-ATRP. The optical properties of these stimuli-responsive devices were investigated by both in-situ and static SPR analysis. Also, we demonstrate that bimetallic nanostructures containing another type of metal NP at the stimuli-responsive polymer periphery exhibit a controlled optical sensing property based on LSPR coupling phenomenon.

Q1.00018 Supramolecular Nanocomposites: Effects of the Aspect Ratio of Nanorods, KARI THORKESSLON, Materials Science and Engineering, University of California, Berkeley, TING XU, Materials Science and Engineering, Chemistry, University of California, Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — Anisotropic particles display many unique electrical, mechanical, and optical properties useful in applications ranging from photovoltaic devices, plasmonic devices, and sensors to mechanically strengthened composites. These properties depend not only on size and shape, but also on spatial distribution and orientation. It is thus desirable to control both distribution and orientation with methods applicable to a wide range of size and shape. We have recently demonstrated control over spatial distribution and in some cases local orientation of nanorods by using a supramolecular approach to tailor the conformational entropy of block copolymer chains [1]. Alkyl-passivated nanoparticles can in this way be arranged into aligned arrays, sheets, continuous networks, and clusters. Here, we expand the application of this method to nanorods with a range of aspect ratios, showing that the spatial distribution of the nanorods can be controlled regardless of length, and orientation can also be finely controlled in the case of lengths comparable to the BCP periodicity. Findings will be accounted for by considering the interparticle interactions, the particle-supramolecule interactions and the phase behavior of supramolecules.

Q1.00019 Multi-Color Emission of Hybrid Block Copolymer-Quantum Dot Microspheres by Controlled Quantum Dot Spatial Isolation, KANG HEE KU, MINSOO KIM, KWANYEOL PAEK, JAE MAN SHIN, SUNHAENG CHUNG, KAIRST, SE KYU JANG, KEPRI, WEON-SIK CHAE, KBSI, GI-RA YI, Sungkyunkwan University, BUMJOON KIM, KAISET, SE KYU JANG COLLABORATION, WEON-SIK CHAE COLLABORATION, GI-RA YI COLLABORATION — Fluorescent quantum dots (QDs) are promising candidates for multi-color or white light-emitting systems, however, most current systems involve undesired Forster resonance energy transfer (FRET) between QDs. Herein, we developed multi-color emitting hybrid microspheres with block copolymers (BCPs) and QDs through control of the locations of different-colored QDs in BCP micelles. Hydrogen interaction assisted method was exploited to confine QDs within the BCP spheres without sacrificing any quantum yield efficiency. BCP microspheres with raspberry-like surface structures were prepared by an evaporation-induced self-assembly from an emulsion. When different-colored QDs were independently incorporated into isolated micelles, FRET was completely suppressed because the size of the protective micellar corona was greater than the Förster radius. In contrast, FRET was observed when QDs were concurrently incorporated into the same micelle cores. This spatial control of QDs in micelles was confirmed by TEM, EDX, PL, and FLIM measurements. Through the isolated BCP micelles, ratiometric control of different colored QDs can display a wide range of colors.

Q1.00020 NIR fluorescent chitosan-based nanoparticles for tracking and delivery of cancer therapeutic molecule in living systems, GIULIA SUARATO, AMANDA CHIN, Materials Science and Engineering, Stony Brook University, New York, USA, YIZHI MENG, Materials Science and Engineering, Chemical and Molecular Engineering, Stony Brook University, New York, USA — Tumor metastasis is associated with the epithelial-to-mesenchymal transition (EMT), in which cells lose their polarized phenotype to acquire the asymmetry and motility of mesenchymal cells. Among the many molecular determinants for EMT is bone morphogenetic protein-7 (BMP-7), a critical regulator of skeletal tissue formation and kidney development. Current treatments for metastatic cancer primarily involve surgery and chemotherapy, both with considerable side effects. Therefore the goal of our research is to evaluate the ability of BMP-7 to reverse EMT using a delivery system based on glycol chitosan nanoparticles (GCNP), naturally biodegradable. The GCNP are labeled with Cy5.5, a near infrared (NIR) excitable dye that enables non-invasive imaging in living systems. The chitosan shell provides affinity for the cell surface and protection from intracellular enzymes during transport. Preliminary data show that Cy5.5-GCNP vehicles were successfully delivered to murine preosteoblast (MC3T3-E1), rat osteosarcoma (ROS) 17/2.8 and human embryonic kidney (HEK298) cells. Release kinetics using a model protein (BSA) and BMP-7, and the stability of the protein nano-cargo are currently being evaluated. Cell morphology will be examined with immunofluorescence microscopy.
Q1.00021 Do attractive interactions slow down diffusion in polymer nanocomposites? CHIA-CHUN LIN, SANGAH GAM, University of Pennsylvania, JEFFREY S. METH, DuPont Co., NIGEL CLARKE, University of Sheffield, KAREN I. WINYE, RUSSELL J. COMPOSTO, University of Pennsylvania — Diffusion of deuterated poly(methyl methacrylate) (dPMMA) is slowed down in PMMA matrix filled with spherical silica nanoparticles (NPs) ranging from 13 to 50 nm in diameter. The normalized diffusion coefficients (D/D_0) decrease as the volume fractions increases, and this decrease is stronger as NPs size decreases. When plotted against the confinement parameter, ID/2R_g, where ID is interparticle distance and 2R_g is probe size, D/D_0 collapse onto a master curve. In the strongly confined region where ID < 2R_g, D/D_0 decrease dramatically up to 80 %, whereas in the weakly confined region where ID > 2R_g, D/D_0 decrease moderately. Even when ID is eight times larger than 2R_g, D/D_0 is reduced by 15 %, which reveals an attractive system that is not significantly altered by center of mass polymer diffusion in polymer nanocomposites.

Q1.00022 Confinement and Interfacial Effects in Polymer Nanocomposites ADAM HOLT, University of Tennessee, JOSHUA SANGORO, YANGYANG WANG, ALEXANDER AGAPOV, Oak Ridge National Laboratory, ALEXEI SOKOLOV, Oak Ridge National Laboratory & University of Tennessee — The influence of different nanoparticles on segmental and chain dynamics of poly(2-vinylpyridine) nanocomposites is investigated by broadband dielectric spectroscopy (BDS), dynamic mechanical spectroscopy (DMS), and calorimetry. While remarkable changes in dynamics are observed with increasing nanoparticle loading, only weak effects in the segmental mobility are found. These results are discussed in the context of recent studies of polymer nanocomposites.

Q1.00023 Thermally Switchable Aggregation of Gold Nanoparticles in Polymer Nanocomposites KUHYOUNG HEO, CAROLINE MIESCH, TODD EMRICK, RYAN HAYWARD, Department of Polymer Science & Engineering, University of Massachusetts Amherst — The level of dispersion or aggregation of nanoparticles is a key factor in determining the performance of polymer-based nanocomposites for a wide range of applications. However, controlling this dispersion of nanoparticles can often be challenging due to the interplay between chemical and physical interactions between the polymer and the particles. Here, we introduce a simple method of confining the aggregation state of gold nanoparticles based on hydrogen bonding between the nanoparticle ligands and the matrix. Strong hydrogen bonding interactions provides almost uniform dispersion of poly(styrene=4-vinylpyridine) functionalized gold nanoparticles for annealing temperatures well above the glass transition temperature of the poly(styrene-4-hydroxystyrene) matrix. However, annealing at higher temperatures diminishes the strength of hydrogen bonds, leading to the formation of aggregates. This aggregation was found to be largely reversible, with nanoparticles dispersing once again by annealing the nanocomposites at reduced temperature. We track the thermal switching behavior during a series of heating/cooling cycles through changes in optical properties and by transmission electron microscopy.

Q1.00024 Peptides (P1, P2 and its mutations) binding with a graphene plane: an all-atom to all-residue hierarchical coarse-grained approach ZHIFENG KUANG, BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — Binding of peptide P2 (EPLQLKM) [1] and its mutations (P2G, P2Q) to a graphene plane are studied by a coarse-grained molecular dynamics simulation. Our hierarchical coarse-grained approach involves all-atom MD simulation to assess the binding interaction of each residue with the graphene sheet. Data from all-atom simulations are then used as input to phenomenological interaction in a coarse-grained MC simulation [2]. Binding of each peptide and its residue in corresponding sequence (P2, P2G, P2Q) are evaluated by analyzing the adsorption of each residue, its mobility, and structural profiles. Although it is difficult to identify overall morphological differences in adsorbed peptides by visual inspections, quantitative analysis of the conformational changes of adsorbed peptides shows variations in size among P2E and its mutations. Results on binding of peptide P1 (HSSYWAFNNKT) may also be presented if data become available.

This work is supported by the Air Force Research Laboratory.

Q1.00025 Syntactomer Peptide Assembly on Deformable Silicone Elastomer Surfaces JULIE N. L. ALBERT, JAN GENZER, North Carolina State University, Chemical and Biomolecular Engineering — Surfaces of biocompatible poly(vinylmethylsiloxane) (PVMS) networks can be functionalized readily through modification of pendant vinyl groups. In this work, we also took advantage of network elasticity to examine how the conformation of surface-grafted peptides depended on their grafting density (i.e., the areal density of peptides). PVMS networks were cross-linked via reactive end groups, leaving the pendant vinyl groups available for peptide attachment via a carbonyl acid terminated thiol linker. To control grafting density, the networks were stretched uniaxially up to ∼30 % strain during the attachment of the thiol linker (via thiol-ene click chemistry) and the peptide (via sulf-NHS/EDC coupling chemistry). After deposition, the strain was released. The resultant peptide-modified PVMS networks were imaged using scanning probe microscopy. The specific peptides of interest are called “syntactomers” because they are made up of repeating amino acid sequences much like a polymer is made up of repeating monomers units. In solution, these peptides display interesting pH-sensitive LCST and UCST phase behaviors that may impart surfaces with pH- and temperature-responsiveness in addition to biocompatibility.

Q1.00026 Peptide Length Determines Equilibrium Secondary Structure in Protein-Analogous Micelles MATTHEW TIRRELL, University of Chicago, RACHEL MARULLO, Cooper Vision, MARK KASTANTIN, University of Colorado — This work seeks improved bottom-up design of bioinspired materials built from peptide-amphiphiles, which are a class of bioconjugates whereby a biofunctional peptide is covalently attached to a hydrophobic moiety that drives self-assembly in aqueous solution. Specifically, this work highlights the importance of peptide length (i.e. molecular weight) in determining the equilibrium secondary structure of the peptide as well as the self-assembled (i.e. micelle) geometry. Peptides used here repeat a seven-amino acid sequence between one and four times to vary peptide length while maintaining similar peptide-peptide interactions. Without any hydrophobic tail, these peptides all exhibit a combination of random coil and α-helical structure. Upon self-assembly, however, short peptides are prone to β-sheet structure and cylindrical geometry while longer peptides remain helical in spherical micelles. The transition to β-sheet structures in short peptides is kinetic, whereby amphiphiles first self-assemble with helical peptide structure, then overcome an activation barrier as they transition to their equilibrium β-sheet structure at a rate that depends on both temperature and ionic strength. These results identify peptide length as an important control over equilibrium peptide secondary structure and micelle geometry. Furthermore, the kinetic nature of the helix-to-sheet transition opens the door for shape-changing bioinspired materials with tunable conversion rates.

Q1.00027 Using Lipid Vesicles to Achieve Selective Removal or Deposition of Janus Particles on Rough Surfaces EMILY CRABB, NICHOLAS MOELLERS, XIN YONG, ISAAC SALIB, ANNA BALAZS, Chemical Engineering Dept., University of Pittsburgh — Using dissipative particle dynamics (DPD), we explore the interaction between a nanoscopic lipid vesicle and Janus nanoparticles that are localized on rough hydrophilic substrates. We have previously shown that a fluid-driven vesicle can adsorb and transport up to four nanoparticles on a flat hydrophilic surface. Furthermore, we showed that it is possible to induce pick-up and drop-off of particles by varying parameters such as particle composition and particle-substrate attraction. We now introduce a nano-scale crack that spans the substrate’s width onto the otherwise flat surface and determine under what conditions the vesicle either removes the particle or deposits the particle into this niche. In this way, our model can describe an attractive system that is not significantly altered by center of mass polymer diffusion in polymer nanocomposites.
**Q1.00028** Target Diffusion and Concentration Control of Varying Hydrophobicity Drugs in an Injectable Solid Self-Assembling Peptide Hydrogel, JESSIE E.P. SUN, University of Delaware, SIGRID LANGHANS, SEUNG JOON LEE, Al DuPont Children’s Hospital, SAMER SATAYHE, University of Delaware, JOEL P. SCHNEIDER, National Cancer Institute at Frederick, DARRIN J. POCHAN, University of Delaware — We studied diffusion profiles of varying hydrophobicity drugs in a beta-hairpin peptide hydrogel solid that is shear thinnable, injectable, and immediate reheals after shear. These rheological properties result from its entangled and branched fibrillar nanostructures, formed from intramolecular folding and consequent intermolecular assembly of the peptides. Different chemotherapeutic drugs at different concentrations with greatly differing properties were encapsulated to show direct targeting drug delivery. Using in vitro and spectroscopy techniques, we showed controlled, sustained diffusion of the drugs. We were able to protect and keep active, hydrophobic agents that otherwise would be deactivated through traditional delivery methods. We also showed that we can maintain low, targeted, and constant dosages, preserving surrounding areas from lack of target specificity of certain drugs.

**Q1.00029** Expanding Cancer Detection Using Molecular Imprinting for a Novel Point-of-Care Diagnostic Device, YINGJIE YU, MIRIAM RAFAILOVICH, YANTIAN WANG, YEONA KANG, LINGXI ZHANG, BASIL RIGAS, Department of Materials Science and Engineering, State University of New York at Stony Brook, DIVISION OF GASTROENTEROLOGY, SCHOOL OF MEDICINE TEAM — We propose the use of a potentiometric biosensor that incorporates the efficient and specific molecular imprinting (MI) method with a self-assembled monolayer (SAM). We first tested the biosensor using carcinoembryonic antigen, CEA, a biomarker associated with pancreatic cancer. No change in detection efficiency was observed, indicating that the sensor is able to discriminate for the template analyte even in concentrated solution of similar substances. In addition, we use biosensor to discriminate normal fibrinogen and damaged fibrinogen, which is critical for the detection of bleeding disorder. Computer simulations of the protein structure were performed in order to establish the changes in morphology and determine the sensitivity of the biosensor to conformational changes in the proteins. We found that even small changes in PH can generate rotation of the surface functional groups. Yet, the results show that only when the detection and imprinting conditions are similar, robust signals occurs. Hence we concluded that both morphology and surface chemistry play a role in the recognition.

**Q1.00030** Reconstruction of Bone Nanostructure using Hierarchically Ordered Polymer Nanofibers, XI CHEN, WENDA WANG, SHAN CHENG, BIN DONG, CHRISTOPHER LI, Drexel University — Natural bone is comprised of hydroxyl apatite (HA) crystals periodically templated by collagen fibers with precisely controlled crystal orientation. No synthetic materials can mimic natural bone with controlled mineral orientation and periodicity. Herein we report that this structural challenge can be met using hierarchically ordered nanofiber shish kebabs (NFSKs), constructed via combination of electropinning polycaprolactone (PCL) and controlled crystallization of PCL-β-poly acrylic acid (PCL-β-PAA). These NFSKs were employed as a template to control the nucleation and growth of hydroxyapatite nanocrystals. HA crystals were formed on such templates with controlled orientation and periods. Such a biomimetic structure serves as a promising bone scaffold material for tissue engineering.

**Q1.00031** Mechanics and geometry in the seashell-like (Turritella) surface, QIAOHANG GUO, ZI CHEN, Washington University in St. Louis, WEI LI, KUN REN, JUNJIE LIN, Fujian University of Technology, LARRY A. TABER, Washington University in St. Louis, WENZHE CHEN, Fujian University of Technology — Helical structures are ubiquitous in nature and engineering, ranging from DNA molecules to plant tendrils, from sea snail shells to nanoribbons. While the helical shapes in natural and engineered systems often exhibit nearly uniform radius and pitch, helical shell structures with changing radius and pitch, such as seashells and some plant tendrils, add to the variety of this family of aesthetic beauty. Here we report the first biomimetic seashell-like structure resulting from mechanics of geometric frustration. In previous studies, the total potential energy is everywhere minimized when the system achieves an equilibrium. In this study, however, the local energy minimization cannot be realized as a result of the geometric incompatibility, and hence the whole system deforms into a shape with a global energy minimum whereby the energy in each segment may not necessarily be locally optimized.

**Q1.00032** Bulk Heterojunction Polymer Solar Cells Based on Ternary Blend System, YU GU, FENG LIU, University of Massachusetts - Amherst, CHENG WANG, Advanced Light Source, Lawrence Berkeley National Laboratory, THOMAS RUSSELL, UNIVERSITY OF MASSACHUSETTS - Amherst — To enhance the absorption of the solar light, we mixed two hole-transporting polymers that are active in complementary wavelength ranges of the solar spectrum, e.g., P3HT and PCPDTB, with one electron transporting material, PCBM, to fabricate the single active layer for bulk heterojunction solar cells. This simple one-step method has been shown to efficiently improve the device performance compared with the corresponding binary references. Multiple scattering techniques and transmission electron microscopy were used to determine the morphology for the ternary blend. It is shown that when keeping a low ratio of PCPDTB in the ternary blend, P3HT could still crystallize and phase-separate from other amorphous components. A continuous network of P3HT fibril bundles was formed, PCPDTB/PCBM/amorphous P3HT filled the interfibrillar region and PCPDTB wrapped the P3HT fibrils. Such morphology is compatible with the well aligned HOMO-LUMO levels of the three components and the sensitization effect of PCPDTB. As a result, PCPDTB benefits the charge transfer; the two polymers act not only individually but also synergistically. 1This work was supported by the Department of Energy supported Energy Frontier Research Center at University of Massachusetts and the NSF-supported Materials Research Science and Engineering Center at University of Massachusetts.

**Q1.00033** Characterization of Nanostructure and Electrical Properties of Polymer- Fullerene Bulk Heterojunction Solar Cells, DONG WANG, FENG LIU, XIAOBO SHEN, University of Massachusetts Amherst, KEN NAKA-JIMA, Tohoku University, THOMAS RUSSELL, University of Massachusetts Amherst — The ability to control and optimize the active layer morphology is critical for achieving high power efficiency with bulk heterojunction (BHJ) organic photovoltaic (OPV) devices. Here, we fabricated three types of polymer-fullerene BHJ active layers: diketopyrrolopyrrole (DPP)/PCBM, poly[N-9′-heptadecyl-2,7-carbazole-alt-5,5-(4,7-di-2-thienyl-2′,1′,3′'-benzo[b]thiadiazole)] (PCDDBT)/PCBM, and poly(3-hexylthiophene) (P3HT)/PCBM. A comparative study of the nanostructure and electrical properties resulting from different donors and annealing processes was done by conductive atomic force microscopy (c-AFM) grazing incidence small angle scattering (GI-XAS), wide angle scattering (GI-XAS), and transmission electron microscopy (TEM). To obtain a signal from the c-AFM, a percolated pathway for either electrons or hole is required, with details on the internal structure of the assemblies being provided by GI-XAS and morphology of the assemblies being provided by GI-XAS and TEM.
Q1.00034 Processing Solvent Dependent Morphology of Diketopyrrolopyrrole (DPP) based Low Band Gap Polymer and PCBM Blends, SUNZIDA FERDOUS, FENG LIU, THOMAS RUSSELL, Polymer Science and Engineering, University of Massachusetts-Amherst — Solution processing of polymer semiconductors is widely used for fabrication of low cost organic solar cells. Recently, mixed solvent systems or additive based systems for fabricating polymer solar cells have proven to be beneficial for obtaining high performance devices with multi-length scale morphologies. To control the morphology during the processing step, one needs to understand the effect of solvent as it evaporates to form the thin film structure. In this study, we used diketopyrrolopyrrole (DPP) based low band gap polymer and phenyl-C61-butyric acid methyl ester (PCBM) blend in a series of mixed solvent systems consisting of a good solvent for both of the active material components, as well as different solvents that are good solvents for PCBM, but poor solvents for the polymer. Different evaporation times of the poor solvents during the drying process, and different solubility of the polymer in these poor solvents as well as their interaction with the substrate play an important role in the final morphology. In-situ GIWAXS studies were performed to observe the evolution of the structure as the solvent evaporates. The final morphologies of the thin film devices were also characterized by AFM, TEM, and various x-ray scattering techniques to correlate the morphology with the obtained device performances.

Q1.00035 The Effect of Binding Groups on the Seebeck Coefficient of Phenyl Derivative Molecular Junctions1, WILLIAM CHANG, UC Berkeley, CHENGKANG MAI, UC Santa Barbara, MICHELE KOTIUGA, JEFFREY NEATON, Lawrence Berkeley National Lab, GUI BAZAN, UC Santa Barbara, RACHEL SEGALMAN, UC Berkeley — Thermoelectrics currently suffer from low efficiencies due to inverse coupling of the Seebeck coefficient and electrical conductivity, limiting the power factor. Decoupling of these two physical properties has previously been achieved with molecular junctions. Larger phenyl derivative molecules with an Au binding group Au-C has on the Seebeck coefficient. Phenyl derivative molecules with an Au direct binding group show a significantly lower Seebeck coefficient than molecules with an Au-S binding group. This lower Seebeck coefficient is explained by theoretical calculations as a broadening in the transmission function due to the direct bonding group. This demonstrates the importance of the metal-molecule interface and binding group selection in tuning the transmission function, and the resultant conductance and Seebeck coefficient. This result will lend further insight in rational design for molecules with higher power factors. 1We would like to acknowledge support from Office of Naval Research - ONR/AFOSR BAA 10-026

Q1.00036 A Facile Route to Large-Scale Hierarchically Structured Polymer Assemblies with Enhanced Electrical Conductivity, WEI HAN, Georgia Institute of Technology, MING HE, Fudan University, MYUNGHWAN BYUN, University of Massachusetts, BO LI, ZHIQUN LIN, Georgia Institute of Technology — By subjecting a drying droplet containing conjugated homopolymer to a judiciously designed geometry consisting of a cylinder situated on a flat substrate (i.e., cylinder-on-flat geometry), a set of highly ordered straight or wavy stripes at the microscopic scale over a large area were yielded, in which each microscopic stripe was composed of bundles of nanofibers or node-like nanodomains (i.e., forming hierarchical assemblies). These hierarchical patterns of conjugated homopolymers and all-conjugated diblock copolymer exhibited good electrical properties. Quite intriguingly, the crystallinity of the as-prepared assemblies of all-conjugated diblock copolymer was largely improved after the solvent vapor annealing, resulting in four times increase in electric conductivity. This facile, scalable deposition technique based on controlled evaporative self-assembly renders the crafting of hierarchically structured semicrystalline conjugated optoelectronic materials, and may provide a paradigm to develop high-performance electronic devices in a simple and controllable manner.

Q1.00037 Random Conjugated Copolymers with Panchromatic Absorption for High-Efficiency Polymer Solar Cells, JAE WOONG JUNG, WON HO JO, Seoul National University — One of the most important issues for polymer solar cells (PSCs) is to develop conjugated polymers with broad absorption in the visible-light range and vertical charge transport. Particularly, the broad light absorption of the polymer is important to enhance the power conversion efficiency because these have absorption leads to low current in comparison with other inorganic-based solar cells. A fascinating approach to extend light absorption is the synthesis of copolymers composed of several chromophores. Among various building blocks, diketopyrrolo[3,4-c]pyrrole (DPP) and 6,6’-[3,3’]-biindolylidyene-2,2’-dione (isoindigo) have attracted much interest since they are easily accessible and exhibit promising optoelectronic properties. Here, we report random conjugated copolymers consisting of DPP and isoindigo as co-electron acceptor of donor-acceptor conjugated polymer. The random copolymers exhibited not only broad light absorption but also low-lying HOMO levels. Also, the predominant face-on orientation of the copolymers is beneficial for vertical charge transport in PSCs. The combination of excellent optoelectrical properties and favorable molecular conformation makes copolymers promising candidate for active material in high performance PSCs.

Q1.00038 Synthesis of Graphene Nanoribbons with Various Widths and Its Application to Thin-Film Transistor, KYUNG TAE KIM, WON HO JO, Seoul National University — Although graphene itself is a zero-bandgap semimetal, graphene nanoribbon (GNR) with a width smaller than 10 nm exhibits semiconductor behavior that renders them suitable for active materials of electronic devices. Several methods have been reported to produce GNRs, such as lithography, unzipping of CNTs, mechanical exfoliation and CVD. However, the uncontrollable character of these methods or in some case the harsh conditions restrict severely the quality of the resulting graphenes and consequently limit their applicability below a certain width. Here we report the synthesis of graphene nanoribbons with various widths and lengths. For synthesis of GNRs, we first synthesized polymers with phenylene, naphthalene and anthracene units by the Suzuki coupling reaction between dibromine monomer and diboron ester monomer. The polymers were then converted into the corresponding GNRs through intramolecular cyclodehydrogenation reaction. The cyclodehydrogenation were identified quantitatively by NMR analysis. All GNR-based TFTs showed ambipolar transport behavior. The anthracene-based GNR exhibits the best TFT performance among three GNRs due to longer conjugated length, larger width and stronger π-stacking as compared to phenylene- and naphthalene-based GNRs.

Q1.00039 Tuning the crystal structure of contorted hexabenzocoronene thin films for transistors applications, ANNA HISZPANSKI, Chemical and Biological Engineering Department, Princeton University, MATTHEW BRUZEK, Chemistry Department, University of Kentucky, ARTHUR WOJ, Cornell High Energy Synchrotron Source, JOHN ANTHONY, Chemistry Department, University of Kentucky, YUEH-LIN LOO, Chemical and Biological Engineering Department, Princeton University — Though the structure of organic semiconductors in the active channels of thin-film transistors is known to impact device performance, controlling such structure has been a long-standing challenge. We demonstrate the ability to fine-tune the crystal packing of semiconducting contorted hexabenzocoronene (HBC) thin films via solvent-vapor annealing. Solvent-vapor annealing with weakly hydrogen-bonding solvents having large molar volumes preferentially yields the P21/c crystal structure of HBC. Annealing with solvent vapors having smaller molar volumes and stronger tendencies to hydrogen-bond coaxes HBC films to adopt a previously-unpublished crystal structure that is similar to that of the Pbcn structure. Elucidating the structures of HBC thin films when they are exposed to a myriad of solvent vapors has allowed us to produce a processing diagram, with which we have been able to predictively access different crystal structures for thin-film transistor applications.

Q1.00040 Active layer morphologies for device simulations, JUTTA LUETTMER-STRAHMANN, KIRAN KHANAL, Departments of Physics and Chemistry, The University of Akron — The morphology of the active layer has a strong effect on charge generation and transport in organic photovoltaics. In bulk heterojunction devices, amorphous and crystalline regions with varying compositions coexist due to microphase separation and crystallization of the blend components. Accounting for these effects in device simulations is difficult since the size of the active layer is too large to generate realistic morphologies from molecular simulations of the constituents. In this work we perform Monte Carlo simulations of a coarse-grained lattice model of polymer mixtures to generate microphase separated layers with ordered and disordered regions. We employ external fields and surface interactions to control the morphologies and investigate the effect of domain size and charge on transport charge.
Q1.00041 Thermally-Induced Dewetting in Ultra-Thin C$_{60}$ films on Copper Phthalocyanine . TERRY MCAFEE, HARALD ADE, DANIEL DOUGHERTY, North Carolina State University — Organic photovoltaics have made significant advances in the past decade. These advances have occurred primarily by the synthesis of new materials that manipulate the bandgap to improve the short circuit currents and open circuit voltages. Domain size and orientation of the donor and acceptor materials has shown to also have a significant impact on device performance, and must be better understood and controlled to achieve organic solar cells that are a feasible alternative energy source. The evolution of thermally-annealed ultra-thin fullerene-C$_{60}$ layers on copper phthalocyanine is examined by Atomic Force Microscopy and Near Edge X-Ray Absorption Fine Structure spectroscopy. Annealing at 105°C causes 2 nm thick C$_{60}$ films to de-wet the copper phthalocyanine substrate surface. Coarsening of C$_{60}$ clusters is observed that creates mounds that exceed the nominal C$_{60}$ thickness by more than an order of magnitude. Sequential deposition and annealing of C$_{60}$ layers alternated with a donor material such as CuPc could be utilized to engineer a Bulk Heterojunction structure with C$_{60}$ domain sizes catered to the exciton diffusion length.

Q1.00042 Distinguishing excitonic from vibronic oscillations in ultrafast spectroscopy , JACOB KRICHER, University of Ottawa, JOEL YUEN, Harvard University, ALLAN JOHNSON, University of Ottawa, JOSEPH GOODKINNIGHT, ALAN ASPURU-GUZIK, Harvard University — Ultrafast experiments on photosynthetic and conjugated organic systems have indicated that coherent delocalization of exciton states significantly contributes to exciton transport, even up to room temperature. Oscillations in 2D spectra due to excitonic delocalization can be similar to those from vibronic oscillations, which are not important for exciton transport. We describe a straightforward experiment — broadband pump-probe — to distinguish between ultrafast oscillations from excitonic or vibronic-only sources. We consider anharmonic molecular oscillators and consider the requirements for how broadband (short in time) the experimental pulses must be to distinguish excitonic from vibronic oscillations.

Q1.00043 Structure development of bilayer PCDTBT and PCBM films , HSIN-WEI WANG, THOMAS RUSSELL, TODD EMRICK, UMass Amherst — Poly[N-9'-hepta-decanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)] (PCDTBT) is a promising low band gap material, with power conversion efficiency approaching 6% when blended with PCBM$_{70}$. However, unlike the benchmark P3HT:PCBM system, annealing at high temperature results in performance reduction. To gain a deeper understanding of this material, bilayer films of crystalline PCDTBT and PCBM were prepared, and the kinetics associated with the structure development were investigated. It was found that the diffusion of PCBM disturbs the ordering of PCDTBT along (100) direction. A decrease in domain size was also observed by transmission electron microscopy.

Q1.00044 Effects of supercritical carbon dioxide on immobile bound polymer chains on solid substrates 1. MANI SEN, Stony Brook University, MITSUNORI ASADA, Kuraray Co., NAISHENG JIANG, MAYA K. ENDOH, Stony Brook University, BULENT AKGUN, SUSHIL SATLIA, Center for Neutron Research, NIST, TADANORI KOGA, Stony Brook University — Adsorbed polymer layers formed on flat solid substrates have recently been the subject of extensive studies because it is postulated to control the dynamics of technologically relevant polymer thin films, for example, in lithography. Such adsorbed layers have been reported to hinder the mobility of polymer chains in thin films even at a large length scale. Consequently, this bound layer remains immobile regardless of processing techniques (i.e. thermal annealing, solvent dissolution, etc). Here, we investigate the use of supercritical carbon dioxide (scCO$_2$) as a novel plasticizer for bound polystyrene layers formed on silicon substrates. In-situ swelling and interdiffusion experiments using neutron reflectivity were performed. As a result, we found the anomalous plasticization effects of scCO$_2$ on the bound polymer layers near the critical point where the anomalous adsorption of CO$_2$ molecules in polymer thin films has been reported previously.

1Acknowledgement: We acknowledge the financial support from NSF Grant No. CMMI-084626.

Q1.00045 A Length Scale for the Free Surface of Polymer Films , ETHAN GLOR, MARY KLING, NOLAN AVERBUCH, ZAHLRA FAKHRRAAI, University of Pennsylvania — Recent work in polymer physics shows that the relaxation dynamics near a free surface of a thin polymer film are significantly different from that of the bulk polymer. While experiments directly probing the surface and bulk relaxation dynamics are rare, the effect of this difference can be seen in the properties of some polymer thin films. For instance, studies have shown that polystyrene thin films exhibit a decreased glass transition temperature with decreased thickness. A common explanation for this observation is that the mobile surface occupies a greater percentage of a thin film, thus the average relaxation dynamics of the film is affected, and the glass transition temperature decreases. Despite extensive research in this area, little is known about many fundamental questions of this mobile surface layer, including the penetration depth of the layer and the mechanism by which the free surface of a polymer film is more mobile. In this study, we use ellipsometry to measure the Tg of polystyrene films of various film thicknesses, molecular weights, and at various cooling rates. From these experiments, we estimate both a length scale and molecular weight dependence for the depth of enhanced mobility near the free surface.

Q1.00046 Effect of Adjacent Rubber Layers on the Physical Aging Rate of Polymer Glasses , PHILLIP RAUSCHER, CONNIE ROTH, Department of Physics, Emory University, Atlanta, GA 30329 — Recent advances in block copolymer synthesis have led to new routes for forming nanostructured polymer blends putting glassy and rubbery phases in intimate contact. The long-term stability of these systems is crucial for their performance and functionality. In order to investigate the effect of glassy-rubber interfaces between neighboring polymer domains on the local stability and physical aging of the confined glassy layers, we have modified our streamlined ellipsometry method to be able to determine the physical aging rate of thin glassy layers adjacent to rubber layers. We present results demonstrating how ellipsometry can be used to measure the physical aging rate of glassy polystyrene (PS) layers atop rubbery poly(n-butyl methacrylate) (PnBMA) layers. With decreasing PS layer thickness, down to 55 nm, we observe a slight increase in the aging rate. This is in strong contrast to single layer PS films, which show a decrease in aging rate with decreasing thickness due to the local Tg reduction at the free surface. The slight increase in aging rate of the glassy PS layers atop rubbery PnBMA cannot be explained by any shift in local Tg suggesting that this faster aging rate caused by the presence of the rubbery-glassy interface must be due to some separate mechanism.

Q1.00047 Oxidatively stable polyaniline derivatives for electrodes in energy storage1. JODIE LUTKENHAUS, JU-WON JEON, Texas A&M University, LUTKENHAUS LABORATORY TEAM — Conjugated polymers have been explored as electrodes in batteries and pseudocapacitors for over 30 years. Yet, their widespread implementation has been hindered for several reasons such as oxidative stability, low capacity, and rate limitations associated with ionic mobility relative to current state-of-the-art. On the other hand, conjugated polymers have much to offer because of their good electronic conductivity, high Coulombic efficiency, and theoretical capacities comparable to those of metal oxides. Our lab’s current goal is to overcome the aforementioned challenges, so that conjugated polymeric electrodes can be suitable used in energy storage for applications such as mechanically flexible energy storage and structural power system. This talk will present one of several experimental approaches towards synthesis and processing of polyaniline that achieve oxidatively stable, high capacity, ioniically mobile electrodes. This derivative is a water-processable colloid of intimately mingled polyaniline and polyacryl, where the polyacid acts as the dopant. The origin of the oxidative stability is investigated using computation modeling.

1This work is supported in part by the Welch Foundation.
**Q1.00048 Conjugated block copolymer photovoltaics with near 3% efficiency**, CHANGHE GUO, The Pennsylvania State University, YEN-HAO LIN, Rice University, MATTHEW WITMAN, The Pennsylvania State University, KENDALL SMITH, Rice University, CHENG WANG, ALEXANDER HEXEMER, Lawrence Berkeley National Lab, RAFAEL VERDÚZCO, Rice University, ENRIQUE GOMEZ, The Pennsylvania State University — Conjugated polymer blend solar cells are devices where the active layers are composed of polymer donor and polymer acceptor pairs. These devices suffer from macrophase separation in the active layer, limiting efficiency. The self-assembly properties of block copolymers have the potential to overcome the thermodynamic incompatibility between different polymers and form unique nanostructures for efficient photovoltaic operation. Using a poly(3-hexylthiophene) - poly(9,9-diocetylfluorene)-2,7-diy)alt-[4,7-bis(thiophen-5-yl)-2,1,3-benzothiazoladiazole]-2,7-diyl] conjugated block copolymer (P3HT-PFOTBT), we demonstrate for the first time that devices composed of donor-acceptor block copolymers can work as solar cells with efficiencies around 3%. Lamellar morphologies formed in block copolymer thin films have been characterized using resonant soft X-ray scattering.

**Q1.00049 Unconventional Routes for the Enhancement of the Efficiency of Dye-Sensitized Solar Cells (DSSCs) Based on Self-Assembled Block Copolymer Nanotemplates**, YOONHEE JANG, DONGHA KIM, Ewha Womans University — We introduce distinctly different and creative two strategies for improving the efficiency of TiO$_2$-based DSSCs by incorporation of tailored hybrid nanostructures prepared from self-assembled block copolymer nanotemplates. Firstly, carbonized TiO$_2$ thin layer was incorporated into the interface either between the transparent conductive electrode and TiO$_2$ NP layers or between the electrolyte and TiO$_2$ NP layers. Massively-ordered arrays of TiO$_2$ dots embedded in the carbon matrix were fabricated via direct carbonization of UV-stabilized PS-b-P4VP block copolymer films containing TiO$_2$ sol-gel precursors. DSSCs containing carbon/TiO$_2$ thin layers exhibited remarkably enhanced overall power conversion efficiency compared with DSSCs based on neat TiO$_2$ NPs. Secondly, we introduce a new class of organic/inorganic 1D photonic crystals exhibiting stop bands in the specific wavelength range, which was created by stepwise layer-by-layer deposition of UV-crosslinked BCP reverse micelle layers. The simple yet novel 1D layered BCP films have been introduced into the back-side of the counter electrodes as light reflector in DSSCs system to increase the light harvesting of dye.

**Q1.00050 Microwave energy application on carbon cathode for high efficient microbial electrosynthesis**, HUARONG NIE, MENGMENG CUI, Department of Polymer Science & Engineering, University of Massachusetts, Amherst, TIAN ZHANG, DEREK LOVELY, Department of Microbiology, University of Massachusetts, Amherst, THOMAS RUSSELL, Department of Polymer Science & Engineering, University of Massachusetts, Amherst — Microbial electrosynthesis represents a promising strategy of energy storage through microbial conversion of carbon into the back-side of the counter electrodes as light reflector in DSSCs system to increase the light harvesting of dye.

**Q1.00051 Ordered Mesoporous Carbon/Iron Oxide Nanoparticle Composites for Supercapacitor Applications**, YING LIN, XINYU WANG, JAMES WATKINS, Department of Polymer Science and Engineering, University of Massachusetts Amherst — Novel mesoporous carbon/iron oxide composites were synthesized through a simple carbonization procedure of blends of block copolymer precursors containing the source of carbon, i.e., polyacrylonitrile-block-poly(t-butyl acrylate) (PAB-b-PAN) with iron oxide nanoparticles. The addition of functionalized nanoparticles that selectively hydrogen bond with PAN segments was shown to induce order in otherwise disordered systems. The ordered mesostructure of the composites was confirmed by both small x-ray scattering and transmission electron microscopy. The preparation of nanocomposites with pore structure was enabled by the high 2Dlity preservation of the phase-separated nanostructure between two polymer blocks driven by nanoparticle additive upon carbonization at 700°C. The electrochemical performance of the composite films was compared to that of the neat carbon and the mesoporous carbon without iron oxide nanoparticles. The mesoporous structure together with the high iron contents in such materials make them particularly promising for use in supercapacitor applications.

1This work was supported by the NSF Center for Hierarchical Manufacturing at the University of Massachusetts (CMMI-0531171).

**Q1.00052 Control ion transport by tuning the crystalline morphology in polyethylene oxide-based solid electrolyte**, SHAN CHENG, CHRISTOPHER LI, DERRICK SMITH, Drexel University — The crystalline structure of polyethylene oxide (PEO) strongly affects the ion transport in solid PEO-Lithium salt electrolytes. Four possible phases can exist in a PEO-LiClO$_4$ electrolyte membrane, e.g. crystalline PEO, amorphous PEO, amorphous PEO-Li complex and crystalline PEO-Li complex. It has been widely accepted so far that ion can transport through either amorphous PEO phase or PEO-Li crystalline complex phase. The ion conduction mechanism of the former is based on ion hopping as well as PEO segment motion. In the latter case two PEO chains form cylindrical channels within which Lithium cation can transport. In this presentation, we will show that tuning the crystalline morphology can optimize ion conduction. This can be achieved by controlling the orientation of the PEO lamellae as well as PEO-Li crystalline complex to optimize the ion conducting pathways.

**Q1.00053 Tunable morphology of P3HT: PCBM films by combinatorial methods for bulk heterojunction solar cells**, YAN SUN, GURPREET SINGH, ALAMGIR KARIM, University of Akron — P3HT: PCBM films for bulk heterojunction (BHJ) solar cells were processed by dynamic annealing method termed as cold zone annealing (CZA) with varying velocities in conjunction with a confining and conformal surface energy controlled polydimethylsiloxane (PDMS) capping layer on top. Morphologies and optical properties of P3HT: PCBM were investigated by atomic force microscopy, optical microscope and UV-Vis absorption spectroscopy. Effect of CZA annealing rate and surface energy of PDMS as well as CZA annealed films without PDMS on P3HT: PCBM morphologies were compared. It was observed that the growth of large PCBM crystals can be suppressed with the confining PDMS under CZA annealing conditions. The thermal expansion of PDMS is several times the BHJ film, so that there is significant shear effect on the BHJ under the confined annealing process. High resolution TEM was used for further investigation of the film morphology and the orientation of the P3HT in the BHJ was studied by UV-Vis absorption spectroscopy with polarized incident light and grazing incidence wide angle X-ray spectroscopy (GIWAXS) at a synchrotron source.

2Work supported by Department Of Energy - Office of Basic Energy Sciences

**Q1.00054 The influence of ion content on mobility and ion aggregation in PEO-based single-ion conductors**, DAVID CALDWELL, JANNA MARANAS, Pennsylvania state university — PEO-based ionomers reduce concentration polarization in solid polymer electrolytes by binding the anion to the polymer backbone. Ionomers have significant ion aggregation compared to PEO/salt systems, and the influence of these aggregates is unclear. When ion transport is coupled to the segmental dynamics of the polymer, aggregation will always reduce ion motion and conductivity. However, the conductivity of PEO ionomers is not sensitive to the degree of aggregation. We present results of molecular dynamics simulations where ion content is systematically varied. We consider the influence of ion content on ion aggregation, polymer mobility and cation motion.
Q1.00055 X-ray absorption spectroscopy of reaction intermediates of lithium-sulfur batteries dissolved in polymer electrolytes. KEVIN WUJICK, NITASH BALSAARA, University of California, Berkeley — Lithium polysulfide reaction intermediates formed during the charge and discharge reactions of a lithium-sulfur battery are known to diffuse out of the cathode during cycling, thus lowering battery capacity and lifetime. While numerous techniques have been developed to confine intermediates to the battery cathode, little is known about the complex reaction mechanism responsible for their formation. Work to understand the reaction mechanism requires an experimental technique capable of distinguishing the various lithium polysulfide intermediates formed during the charge/discharge reactions. We report on the use of x-ray absorption spectroscopy (XAS) to distinguish lithium polysulfide molecules in polymer electrolytes. Polysulfide intermediates dissolved in poly(ethylene oxide) and a block copolymer of polystyrene-poly(ethylene oxide) were probed at the oxygen, carbon, and sulfur K-edges. Simulated x-ray spectra based on ab-initio molecular dynamics were used to interpret experimental x-ray spectra. Theories regarding the physical and chemical nature of the polysulfide–polymer electrolyte interaction were developed.

Q1.00056 Investigation of PVDF/TiO$_2$ Composite Films for Use in the Capacitive Storage of Energy. JOEL IWAGOSHI, Northern Arizona University — Research on alternative energies has become an area of increased interest due to environmental concerns. Fluctuations due to changing environmental conditions cause instability in the electrical grid. Capacitors made from composite polymer/nanoparticle thin films have been shown to be an economically viable solution. Precise compositional tuning of the two materials in the film can lead to high energy density storage capacitors. Through thermal vapor deposition, we synthesized dielectric thin films of polyvinylidene fluoride (PVDF) containing the ceramic nanoparticle titanium dioxide (TiO$_2$). Film composition was analyzed XPS and EDX. Films have been produced with a TiO$_2$ content up to about 8%. Nanoparticle cluster size was examined using intermittent AFM. Images from this technique confirm uniform TiO$_2$ dispersion with cluster size less than 150 nm. Our research provides a framework to the understanding of PVDF:TiO$_2$ composite film. These results will lead to the investigation of PVDF/TiO$_2$ high density energy storage capacitors. These capacitors can potentially increase the efficiency of alternative energy sources already in use.

Q1.00057 Rational Design of POSS-Based Janus Particles into Supramolecular Structures: Symmetry Breaking and Shape Commensuration. ZHAO WANG, YIWEN LI, WEN-BIN ZHANG, STEPHEN Z.D. CHENG, Department of Polymer Science, The University of Akron — The synthesis, self-assembly and applications of structured nanoparticles have significantly intensified over the past decade. In the recent year, a series of precisely defined polyhedral oligomeric silsesquioxane (POSS)-based molecular dumbbell-like Janus particles has been prepared. It was found that those non-spherical POSS Janus nanoparticles processing equally sized blocks could self-organize into a bi-layered structure with a head-to-head, tail-to-tail type of packing in its bulk state. The driving force of this hierarchical structure formation was attributed to the symmetry breakings of both geometrical sense (molecular shape) and chemical sense (selective amphiphilic interactions) of dumbbell-like Janus particles. Based on this modal system, we further developed a family of POSS-based structured nanoparticles for supramolecular structure formation in the solid state. It was found that the snowman-like Janus particle with two POSS cages in different sizes (a Janus particle with long alkyl chains on one POSS and carboxylic groups on the other) could self-assemble into frustrated lamellar structure (1.5 layered structure). Meanwhile, the supramolecular structure of corresponding micemyoue-like Janus particle (long alkyl chains on one POSS and carboxylic groups on the other two POSS cages) could recover into normal lamellar structure (bi-layered structure). The self-assembly behaviors of those shape-persistent nanoparticles are absolutely different from those of di-block copolymers.

Q1.00058 Self-Assembly of Giant Gemini Surfactants Based on Polystyrene- Hydrophilic Polyhedral Oligomeric Silsesquioxane Shape Amphiphiles. YIWEN LI, ZHAO WANG, STEPHEN CHENG, Department of Polymer Science, The University of Akron, Akron, OH, 44325 — A series of giant gemini surfactants consisting of two hydrophobic carboxylic acid-functionalized polyhedral oligomeric silsesquioxane (APOSS) heads and two hydrophobic polystyrene (PS) tails covalently linked via rigid spacers (PS-(APOSS)$_2$-PS) was designed and synthesized. Our current study revealed a morphological transition from vesicles to wormlike cylinders and further to spheres as the degree of ionization of the carboxylic acid groups on POSS heads increases in their micelle solution. PS tails were found to be less stretched in micellar cores of PS-(APOSS)$_2$-PS than those of the corresponding single-chained giant surfactant. It was also observed that the PS tail conformations in the micelles were also affected by the length of rigid spacers where the one with longer spacer exhibits stretched PS chain conformation. Both findings could be explained by the topological constraint imposed by the short rigid spacer in giant Janus surfactants. This constraint effectively increases the local charge density and leads to an anisotropic head shape that requires a proper re-distribution of the APOSS heads on the micellar surface to minimize the total electrostatic repulsive free energy. Moreover, their supramolecular structures in bulk were also found to be strongly affected by rigid spacer effects. Our study has general implications in the basic physical principles underlying their self-assembly behaviors in solution and bulk states.

Q1.00059 Hierarchical Structure from the Self-Assembly of Giant Gemini Surfactants in Condensed State. HAO SU, ZHAO WANG, YIWEN LI, STEPHEN CHENG, Department of Polymer Science, the University of Akron — In the past a few years, a new class of amphiphiles with both asymmetrical shapes and interactions named “shape amphiphiles” has been significantly intensified. Recently, a new kind of shape amphiphiles called “Giant Gemini Surfactants” consisting of two hydrophilic carboxylic acid-functionalized polyhedral oligomeric silsesquioxane (APOSS) heads and two hydrophobic polystyrene (PS) tails covalently linked via rigid spacers (p-phenylene versus biphenylene) has been successful behavior of giant gemini surfactants. We currently continue to investigate the space effects on the self-assembly behaviors of giant gemini surfactants in condensed state by utilizing DCS, SAXS and TEM. Preliminary results showed that giant gemini surfactants with different spacer have diverse phase behaviors. As we use the same 3.2k PS chains, the giant gemini surfactant with p-phenylene spacer showed double gyroid morphology, while the one with biphenylene spacer revealed cylindrical morphology. This study expands the scope of giant gemini surfactants and contributes a lot to the basic physical principles in self-assembly behavior.

Q1.00060 Curvature-directed crystallization of isotactic poly(propylene) in nanopores. DARIYA REID, BRIDGET EH Lingler, JODIE LUTKENHAUS, Texas A&M University — Properties of a cylindrically confined polymer may greatly differ from its properties in bulk state when the geometrical restrictions approach the size of the polymer itself. Confinement of polymer dielectrics, such as isotactic polypropylene (IPP), in nanoporous templates can potentially enhance the dielectric properties of the material via directed crystallization. IPP was melt-wetted into nanoporous templates of varying diameter (15 - 200 nm) in order to study the effect of pore dimensions on crystallization. Using differential scanning calorimetry (DSC) and X-ray diffraction (XRD), it is shown that IPP crystallizes into the α-phase and preferentially orients along the long axis pore. A transition from hetero to homogeneous crystallization was observed in relation to pore diameter. The isothermal crystallization kinetics was analyzed using Avrami analysis. As the pore diameter decreases crystallization shifts to a multi-mode process, whose origins will be discussed in this presentation.

1This work has been supported by ACS PRF.
Q1.00061 Fabrication of Micropatterns using Salt Crystals from Solvent Evaporation\(^1\). DONG-EUN LEE, SEILING JAE GO, DONG HYUN LEE, Dankook University — Herein, we investigated the crystallization behaviors of sodium carbonate (Na\(_2\)CO\(_3\)) from highly diluted aqueous solutions. Aqueous Na\(_2\)CO\(_3\) solutions which were applied on substrate surfaces by either dropping or draining exhibited a variety of well-defined crystal structures over large areas during water evaporation. It was also found that both sizes and shapes of salt crystals could be effectively controlled by the experimental conditions such as their concentration, evaporation rate, temperature and humidity. Furthermore, it was observed that the salt crystals could be oriented to specific direction as the evaporation of water occurred on the tilted substrates. The crystals of Na\(_2\)CO\(_3\) were then employed as the master pattern to fabricate the soft mold of poly(dimethylsiloxane) (PDMS). Then silver (Ag) inks were filled into the pores of PDMS molds and transferred to various substrates by imprinting techniques to produce electrically conductive electrodes for potential electric devices.

\(^1\)The National Research Foundation of Korea (NRF) grant (2011-0013084) and Gyeonggi Regional Research Center (GRRC) Program (2012-11150)

Q1.00062 Small Molecule-Guided Thermoresponsive Supramolecular Assemblies. BENJAMIN J. RANCATORE, CLAYTON E. MAULDIN, Department of Chemistry, UC Berkeley. JEAN M.J. FRECHET, College of Chemistry, UC Berkeley, TING XU, Department of Materials Science and Engineering, UC Berkeley — Small organic molecules with strong intermolecular interactions have a wide range of desirable optical and electronic properties and rich phase behavior. Incorporating them into block copolymer (BCP)-based supramolecules opens a new route to generate functional responsive materials. A quatertiary amine semiconductor containing alkyl and phenolic moieties was hydrogen-bonded to the 2-vinylpyridine groups of a block copolymer, polystyrene-b-poly(2-vinylpyridine) or a homopolymer, poly(2-vinylpyridine) (1.2). Hierarchical co-assemblies of oligothiophene and BCP with a number of potentially useful morphologies for optoelectronic materials were obtained. Crystallization of the oligothiophene from a melt not only induced chain stretching of the BCP block the oligothiophene was hydrogen bonded to, but also changed the conformation of the other BCP coil block, which led to an over 70% change in the BCP periodicity. The present studies have demonstrated the experimental feasibility of generating thermoresponsive materials that convert heat into mechanical energy and provides access to large BCP periodicities using fairly low molecular weight BCP. References: (1) Rancatore et al., ACS Nano 2010, 4, 2721. (2) Rancatore et al., Macromolecules 2012, 45, 8292.

Q1.00063 Polymer single crystal membrane from liquid/liquid interface, WENDA WANG, CHRISTOPHER LI, Drexel University. SOFT MATTER RESEARCH GROUP-DREXEL UNIVERSITY TEAM — Vesicles, mimicking the structure of cell membrane at the molecular scale, are small membrane-enclosed sacks that can store or transport substances. The weak mechanical properties and the nature of environment-sensitivity of the current available vesicles: liposomes, polymersomes, colloidosomes limit their applicabilities as an excellent candidate for targeting delivery of drugs/genes in biomedical engineering and treatment. Recently, we developed an emulsion-based method to grow curved polymer single crystals. Varying the polymer concentration and/or the emulsification conditions (such as surfactant concentration, water-oil volume ratio), curved crystals with different sizes and different openness could be obtained. This growing process was attributed to polymer crystal growth along the liquid/liquid interface. In addition, the liquid/liquid interfacial crystal growth is promising for synthesis of enclosed hollow sphere.

Q1.00064 Rate of Formation of Trigonal Phase in Blends of Homogeneous Propylene 1-Hexene Copolymers, HAMED JANANI, GABRIEL TRUJILLO, RUFINA ALAMO, Florida State University. FAMU-FSU College of Engineering — Blends of polyolefins such as polyethylenes, polypropylenes or their copolymers are often used to balance the strengths of each component towards improving processing, physical properties and performance. The final properties depend on the semicrystalline state acquired upon melt-solidification which is highly impacted by the state of melt miscibility. In this work we have assessed the critical composition difference for melt miscibility of propylene 1-hexene copolymers (PH) and selected a miscible pair with 11 and 21 mol% of 1-hexene respectively. PH21 crystallizes in a trigonal packing, while PH11 develops monoclinic crystals (at low undercooling) or the mesomorphic form (at high undercooling). In situ DSC and WAXD analysis indicate that while the content of trigonal phase decreases with increasing PH11, the rate of formation of trigonal phase in the whole range of undercooling increases with addition of PH11, which as a pure component does not form trigonal phase. The unexpected enhanced kinetics of formation of trigonal phase with blending is attributed to the increasing composition of 1-hexene in the melt during isothermal crystallization of the blend.

Q1.00065 The Thickness And Stretch Dependence Of The Electrical Breakdown Strength Of An Acrylic Dielectric Elastomer, JIANGSHI HUANG, ZHIGANG SUO, DAVID CLARKE, Harvard University — The performance of dielectric elastomer actuators is limited by electrical breakdown. Attempts to measure this are confounded by the voltage-induced thinning of the elastomer. A test configuration is introduced that avoids this problem: A thin sheet of elastomer is stretched, crossed-wire electrodes attached, and then embedded in a dielectric elastomer actuators is limited by electrical breakdown. Attempts to measure this are confounded by the voltage-induced thinning of the elastomer. The applied electric field at breakdown \(E_B\) is found to depend on both the deformed thickness, \(h\), and the stretch applied, \(\lambda\). For the acrylic elastomer investigated, the breakdown field scales as \(E_B = 51 h^{-0.25} \lambda^{0.63}\). The test configuration allows multiple individual tests to be made on the same sheet of elastomer.

Q1.00066 Crystal Engineering of Tetrahedral ‘Nano Molecules’ Constructed by POSS Cages, MINGJUN HUANG, SHAN MEI, STÉPHEN CHENG, Department of Polymer Science, the University of Akron — Functional hybrid materials provide us a powerful approach to acquire novel hierarchical structures and exceptional properties. Designed nanoparticle building blocks with specific interactions can self-assemble into targeted ordered structures with intriguing shapes, sizes and functionalities. Classical high symmetric ‘nano atoms’, Polyhedral Oligomeric Silsesquioxane (POSS) can be utilized to construct ‘nano molecules’ with different symmetry, which can further act as novel nanoparticle building blocks. Very interesting rigid tetrahedral ‘nano molecules’ covalent linking four POSS cages were synthesized. Their close packing structures in crystal were determined by transmission electron microscopy (TEM) and wide angle X-ray diffraction (WAXD).

Q1.00067 Dielectric Characterization of Poly(styrene-b-methyl methacrylate) Block Copolymer Films\(^1\), CHRISTOPHER GRABOWSKI, MICHAEL DURSTOCK, RICHARD VAIA, Air Force Research Laboratory, Wright Patterson Air Force Base — Polymer films that incorporate nanoscale features have been previously investigated for their suitability as dielectric insulating materials, such as mixtures of high dielectric strength polymers with high permittivity nanoparticle. Block copolymers, due to their highly customizable molecular-scale morphologies, may exhibit useful energy storage properties. Spherical, cylindrical, or lamellar morphologies can all be generated by altering block size ratio. We report the dielectric study of thin, submicron supported polystyrene-b-methyl methacrylate) linear block copolymer films. Energy storage capabilities will be determined through dielectric strength and permittivity measurements. As both polymer blocks have similar permittivity, field enhancement effects that typically occur in inorganic nanoparticle/polymer composites are limited. Our experiments with block copolymers will more directly test how dielectric breakdown is influenced by interfacial interactions.

\(^1\)We thank AFSOR and AFRL for their financial support.
Multilayer Films, CRAIG LEWIS, JUNG-KAI TSENG, MATHEW MACKEY, ERIC BAER, LEI ZHU, Case Western Reserve University, LEI ZHU

GROUP TEAM — Because of significant dielectric and resistivity constants for polycarbonate (PC) and poly(vinylidene fluoride) (PVDF), the Maxwell-Wagner-Sillars interfacial polarization effect is observed in PC/PVDF multilayer films and is able to increase the overall electric displacement. However, based on the dielectric displacement-electric field (D-E) loop study, the PC/PVDF 50/50 32 layer film has higher dielectric constant calculated from the slope of D-E loop as compared to the 256 layer film. In other words, the maximum D decreases with decreasing the PC layer thickness. Since the electron tunneling is significant for thinner PC layers (i.e., internal conduction), the interfacial polarization is decreased. This study elucidates the relationship between the maximum D and the PC layer thickness, as well as the dielectric behavior at high temperatures.

Diffusion of gaseous and supercritical CO₂ through polycarbonate¹, MICHAEL GOODMAN, RAHMI OZISIK, Rensselaer Polytechnic Institute — The design of polymeric materials for applications such as separation membranes and nanostructured foams requires prediction of gas transport properties under a wide range of pressures. In the current study, transport of CO₂ both in gaseous and supercritical state through samples of polycarbonate at 51 °C and pressures from 15 to 2000 psi was measured using an asymptotic time lag apparatus. Through volumetric calibration, the traditional analysis was extended to yield permeability (P) and solubility (S), in addition to the usual asymptotic diffusivity (Dₒ). Nonlinear least squares fitting to a truncated series solution then provided an alternative measurement of the (transient) diffusivity (Dₜ), as well as the surface concentration (Cₒ) of adsorbed gas. At 1 atm, Dₛ and Dₛ were within a factor of 2 from selected handbook values; and with increasing pressure, both exhibited an overall downward trend, consistent with other studies, but an unexpected dropoff occurred between 1350 and 1500 psi. As expected, Cₒ showed an overall increase with pressure, but as with P and S, displayed a peculiar drop between 1350 and 1500 psi. Measurement of Cₒ in polycarbonate has never been done before and constitutes a novel feature of this study.

Scaling of the strain hardening modulus with nanoparticle loading and the rejuvenated yield stress in polymer nanocomposites, ROBERT HOY, University of South Florida, ALAN LESSER, University of Massachusetts, JOSEF JANCAR, Brno University of Technology — We examine the nonlinear mechanics of polymer glasses by using silica nanoparticles as “probes” that alter the segmental packing and relaxation dynamics of glassy PMMA. At low T = Tₒ − 80K, the scalings of both the strain hardening modulus Gₛ and the rejuvenated yield stress σᵧ with NP loading (i.e. the silica volume fraction νₛ) are predicted by a simple volume-replacement model. At higher T = Tₒ − 20K, this scaling breaks down, indicating substantially interface-retarded dynamics and packing frustration. At high strain rates, Gₛ scales linearly with σᵧ, with a νₛ-dependent offset. This linear scaling breaks down at lower strain rates ˙ε < C ℎ(νₛ). Surprisingly, C ℎ increases with increasing νₛ, violating the intuitive expectation that NP filling would increase the controlling relaxation times. We explain this phenomena in terms of the increasing dynamical heterogeneity induced by filler particles.

Physical Property Requirements of Ion-exchange Polymer Membranes for Acid-base Flow Batteries, SUPACHAREE RODDECHA, PETER THAYER, JACOB JORNE', MITCHELL ANTHAMATTEN, University of Rochester — Flow batteries offer feasible solutions to grid-scale storage of intermittent power. We are developing a new type of flow battery that reversibly controls an acid-base neutralization reaction. The battery consists of two highly reversible hydrogen gas electrodes that are exposed to low and high pH process streams. A brine solution runs between the acid and base streams and is separated by cationic and anionic exchange membranes. For both charge and discharge phases, hydrogen gas is produced at one electrode and consumed at the other. During charging, an external potential is applied across the two electrodes to electrochemically produce acid and base from the brine solution. Discharge involves electrochemical neutralization of acid and base streams, resulting in current flow through an external load. Several charge and discharge cycles were performed to demonstrate proof of concept. Experiments were conducted to determine the physical property requirements of the ionic exchange polymer layers. Properties including ion conductivity, permselectivity, and membrane stability will be discussed.

Magnetic fields-directed self-assembly of soft nanomaterials for energy harvesting and storage, PAWEL MAJEWSKI, MANESH GOPINADHAN, CANDICE PELLIGRA, CHINEDUM OSUJI, Yale University — We utilize magnetic fields to impose long range order in self-assembled soft materials including block copolymers, polymer-nanowire composites, and surfactant mesophases. Due to the space-pervasive nature of magnetic fields, this method can be utilized to produce arbitrarily large volumes of highly anisotropic materials with a quality of the alignment frequently approaching that of single crystals as assessed by X-ray scattering. The high fidelity of the alignment allows us to systematically explore and characterize the anisotropy of the charge transport in these materials. We present the results for improving charge transfer in cobalt doped ZnO nanowire-polythiophene composites for photovoltaic applications by the alignment of the nanowires. In block copolymers, we focus on enhancing Li-ion transport and storage properties requirements of the ionic exchange polymer layers. Properties including ion conductivity, permselectivity, and membrane stability will be discussed.

Fluctuation Effects on Phase Behavior of Gradient Copolymer Systems, GUNJA PANDAV, VENKAT GANESAN, University of Texas at Austin — We consider the effect of sequence polydispersity on fluctuation induced shift in order-disorder transition (ODT) temperature for symmetric systems of gradient copolymers. Using single chain in mean field simulations, a systematic change in scaling prediction for shift in ODT with Ginzburg parameter is reported. We demonstrate that gradient strength and overall blockiness of sequences has a significant impact on shift in ODT temperature. The weak gradient copolymers having high compositional polydispersity mimic random copolymers whereas, strong gradient copolymers possess inherent blockiness and are close to diblock copolymers. The blockiness parameter has a minimal impact on shift in ODT in strong gradient copolymers. Also, ternary blends of homopolymer/gradient copolymer are investigated to capture effect of compositional polydispersity on phase diagram and formation of microemulsion structures.

Influence of substrate confinement on the phase-correlation in the capillary breakup of lithographically patterned polymer stripes¹, ZHENG ZHANG, YIFU DING, University of Colorado at Boulder — We study the simultaneous capillary breakup of parallel polymer stripes, which were partially embedded in an immiscible polymer and confined on elastic substrates. Polystyrene (PS) and Poly(methyl methacrylate) (PMMA) were used because of their immiscibility. When annealed at a temperature above the glass transition temperature of both polymers, capillary instabilities of the stripes were observed. We found that substrate-induced confinement influenced the phase-correlation in the breakup of neighboring stripes. With the increase of substrate confinement, the simultaneous breakup of the parallel polymer stripes transitioned from non-correlated to in-phase, irrespective of the viscosity ratio between PS and PMMA.

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²The authors acknowledge the funding support from the National Science Foundation under Grant No. CMMI-1031785. Acknowledgment is made to the donors of the Petroleum Research Fund for partial support of this research (Grant Number: ACS-PRF 50581-DN17).
Q1.00075 The Structural Change Depending on the Buckling Direction and Alignment of Block Copolymer Thin Films, DOKYEONG Kwon, HYO SEON SUH, KOOKHEON CHAR, National University — Buckling of thin films on elastomeric substrates such as polydimethylsiloxane (PDMS) is the well-known phenomenon in buckling instability originating from the moduli mismatch between a substrate and a thin film placed at the top. Recently, many studies on the microstructure created by the buckling have been reported but most of the work has employed either metal or semiconductor thin films and few studies utilized block copolymer (BCP) thin films as the top layer. Here, we present the buckling of oriented BCP thin films placed on top of PDMS substrates, resulting in hierarchical structures combining nanostructured BCP with microstructured buckling. Buckling instability was induced by applying a mechanical stress to the BCP-PDMS bilayer. Due to the buckling of BCP thin films, we observed the structural change of the films depending on the alignment of BCP domains with respect to the buckled direction of a substrate, which could give us insights on the buckling of mechanically heterogeneous films. This work could even be extended to a new patterning technique, utilizing both BCP thin film lithography and the microscale patterning induced by buckling.

Q1.00076 The formation of standing cylinders in block copolymer films by irreversibly adsorbed polymer layers on substrates1. JUN SHANG, NAISHENG JIANG, MAYA ENDOH, TADANORI KOGA, Department of Materials Science and Engineering, Stony Brook University — Block copolymers offer a simple and effective route to produce standing cylindrical nanostructures with regularity on the order of 10-100 nm, the length scale that is desirable for many advanced applications. However, these formations have been especially troublesome due to the fact that preferential interactions between one of the blocks and the surfaces will induce parallel alignment of the cylinders in order to minimize interfacial and surface energy. Here we introduce an alternative simple method utilizing an irreversibly adsorbed polymer layer (a “Guiselin” brush) as a neutral “substrate” formed on solid substrates for the arrangement of standing cylindrical nanostructures. The effect of polymer adsorbed layer on the long range ordering of asymmetric cylinder forming poly(styrene-block-ethylene/butylene-block-styrene) (SEBS) triblock copolymer thin films were investigated by using a combination of grazing incidence small angle x-ray scattering and atomic force microscopy techniques. We found that the SEBS, which forms cylinders lying parallel to the surface when prepared on silicon substrates, show standing cylindrical structures on selected Guiselin brush layers after prolonged thermal annealing. The details will be discussed in the presentation.

Q1.00077 Sequences of Mixed Ions in Polypeptoid Surfaces, HILDA BUSS, WENDY VAN ZOELEN, NATHAN ELLEBRACHT, University of California, Berkeley, RONALD ZUCKERMANN, Lawrence Berkeley National Lab, RACHEL SEGALMAN, University of California, Berkeley — Polypeptoids, a unique, sequence specific class of polymers, are used to investigate the influence of charge spacing, grouping, and chemistry on the surface properties of polymer coatings. Short peptoid oligomers composed of cationic and anionic groups, and superhydrophobic (fluorinated) functionalities were attached to a synthetic backbone to form comb-shaped molecules. These molecules display different surface chemistry as a function of side chain composition, as indicated by near edge X-ray absorption fine structure spectroscopy (NEXAFS). A 50:50 ratio of peptoid:fluorinated functionality resulted in optimal surface segregation of the comb block while preventing surface reconstruction upon immersing the polymer films in water. Antifouling experiments with the green algae Ulva showed that polymers with non-ionic peptoid functional groups resulted in superior antifouling coatings compared to polymers with charged peptoids. The effects of decreasing the peptoid charge spacing even further (zwitterionic side chains) and exploring stronger ionic moieties, such as phosphate groups, will also be discussed.

Q1.00078 Self-Consistent Field Simulation of Block Copolymer Thin Films Located on Topographic Pattern, JUNG GUN BAE, Nano-Structured Complex Fluids Lab, School of Chemical and Biomolecular Engineering — Motivated by recent experiments of directed self-assembly of AB diblock copolymer (BCP) thin film induced from patterned substrates, there is need to compare with simulation. We employ self-consistent field theory (SCFT) simulation which is known as well fitted. Especially, we investigated the effect of each roughness factors, such as period and depth of eroded line patterns. The higher-order accurate and stable pseudo-spectral method is adopted to numerically solve the SCFT equations and appropriate cavity function is also employed to represent the square wave patterns. There is some correspondence between the orientation of BCP micro-domain period and depth of eroded line patterns. The higher-order accurate and stable pseudo-spectral method is adopted to numerically solve the SCFT equations and appropriate cavity function is also employed to represent the square wave patterns. There is some correspondence between the orientation of BCP micro-domain period and depth of eroded line patterns. The higher-order accurate and stable pseudo-spectral method is adopted to numerically solve the SCFT equations and appropriate cavity function is also employed to represent the square wave patterns. There is some correspondence between the orientation of BCP micro-domain period and depth of eroded line patterns. The higher-order accurate and stable pseudo-spectral method is adopted to numerically solve the SCFT equations and appropriate cavity function is also employed to represent the square wave patterns. There is some correspondence between the orientation of BCP micro-domain period and depth of eroded line patterns.

Q1.00079 Sulfonated block copolymer thin films for fast responsive dual-mode humidity sensors, EUNYEONG KIM, MOON JEONG PARK, POSTECH — Polymer electrolytes have been widely used to fabricate humidity-sensing devices by taking advantages of easy fabrication and low cost. In present study, we developed humidity sensors from sulfonated block copolymer thin films with tailored hygroscopic properties. The films exhibit hexagonal cylindrical morphology where hydrophobic cylinders are dispersed within a hydrophilic matrix. Under the level of humidity, it has been revealed that the films self-display discernible reflective color changes, which cover almost entire visible light spectrum from violet (RH = 20%) to red (RH = 95%). This is due to fact that the hydrophilic matrix absorbs water yielding anisotropic swelling of the film along the film thickness direction. In addition, the sensors exhibit a few orders of magnitude changes in impedance with exposure to humid air owing to the strong polyelectrolyte characteristics. To the best of our knowledge, our system is the first example of dual-mode humidity sensor among any existing humidity sensors. What is most interesting is that the time to complete the changes in color and/or impedance was only 5s regardless of RH gradients, as rationalized by well-connected hydrophilic matrices, offering short water diffusion pathways in nanostructured block copolymer thin films.

Q1.00080 Nanomanufacturing of Gold Nanoparticle Arrays Using Peptide-Derivatized Block Copolymer Templates, TINGLING RAO, Department of Polymer Science, University of Akron, GURPREET SINGH, Department of Polymer Engineering, University of Akron, SIBAI XIE, Department of Polymer Science, University of Akron, ALAMGIR KARIM, Department of Polymer Engineering, University of Akron, MATTHEW BECKER, Department of Polymer Science, University of Akron — Collective surface plasmons (SPs) displayed by two-dimensional (2-D) Au nanostructures are important for applications such as plasmonics and plasmonic sensing. However, methods for fabricating programmable highly-ordered arrays of Au nanoparticles with nanoscale precision are limited. Here, we report a peptide-derivatized block copolymer based route towards continuous fabrication of Au nanoparticle superlattice with tunable structures. We successfully obtain discrete, hexagonally-packed Au nanoparticle hierarchical structures with Au-to-Au nanoparticle spacing is precisely controlled by the underlying PMMA cylindrical phase of the block copolymer (BCP). Dynamic thermal field processing techniques offer a facile and continuous route to tune the BCP assembly, thus enabling versatile arrangement of Au nanostructures from Au-dots to Au-lines. Our method may open a cost-effective way towards assembly of 2-D Au nanoparticles with tunable structures by carefully tuning molecular parameters – a promising step to novel nanodevices.

1 Akron Functional Materials Center (AFMC) and The University of Akron Research Foundation
Q1.00084 In-situ Grazing-incidence Small-angle X-ray Scattering Study of Diblock Copolymer Thin Films during Solvent Annealing

XIAODAN GU, University of Massachusetts Amherst.

Lawrence Berkeley National Lab, THOMAS RUSSELL, University of Massachusetts Amherst, UNIVERSITY OF MASSACHUSETTS AMHERST COLLABORATION.

In-situ Grazing Incidence Small Angle X-ray Scattering (GISAXS) experiments on diblock copolymer thin films during annealing in organic solvent vapors were performed to study the underlying mechanism that underpins the self-assembly process. We used two different cylinder forming block copolymers, poly(styrene-block-ethylene oxide) (PS-b-PEO) and poly(styrene-block-2-vinylpyridine) (PS-b-P2VP) that were spin-coated on silicon wafers and then annealed in tetrahydrofuran (THF).

Q1.00085 Analysis of Crystallization on Polymeric Thin Films Deposited on Silicon Dioxide

ETHAN CUMMINGS, James Madison University — Polyvinyl Alcohol (PVA) is a synthetic polymer containing carbon chains with hydroxide groups bonded to every other carbon. Poly[propylmethacryloisobutyl POSS-co-methylmethacrylate] (POSS-MA) is a co-polymer that contains polyhedral oligomeric silsesquioxane (POSS) cages co-polymerized to a poly methyl methacrylate (PMMA) backbone. PVA is dissolved into water at various concentrations and coated onto a silica wafer using spin coating. Various concentrations of 30-40 wt% POSS-MA are dissolved in chloroform and deposited onto the same sample. After spin coating, these samples are analyzed using AFM and ellipsometry. Typical samples of POSS-MA and PVA/POSS-MA thin films exhibit varying rates of solvent removal. Our results show that the films undergo a disorder-to-order transition during swelling. Also, we found that the lateral ordering of the microdomains after deswelling is highly sensitive to the rate of solvent removal.

Q1.00086 Photo-Activated Replication of Thin Film Block Copolymer Patterns

CHRISTOPHER ELLISON, DUSTIN W. JANES, Department of Chemical Engineering, The University of Texas at Austin.

Photo-Activated Replication is the ability to choose any desired pattern shape from a library of templates that has been spin-coated onto a silicon wafer, and to use this pattern to imprint a new structure onto the material that was used to make the template. This technique provides control over the mechanical properties of the new structure, as well as a way to transfer complex patterns from one material to another. We have developed a method for making small, 2D patterns using a photoresist that can be exposed to light through a mask. The photoresist is then developed to create a pattern in the resist, which is then used to print the desired pattern onto the material. The resulting pattern can be used to control the mechanical properties of the material, or to transfer a complex pattern from one material to another. This technique has applications in the fields of microfabrication and nanotechnology, and it is also useful in the design of new materials with desired mechanical properties.
Q1.00087 An Automated System for GISAXS and GIWAXS Measurements. JESSICA JIMENEZ, Jema Technology LLC, ERIC SCHAIBLE, Lawrence Berkeley National Laboratory, MATTHEW CHURCH, Jema Technology LLC, CHRISTINA YEE, ALASTAIR MACDOWELL, DILWORTH PARKINSON, EDWARD DOMNING, BRIAN SMITH, STEVEN ALVAREZ, ALEXANDER HEXEMER, Lawrence Berkeley National Laboratory — Grazing incidence small-angle scattering (GISAXS) and grazing incidence wide-angle scattering (GIWAXS) are important techniques for characterizing thin films, and their use is rapidly expanding. The current bottleneck in conducting GISAXS measurements is the time it takes to load and align samples. In order to meet increasing demand, we are implementing a fully automated system to conduct GISAXS and GIWAXS measurements. A robot arm will load samples from a holding tray onto the measurement stage. Intelligent software will align each sample in turn, and measure each according to user-defined specifications. Users will be able to mail in trays of samples, and will be able to monitor and control their experiments remotely.

Q1.00088 Co-assembly of polymer covered cyclic peptide nanotubes and block copolymer in thin films. CHEN ZHANG, THOMAS LAZZARA, Department of Materials Science and Engineering, University of California, Berkeley, CHANGYI LI, Department of Chemical Engineering, University of California, Berkeley, BRETT HELMES, The Molecular Foundry, Lawrence Berkeley National Laboratory, TING XU, Department of Materials Science and Engineering, University of California, Berkeley — Nanotubular structures have gained prevalent interest for their unique hollow structures and high aspect ratio and their potential applications ranging from molecular separation to nanocomposite membranes. We used nanotube forming cyclic peptide (CP) as the structural motif and studied the self-assembly of polymer conjugated CPs in block copolymer (BCP) matrix in thin films. The co-assembly process is mainly driven by thermodynamic quantities, namely Flory-Huggins polymer-polymer interactions that governs the interaction between CP and BCP, interfacial interactions that affects polymer chain orientation, and thin film commensurability. In addition, due to the dynamic nature of the nanotube formation, the co-assembly process is also pathway-dependent. Thus, processing conditions are critical in co-assembling CP nanotubes and BCP in thin films. Our results show that the initial aggregate state of polymer covered CP nanotubes determines the pathway the system takes and hence the final morphology of the films. The co-assembly of polymer covered CPs and BCPs demonstrates the feasibility of assembling 1D nanotubes in supramolecular thin films and opens up a new avenue for the generation of novel nanotubular structures.

Q1.00089 sPP gel with high mechanical properties and high transparency by supercooling in mixed solvents. KEITA TAKAESU, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — Polymer gels are generally classified into chemical gels and physical gels depending on the types of crosslinking points. Physical gels are known to possess significantly poorer mechanical properties than chemical gels due to relatively weak crosslinking bonds in physical gels such as hydrogen bond and an intermolecular bond. In this work, physical sPP gels with extremely high mechanical properties and high transparency were successfully created by supercooling in mixed solvents. From our previous work, it was found that supercooling of physical gels (sPP/decalin gels) could produce gels with high mechanical properties comparable to chemical gels but maintaining the advantages of physical gels such as stimulus-responsiveness and reversibility, which cannot be realized by using chemical gels. Here, we also used tetrahydroxynaphthalene (tetralin) as solvent. The mechanical properties of sPP/tetralin were degraded by supercooling but intriguingly enhancement in the mechanical properties of sPP gels could be observed by using mixed solvent of decalin and tetralin, which eventually showed twice as high fracture stress as sPP/decalin gels.

Q1.00090 Polymer-induced depletion attraction between nanoparticles in confined conditions. VICTOR PRYMITSYN, VENKAT GANESAN, University of Texas at Austin — We studied the polymer-mediated depletion pair interaction between nanoparticles and/or proteins in polymer solutions in confined conditions. The self-consistent field (SCF) theory for a polymer - nanoparticles systems in confined systems is developed and applied for such systems. As an example, we studied the self-assembly of polymer conjugated CPs in block copolymer (BCP) matrix in thin films near a non-adsorbing wall for which the polymer mediated particle-particle and particle-wall interaction in such systems are known to be a depletion attraction. Our main results for such system are the following: polymer depletion from the wall causes the polymer density to decrease near the wall and reduces the particle-particle depletion attraction near the wall. In a similar manner, the particle-wall attraction is also screened due to presence of another particle. Our results surprisingly suggested a simple scaling to rationalize the wall-mediated interparticle potentials. Specifically, the wall-mediated depletion interactions were shown to be semi-quantitatively captured by the depletion interaction between two particles in an unconfined polymer solution at a density corresponding to the density of the polymer solution at midpoint between the two particles. These results suggest that the phase behavior of

Q1.00091 Application of near-field microwave microscopy in in-situ detection of microfluids under dielectric cover1. WEIQIANG SUN, Key Laboratory for Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, YONG YANG, Institute of Microelectronics, Chinese Academy of Sciences, TAO FENG, SHENGYONG XU, Key Laboratory for Physics and Chemistry of Nanodevices, Department of Electronics, Peking University — Based on the capability of penetrating through low permittivity materials and the sensitivity to impedance of microwave, we have applied the near-field scanning microwave microscopy (NSMM) to the in-situ detection of microfluids packed with dielectric covers. By means of a NSMM system, we obtained two dimensional maps showing the frequency shift and magnitude of the reflection coefficient $\mathbf{S}_{11}$, which correspond well to the spatial distribution and electrical conductance of various microfluidic structures underneath 15-200 µm thick dielectric covers. The spatial resolution and sensitivity are found closely related to the thickness of the cover layer. The underlying physics is discussed in detail. The time-resolvable detection of ion concentration in microfluids is also demonstrated in different conditions for study of transport of particles in microfluids. This technique offers a real-time, in-situ and non-invasive approach for monitoring local chemical reactions, motion of fluids, distribution and concentration of ions in lab-on-a-chip systems, and has a potential to be developed for detection of cells and tissues.

1This work is financially supported by the National Science Foundation of China (Grant 11074010) and the Ministry of Science and Technology of China (Grant 2011DFA61450).

Q1.00092 Evaluating the Role of Interfacial Molecules in Cp Measurements using Differential Scanning Calorimeter1. WILL LINTHICUM, SAMUEL AMANUEL, Dept. of Phys. & Astro., Union College — Differential Scanning Calorimeter (DSC) has been used to evaluate the specific heat capacity of bulk ethylene glycol and physically confined ethylene glycol in porous silica with well-defined porosity. By controlling the pore sizes, we were also able to control the surface to volume ratio of ethylene glycol that comes in contact with the silica walls. Previously, we have demonstrated that about 2.14 nm layers of interfacial cyclohexane molecules do not participate in phase transition. In this case, how the physical size and the interfacial molecules affect the overall specific heat capacity of the silica ethylene glycol system is evaluated in the temperature range 303K - 413K. These empirical results are compared with computed specific heat capacities of composite materials, where the specific heat capacities of the composite systems are evaluated from the weighed average of the individual specific heat capacities. We are seeking means of reconciling the experimental observations with the computed specific heat capacities and looking for correction terms where the role of interface can be accounted.

This work has been supported financially by Union College Faculty Research Fund, NSF-EEC 0939322 and New York State NASA space grant for financial support.
Q1.00093 Analysis of Fluid Dynamics and Reactant Consumption in Microchannel Based Fuel Cells. JOSEPH DALESSANDRO, PETRU FODOR, Cleveland State University — In this work, the fluid dynamics within a membraneless microchannel fuel cell is analyzed computationally. The membraneless design is a result of the laminar nature of the fluid flow at small Reynolds numbers, restricting the fuel and oxidant to the vicinity of the corresponding electrodes, without the need of a proton exchange membrane (PEM). The performance of such cells is limited by the mass transport near the electrodes, with much of the reactants leaving the channel without coming in contact with the catalytic surfaces. We use various strategies similar with those used in grooved micromixers to overcome this limitation. While the flow is still laminar in nature, the addition of ridges to the top and bottom of the cell introduce a transverse element to the fluid flow, increasing reactant consumption and overall cell efficiency. The characteristics of the cells are investigated as a function of the Peclet number.

Q1.00094 Precise measurement of spring constant and friction coefficient of nano-confined T4 DNA. CHRISTOPHER LÜSCHER, JONAS PEDERSEN, RODOLPHE MARIE, ANDERS KRISTENSEN, HENRIK FLYVBJERG, Naotech DTU — A simple method for accurate detection of dynamic parameters for DNA confined in nano-fluidic channels is presented. T4 DNA is stained with YOYO-1 fluorescent dye and studied by epifluorescence under confinement in nonfluidic capillaries with cross-section less than 250 nm. A DNA molecule confined in a nano-channel of width below the molecule’s radius of gyration is stretched to fill a length, L, of the channel. In equilibrium, the DNA will be subject to thermal fluctuations, which are governed by the drag force of the surrounding fluid and by the entropic spring constant of the DNA conformation in the channel. The power spectrum of the end-to-end length is described by a reaction between vibrational modes of the DNA and confined harmonic potentials. A semi-quantitative theory derived from a combination of the DSS derivation at a higher frequency, with which both the entropic spring constant and the friction coefficient of the nano-confined DNA can be determined. With this method, the spring constant and friction coefficient of nano-confined, YOYO-1 stained T4 DNA has been measured with a relative error below 15%.

Q1.00095 Viscoelasticity of Epoxy nano-composites. SURESH AHUJA, Retired — Nanocomposites have been modeled in a multiscale covering from molecular scale (e.g., molecular dynamics, Monte Carlo), microscale (e.g., Brownian dynamics, dissipative particle dynamics, lattice Boltzmann, time-dependent Ginzburg-Landau method, dynamic density functional theory method) to mesoscale and macroscale (e.g., micromechanics, equivalent-continuum and self-similar approaches, finite element method) The presence of layered silicates in nonaqueous polymers changes the viscoelastic behavior of the unfilled matrix from liquid-like to solid-like because of the formation of a three-dimensional percolating network of exfoliated or intercalated stacks. This gel-like behavior is a direct consequence of the highly anisotropic nature of the nanoclays which prevents their free rotation and the dissipation of stress. Particle to particle interactions is the dominant mechanism in fumed silica nanocomposites whereas particle to polymer interaction is the dominant one in colloidal silica nanocomposites at identical filler concentrations. These interactions are balanced in each nanocomposite systems by the silica surface treatments (chain grafting, silane modification) and the molecular weight of the matrix. Two different types of nanocomposite structures exist namely, intercalated nanocomposites where the polymer layers are sandwiched between silicate layers and exfoliated nanocomposites where the layers can be considered individually but remain more or less dispersed in the polymer matrix. YIELD stress from Carreau-Yasuda model has been correlated to exfoliation. Also, equilibrium modulus and zero shear rate viscosity has been used to analyze percolation threshold and sol-gel transition. Nano clays organically functionalized were mixed with Epoxy in a high shear mixer.

Q1.00096 Heterogeneous nanoparticles at water-oil interfaces: Structure, Order, Diffusion, and Implications for the stability of Pickering emulsions1, ALBERTO STRILO, XUAN-CUONG LUU, The University of Oklahoma, MOLECULAR SCIENCE AND ENGINEERING TEAM TEAM — Pickering emulsions find applications, e.g., in food processing, personal care products, and drug delivery. The emulsions stability is naturally related to the structural and dynamical properties of the nanoparticles adsorbed at oil-water interfaces. Such properties are investigated here by means of dissipative particle dynamics simulations, informed by atomistic molecular dynamics simulations results (Langmuir 2011, 27, (9), 5264-5274). Several nanoparticles are considered, including Janus and homogeneous, and of several different shapes (spherical, elliptical, discoid, etc.) Structural and transport properties are quantified as a function of surface density and system composition. Results for radial distribution functions, hexagonal order parameters, and self-diffusion coefficients are reported. We sometimes find unexpected behavior. For example, self-diffusion coefficient maxima are observed in mixed systems. Implications of such observations on macroscopic observables (i.e., the stability of Pickering emulsions) are discussed.

Q1.00097 A Polyhedral Oligomeric Silsesquioxane-Polyoxometalate Hybrid Shape Amphiphile: Facile Synthesis, Characterization and Crystal Structure. HAO LIU, JING WANG, KAN YUE, JING JIANG, WEN-BIN ZHANG, STÉPHEN CHENG, Department of Polymer Science, The University of Akron — This study contains the synthesis and characterization of a novel shape amphiphile composed of two covalently conjugated inorganic nanoparticles, i.e. an isobutyl substituted polyhedral oligomeric silsesquioxane (BPOSS) cage and a Lindqvist-type hexamolybdate ([Mo6O19]2-) cluster, and its crystal structure. The facile one-step coupling strategy was realized via the highly efficient palladium-catalyzed Sonogashira reaction between an alkyne-bearing POSS derivative (BPOSS-Alkyne) and an iodo-functionalized Lindqvist precursor (BPOSS-Lind) in high yield. The precisely defined molecular structure was thoroughly characterized by combination of routine techniques, such as 1H and 13C NMR, FT-IR, and MALDI-TOF mass spectroscopy. The persistent shape and chemical incompatibility of the two building blocks, as well as the rigid p-phenylene ethynylene linker, drive BPOSS-Lind to pack into a monoclinic lattice, which was confirmed by bright field transmission electron microscopy (TEM), selected area electron diffraction (SAED), small angle X-ray scattering (SAXS) and wide angle X-ray scattering (WAXS). This work introduces a new dumbbell-shaped giant hybrid molecule (BPOSS-Lind) and shed light on the packing behavior of this shape amphiphile.

Q1.00098 Hierarchical Assembly of a Diblock Copolymer-based Supramolecule Containing Liquid Crystal Side Chains. PETER BAI, MYUNG IM KIM, TING XU, University of California, Berkeley — Liquid crystalline side chain block copolymers (LCSCBCPs) are a novel class of soft materials that combine the rich morphology of block copolymers with the unique structural and electro-optical properties of liquid crystals. A supramolecular LCSCBCP composed of a cholesteric small molecule, 3-hydroxylphenyl cholesteryl succinate (CHHP) hydrogen bonded to a diblock copolymer, poly(ethylene-block-poly-4-vinylpyridine) (PS-b-P4VP) was investigated for its structural and thermoresponsive properties using DSC, POM, DSC, TEM and SAXS. The supramolecule, PS-b-P4VP(CHHP), retained both block copolymer and liquid crystalline phase behavior in the form of hierarchical assembly on multiple length scales to form lamellar-within-lamellar and lamellar-within-cylinder morphologies. Upon thermal annealing, the supramolecule demonstrated thermoresponsive behavior in the form of a series of morphological transitions from a P4VP(CHHP) majority morphology to a P4VP(CHHP) minority morphology. The observed hierarchical assembly and thermoresponsiveness could potentially be applied towards templated assembly of nanomaterials with unique nanostructures for optical and photonic applications.

Q1.00099 Simulations of liquid crystalline phases of semiflexible polymer melts and blends. KIRAN KHANAL, JUTTA LUETTMER-STRAHMANN, Departments of Chemistry and Physics, The University of Akron — We perform Monte Carlo simulations of a box-harmonic model for polymers and introduce a bending energy so that polymer chains are flexible at high temperatures and rigid like at low temperature. The phase diagram of polymer melts is determined in the temperature-density plane and the isotropic to nematic transition temperature is found to increase with increasing density. Single chain properties show that coupling between density and stiffness effects lead to nematic order. Blending with flexible chains leads to microphase separation and the formation of ordered domains of rods embedded in disordered regions.
Q1.00100 Morphological Control and Characterization of Liquid Crystalline Materials for Organic Electronics Applications, NABIL KLEINHENZ, KARTHIK NAYANI, JUNG OK PARK, MOHAN SRINIVASARAO, ELSA REICHMAN, Georgia Institute of Technology — Pi-conjugated polymers have been widely explored for use in organic electronics applications. However, their performance is largely limited by the material morphology. We present research on the control and characterization of morphology for conjugated polymers that exhibit a liquid crystalline phase, while making use of their unique properties in organic field effect transistors and organic photovoltaics. Synthesis of novel materials as well as studies on processing conditions have been utilized to elucidate the relationships between structure, properties and device performance.

Q1.00101 Length and sequence dependence in the association of Huntington protein with lipid membranes, SUDI JAWAHERY, ANU NAGARAJAN, SILVINA MATYSIAK, University of Maryland, College Park — There is a fundamental gap in our understanding of how aggregates of mutant Huntington protein (htt) with overextended polyglutamine (polyQ) sequences gain the toxic properties that cause Huntington’s disease (HD). Experimental studies have shown that the most important step associated with toxicity is the binding of mutant htt aggregates to lipid membranes. Studies have also shown that flanking amino acid sequences around the polyQ sequence directly affect interactions with the lipid bilayer, and that polyQ sequences of greater than 35 glutamine repeats in htt are characteristic of HD. The key steps that determine how flanking sequences and polyQ length affect the structure of lipid bilayers remain unknown. In this study, we use atomistic molecular dynamics simulations to study the interactions between lipid membranes of varying compositions and polyQ peptides of varying lengths and flanking sequences. We find that overextended polyQ interactions do cause deformation in model membranes, and that the flanking sequences do play a role in intensifying this deformation by altering the shape of the affected regions.

Q1.00102 Interaction of Complex Liquids with Lipid Biomembranes, BENXIN JING, Y. ELAINE ZHU, Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, Indiana 46556, United States — With the emerging of smart molecular probes and functional nanocolloids for various biomedical applications, it becomes critical to understand the interaction of complex liquids with cell biomembranes in order to effectively use them with minimal cytotoxicity. Deciphered mainly by fluorescence imaging and fluorescence correlation spectroscopy, this poster will emphasize some recent studies in our group of how ionic liquids, macroionic nanoclusters, and nanocolloids interact with cell membrane. Using lipid bilayers as model biomembranes, I will show that adsorbed molecules and nanocolloids can not only disrupt the morphology of lipid bilayers, but also induce their phase transition due to sufficiently strong electrostatic interaction. With ionic liquids and macroionic nanoclusters whose dimensions are comparable to lipids, intriguing supramolecular assembly is also observed at lipid bilayer interface, showing a strong dependence on the chemical makeup of adsorbed ionic species.

Q1.00103 Ion Induced Changes in Phosphoinositide Monolayers at Phisiological Concentrations, ADOLPHE KAZADI BADIAMIBLE, Syracuse University, MARTIN B. FORSTNER, Physic Department, Syracuse University, Syracuse, NY, 13244, Syracuse Biomaterials Institute, Syracuse University, Syracuse, NY 13244 — Phosphoinositides (PIPs) play a crucial role in many cellular processes that occur at the plasma membrane such as calcium release, exocytosis or endocytosis. In order to specifically regulate these functions PIPs must segregate in pools at the plasma membrane. A possible mechanism that could induce and regulate such organization of phosphoinositides is their interaction with bivalent cations. Understanding the physicochemical mechanism that can regulate membrane structure is a crucial step in the development of adaptive biomimetic membrane systems. Using Langmuir monolayers, we investigated the effect of calcium and magnesium on the surface pressure-area/lipid isotherm of monolayer of phosphatidylinositol (PI), phosphatidylinositol bisphosphate (PIP2), dioleoylphosphatidylglycerol (DOPG) and palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC). It is found that the decrease of area per lipid, i.e. the increase in aggregation, is mostly dependent on the lipid’s head group charge but ion specific. In addition, we discuss changes in free energy and compressibility of these monolayer-ion systems. 

Q1.00104 Low Temperature Energy Phase Diagrams of Dimer Adsorption on Square Nanotubes With Attractive First Neighbor Interactions, ALAIN PHARES, Villanova University, DAVID GRUMBINE, JR., St. Vincent College — We consider dimer adsorption on a nanotube with square lattice geometry that is an arbitrary number M of atomic sites in normal cross-section. First-neighbor adsorbate-adsorbate interactions, V, are assumed to be attractive while second-neighbor interactions, W, are allowed to be repulsive, attractive or negligible. The effective potential energy per dimer, μ, is the sum of the adsorbate-substrate interaction energy and the chemical potential of dimer molecules in the medium surrounding the nanotube. At low temperature, the energy phase diagrams are two-dimensional with parameters u = W/V and v = μ/V. These diagrams have been generated numerically for increasing values of M. They fall into two categories which depend on whether M is even or odd. The occupational characteristics of the phases have analytic expressions in M. The occupational configurations of, and line boundaries between phases are determined.

Q1.00105 Polymer adsorption from the melts - In-situ x-ray/neutron reflectivity studies on the chain conformations at the polymer/solid interfaces, NAIHSHENG JIANG, JUN SHANG, MAYA ENDOH, Department of Materials Science and Engineering, Stony Brook University, BULENT AKGUN, SUSHIL SATIJA, Center for Neutron Research, NIST, Gaithersburg, TADANORI KOGA, Department of Materials Science and Engineering, Stony Brook University — Adsorbed polymer layers formed on flat solid substrates have recently been the subject of extensive studies due to their strong and can be formed even onto weakly attractive substrate surfaces. In this study, we aim to clarify the detailed structures and thermal properties by the combined use of in-situ x-ray/neutron reflectivity and atomic force microscopy techniques. Various polymers including polystyrene, polybutadiene, poly (2-vinylpyridine), polycarbonate, and poly(methyl methacrylate) were used to prepare equilibrium adsorbed polymer layers on silicon substrates. We report the effects of the intramolecular architectures, molecular weight, and polymer/substrate interactions on the structures, leading to a better understanding of the thermodynamics at the polymer melt/solid interfaces.

Q1.00106 Ionic Interactions for Aqueous Templating of Biofunctional Molecules in Block Copolymer Nanostructures, BRADLEY OLSEN, BOKYUNG KIM, CHRISTOPHER LAM, CHARLOTTE STEWART-SLOAN, EMMANOUIL GKIKAS, Massachusetts Institute of Technology — The use of ionic interactions to direct both biomolecular templating and block copolymer self-assembly into nanopatterned films with only aqueous processing conditions is demonstrated using block copolymers containing both thermally responsive and pH responsive blocks. Reversible addition-fragmentation chain transfer (RAFT) polymerization is employed to synthesize diblock copolymers with one neutral thermoresponsive and one polyiontropic block and the pH-dependent complexation between model proteins or biomimetic J-aggregating chromophores and the polycationic block is demonstrated. Spin casting is used to prepare nanostructured films from the protein-block copolymer and chromophore-block copolymer coacervates. After film formation, the lower critical solution temperature (LCST) of the thermoresponsive block allows the nanomaterial to be effectively immobilized in aqueous environments at physiological temperatures, enabling use of the materials for biomolecule immobilization and controlled release. In the case of protein nanotemplating, the ionic environment in which the protein is confined enables the majority of the protein (80%) to retain its activity, even after having been dehydrated in vacuum and confined in the thin film.

We acknowledge the financial support from NSF Grant No. CMMI-084626.
Q1.00107 Computational Exploration of the Surface Properties of Cs2Te5 Photoemissive Material, ANTHONY RUTH, Student, KAROLY NEMETH, Adjunct Professor of Physics, KATHERINE HARKAY, Physicist at Argonne, LINDA SPENTZOURS, JEFF TERRY, Associate Professor of Physics — Cs2Te is a broadly used photoemissive material due to its exceptionally high quantum efficiency (∼20%). Our group has recently predicted that the acetylization of this material (Cs2TeC2) would lower its workfunction down to about 2.4 eV from ̃3 eV, and preserve its high quantum efficiency. Such a modification is advantageous because visible light can be used in the operation of such a photoemissive device instead of ultraviolet light. To explore other variants of Cs2Te, we conducted DFT-based computational analysis of the photoemissive properties of Cs2Te5 which is a known phase of Cs and Te. Cs2Te5 attracted our attention for its rod-like 1D Te substructures embedded in a Cs matrix. This structure is similar to Cs2TeC2 as Cs2TeC2 contains TeC2 polymeric rods in a Cs matrix. In addition to that, exploration of various Cesium Telluride phases is necessary to better understand the working of Cs2Te photocathodes. We have calculated surface energies, workfunctions, and optical absorption spectra of several different surfaces of Cs2Te5. A comparison of the properties of various Cs2Te5 surfaces and their utilization in photoemissive devices will be presented.

Q1.00108 Measuring graft stability in a tethered polyelectrolyte film by X-ray and neutron reflectivity, MICHAEL D. DIMITRIOU, NIST Center for Neutron Research, CASEY J. GALVIN, NC State Chemical and Biomolecular Engineering Department, SUSHIL K. SATIJA, NIST Center for Neutron Research, JAN GENZER, NC State Chemical and Biomolecular Engineering Department — The instability of tethered polyelectrolym films in mild conditions has recently brought into question the limits of use of such layers in certain technologies, such as anti-fouling coatings. In order to better understand the process of chain degrading in a polymer brush, we have used X-ray reflectivity (XR) and neutron reflectivity (NR) to examine tethered layers of poly(2-dimethylaminoethyl methacrylate) (PDMAEMA). Exposing an ≈ 30 nm thick film of PDMAEMA brushes grafted on flat silica-coated substrates to a range of relative humidities (RH) resulted in reproducible thickness changes as measured by XR, illustrating the need of ambient solvent to induce degrading. The thickness change showed non-linear behavior, increasing rapidly above ≈ 70% RH and swelling to ≈ 230% of its original thickness at ≈ 99% RH. In order to better understand the apparent diffusive process of vapor into the brush, we have exposed brushes to isotopically labeled vapors. Using XR and NR, we examined the extent of modification in scattering length density within the brush using box and gradient models, and discussed the apparent entropic and enthalpic forces at play. We also conducted in situ aqueous measurements of similar samples to comprehend the degrading process of a polymer brush. Through an appropriate choice of model, we detect variations in grafting density as a function of incubation time.

Q1.00109 Self-folding of Polymer Sheets Responding to Light: Applications and Mechanistic Study, YING LUI, MICHAEL DICKEY, JAN GENZER, North Carolina State University — We describe a simple approach to self-folding that uses localized light absorption on a pre-stressed polymer sheet. Self-folding takes advantage of 2D patterning techniques (e.g., lithography, inkjet printing) and converts predefined 2D templates into 3D structures. Self-folding is useful for packaging, actuation, and sensing. Most approaches to self-folding use hinges (regions that fold) that have unique chemical composition from the rest of the sheet, which requires photolithography or other multiple fabrication steps. Our approach employs homogeneous polymer sheets and inkjet printing. The black ink (i.e., the hinge) is patterned using a desktop printer on the sheet. Hinges absorb selectively the light to locally heat the underlying polymer and cause the shrinkage. We study experimentally the key physical parameters (hinge geometry, line width and support temperature) which affect the folding. We also explore various light and ink sources for folding complex 3D structures. Moreover, we model thermal profiles inside the polymer film, and investigate folding dynamics based on thermal shrinkage and rheological properties of polymer networks.

Q1.00110 Formation of Lenses by Liquid Interfacial Surfaces, CHARLOTTE ZIMMERMAN, BENJAMIN CERJAN, MARTHA-ELIZABETH BAYLOR, Carleton College — In this study, we examined the geometry of polymer lenses formed by liquid interfacial surfaces. We observed lenses formed when hydrophobic photo-curable monomer is dropped on the surface of a hydrophilic liquid. Due to intermolecular forces between the monomer and the substrate liquid, the interface is pulled into a curved shape. Upon exposure to UV light, the monomer solidifies while maintaining the boundary interface. The result is a plano-convex, optically-smooth polymer lens. The interfacial surface tension is manipulated by altering the amount of thin film present on the surface of the hydrophilic liquid, producing lenses of different curvatures. The lens curvature is further modified by using various salts that change the polarity of the substrate solution. We will present data demonstrating modification of the lens shape due to specific changes made to the physical and chemical properties of the hydrophilic liquid. We believe this liquid interfacial fabrication technique offers an alternative to current molding techniques for forming polymer lenses.

Q1.00111 Improving the Adhesion of Au Thin Films Onto PMMA Substrates Using Chloroform, COURTNEY WARDWELL, ALAN MO, BRIAN AUGUSTINE, CHRIS HUGHES, THOMAS DEVORE, None, JAMES MADISON UNIVERSITY TEAM — Conventional techniques such as O plasma treatment to improve Au thin film adhesion have resulted in limited success. In this study, the adhesion of 6 nm and 100 nm Au thin films onto 0.8 mm poly(methyl methacrylate) (PMMA) sheets was significantly improved when Au thin film samples were exposed to a saturated chloroform environment after metalization. The shear force required to remove the Au films was calculated by placing samples onto a polished specimen holder at 150–200 μN by using a spring loaded device to apply the force. Au thin samples were characterized through optical microscopy, atomic force microscopy (AFM) and attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR). AFM and optical images show a roughening of the Au thin films after chloroform exposure. ATR-FTIR spectra indicate that residual chloroform solvent remains on the PMMA. Our research indicates chloroform may improve adhesion by relieving the stresses at the PMMA-Au interface. X-ray photoelectron spectroscopy (XPS) studies on chloroform pre-treated PMMA samples show residual solvent at the surface one-week after exposure. We have attributed this to a Lewis acid-base interaction between chloroform and the PMMA surface. We will report on the XPS data of post treated samples.

Q1.00112 Thermodynamics and Preliminary Size Parameters of a Polymer Confined to a Lattice of Finite Size: Matrix Method, CHAD SNYDER, CHARLES GUTTMAN, Materials Science and Engineering Division, NIST, THOMAS DEVORE, None, JAMES MADISON UNIVERSITY — We write equations for the thermodynamic properties and end-to-end distance of a linear polymer molecule confined to walk on a lattice of finite size. A theory is presented wherein the dimension of the space in which the lattice resides can be arbitrary. In this theory, the boundary can be of arbitrary shape and the attraction of the monomers for the sites can be an arbitrary function of each site. The formalism is even more general in that each monomer can have its own energy of attraction for each lattice site. In particular, we look at the effect of energy variation along the lattice with the idea of studying the effect of heterogeneities in the energies of a surface on polymer attachment.

Q1.00113 Influence of Slip on the Rayleigh-Plateau Rim Instability in Dewetting Polymer Films, OLIVER BAEUMCHEN, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, LBS 4M1, KARIN JACOBS, LUDOVIC MARQUANT, SABRINA HAEFFNER, MISCHA KLOS, Saarland University, Department of Experimental Physics, 66123 Saarbruecken, Germany, RALF BLOSSEY, Interdisciplinary Research Institute (IRI), CNRS USR 3078, Villeneuve d’Ascq, France, ANDREAS STUDEN, Mathematical Institute, University of Oxford, Oxford OX1 3LB, UK, BARBARA WAGNER, Technical University of Berlin, Institute for Mathematics, 10623 Berlin, Germany — A dewetting polymer film develops a characteristic fluid rim at its receding edge due to mass conservation. In the course of the dewetting process the rim becomes unstable via an instability of Rayleigh-Plateau type. An important difference exists between this classic instability of a liquid column and the rim instability in the thin film as the growth of the rim is continuously fueled by the receding film. We explain how the development and macroscopic morphology of the rim instability are controlled by the slip of the film on the substrate. A single thin-film model, valid for all slip lengths, captures quantitatively the characteristics of the evolution of the rim observed in our experiments.
Q1.00114 What information can frictional properties of polymer brushes tell us? ZHENYU ZHANG, Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK, MARK MOXEY, ANDREW MORSE, STEVEN ARMES, Department of Chemistry, University of Sheffield, Sheffield, S3 7HF, UK, ANDREW LEWIS, Biocompatibles UK Ltd., Chapman House, Farnham Business Park, Weydon Lane, Farnham, Surrey, GU9 8QL, UK, MARK GOGHEGAN, Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK, GRAHAM LEGGETT, Department of Chemistry, University of Sheffield, Sheffield, S3 7HF, UK — We have used friction force microscopy (FFM) to quantitatively examine surface grown zwitterionic polymer brushes: poly(2-(methacyloyloxy)ethyl phosphorylcholine) (PMPC), and to establish the correlation between its frictional behavior and our two different properties of the substrate: surface energy, \( \gamma_s \), and shear modulus, \( G \), which is a function of the dimensionless parameter \( \gamma_s / G - 1/3 \). Molecular dynamics simulations of nanoparticle detachment show that the Kramers approach fails in the vicinity of the critical detachment force \( f^* \) where activation energy barrier becomes smaller than \( k_B T \).

Q1.00115 Dynamics of Nanoparticle Adhesion\(^1\) J.-M.Y. CARRILLO, A.V. DOBRYNIN, University of Connecticut — We performed molecular dynamics simulations and theoretical analysis of nanoparticle pulling off from adhesive substrates. Our theoretical model of nanoparticle detachment is based on the Kramers solution of the stochastic barrier crossing in effective one dimensional potential well. The activation energy, \( \Delta E \), for nanoparticle detachment first decreases linearly with increasing the magnitude of the applied force, \( f \), then it follows a power law \( \Delta E \propto (f - f_0)^{3/2} \) as magnitude of the pulling force approaches a critical detachment force value, \( f_0 \). These two different regimes in activation energy dependence on magnitude of the applied force are confirmed by analyzing nanoparticle detachment in effective one dimensional potential obtained by Weighted Histogram Analysis Method. Simulations show that detachment of nanoparticle proceeds through neck formation such that magnitude of the activation energy is determined by balancing surface energy of the neck connecting particle to a substrate with elastic energy of nanoparticle deformation. In this regime the activation energy at zero applied force, \( \Delta E_0 \), for nanoparticle with radius, \( R_p \), shear modulus, \( G \), surface energy, \( \gamma_s \), and work of adhesion, \( W \), is a universal function of the dimensionless parameter \( \delta \propto \gamma_s G^{-1/3} R_p^{-2/3} \). Molecular dynamics simulations of nanoparticle detachment show that the Kramers approach fails in the vicinity of the critical detachment force \( f^* \) where activation energy barrier becomes smaller than \( k_B T \).

Q1.00116 Swelling-Induced Hierarchical Structures WEI HAN, BO LI, ZHIQUN LIN, Georgia Institute of Technology — When the two layer structures comprised of the polyvinylpyrrolidone (PVP) thin film as substrate and the upper gradient poly (methyl methacrylate) (PMMA) stripes prepared via self-assembled (CESA) were subjected to ethanol vapor, which is selective solvent for PVP, hierarchical wrinkles were observed due to the osmotically driven swelling associated with solvent-vapor sorption. Due to the confined imposed by the PMMA stripes, the wrinkles aligned perfectly perpendicular to stripes. Quite intriguingly, three-level-hierarchical arrangement of wrinkles containing nanoscale micelles were also produced by CESAs of PS-b-P4VP on the PVP film, followed by the exposure to the ethanol vapor. The patterns were stable in both swollen and dry states, thus creating a versatile approach that is useful for diverse polymers to produce complex patterns with long-range orders.

Q1.00117 Listening in on Friction: Stick-Slip Acoustical Signatures in Velcro SEBASTIAN HURTADO PARRA, LESLIE MORROW, MILES RADZIWILOWSKI, PAUL ANGIOLILLO, Saint Joseph’s University — The onset of kinetic friction and the possible resulting stick-slip motion remain mysterious phenomena. Moreover, stick-slip dynamics are typically accompanied by acoustic bursts that occur temporally with the slip event. The dry sliding dynamics of the hook-and-loop system, as exemplified by Velcro, manifest stick-slip behavior along with audible bursts that are easily acoustically collected. Synchronized measurements of the friction force and acoustic emissions were collected as hooked Velcro was driven at constant velocity over a bed of looped Velcro in an anechoic chamber. Not surprising, the envelope of the acoustic bursts maps well onto the slip events of the friction force time series and the intensity of the bursts trends with the magnitude of the difference of the friction force during a stick-slip event. However, the analysis of the acoustic emission can serve as a sensitive tool for revealing some of the hidden details of the evolution of the transition from static to kinetic friction. For instance, small acoustic bursts are seen prior to the Amontons-Coulomb threshold, signaling precursor events prior to the onset of macroscopically observed motion. Preliminary spectral analysis of the acoustic emissions including intensity-frequency data will be presented.

Q1.00118 Investigating Molecular Level Stress-Strain Relationships in Entangled F-Actin Networks by Combined Force-Measuring Optical Tweezers and Fluorescence Microscopy KENT LEE, DEAN HENZE, RAE M. ROBERTSON-ANDERSON, University of San Diego — Actin is an important cytoskeletal protein involved in cell structure and motility, cancer invasion and metastasis, and muscle contraction. The intricate viscoelastic properties of filamentous actin (F-actin) networks allow for many dynamic roles of actin, thus warranting investigation. Exploration of this unique stress-strain/strain-rate relationship in complex F-actin networks can also improve biomimetic materials engineering. Here, we use optical tweezers with fluorescence microscopy to study the viscoelastic properties of F-actin networks on the microscopic level. Optically trapped microparticles embedded in various F-actin networks are moved through the network using a nanoprecision piezoelectric stage. The force exerted on the microparticles by the F-actin network and subsequent force relaxation are measured, while a fraction of the filaments in the network are fluorescent-labeled to observe filament deformation in real-time. The dependence of the viscoelastic properties of the network on strain rates and amplitudes as well as F-actin concentration is quantified. This approach provides the much-needed link between induced force and deformation over localized regimes (tens of microns) and down to the single molecule level.

Q1.00119 Structure and Dynamics of Polymer nanocomposite hydrogels DI XIU, MIRIAM RAFAILOVICH, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University. NY-11794 — Polymer hydrogels are widely used in fields like food science, tissue engineering and drug delivery. A lot of research has focused on developing hydrogels with novel properties. However, a lack of understanding of the dynamics and structure of the hydrogel has become a big obstacle. We use molecular dynamic simulations, which provide a direct observation of gel formation and gel structures, to study the local structural and dynamic properties of hydrogels. Our work focuses on using coarse-grained molecular simulations to study physically linked polymer nano-composite hydrogels. Our goal is to study how the aspect ratio and shape of the nanofiller introduced to the gel can lead to different mechanical behavior. Our simulation looks at the effects of polymer species, chain length, and water content and the effect on the mechanical properties of the hydrogel.

Q1.00120 Creating Controlled Thickness Gradients in Polymer Thin Films via Flowcoating RALEIGH DAVIS, SAHANA JAYARAMAN, RICHARD REGISTER, Princeton University, PAUL CHAIKIN, New York University — Flow coating is a technique which has a unique capacity to create polymer thin films of virtually any desired thickness profile. The method which allows a user to produce polymer thin films of virtually any desired thickness profile. This has greatly enhanced the throughput of many dynamic roles of actin, thus warranting investigation. Exploration of this unique stress-strain/strain-rate relationship in complex F-actin networks can also improve biomimetic materials engineering. Here, we use optical tweezers with fluorescence microscopy to study the viscoelastic properties of F-actin networks on the microscopic level. Optically trapped microparticles embedded in various F-actin networks are moved through the network using a nanoprecision piezoelectric stage. The force exerted on the microparticles by the F-actin network and subsequent force relaxation are measured, while a fraction of the filaments in the network are fluorescent-labeled to observe filament deformation in real-time. The dependence of the viscoelastic properties of the network on strain rates and amplitudes as well as F-actin concentration is quantified. This approach provides the much-needed link between induced force and deformation over localized regimes (tens of microns) and down to the single molecule level.
Q1.00121 Measuring the Dynamic Parameters of MCF7 Cell Microtubules, CARLY WINTON, MITRA SHOJANIA FEIZABADI, Seton Hall University — Microtubules are the key component of the cytoskeleton. They are intrinsically dynamic displaying dynamic instability in which they randomly switch between a phase of growing and shrinking, both in vitro and in vivo. This dynamic is specified by the following parameters: growing rate, shrinking rate, frequency of catastrophe, and frequency of rescue. In this work, we will present our primary results in which we measured the dynamic parameters of a single microtubule polymerized from MCF7 tubulin in vitro. The results are significant since the MCF7 microtubules are non-neural mammalian consisting of different beta tubulin isotypes in their structures as compared to neural mammalian microtubules, such as bovine brain. The unique dynamic parameters of individual MCF7 microtubules in vitro, which are reported for the first time, indicate that non-neural microtubules can be fundamentally different from neural microtubules.

Q1.00122 Feedback-enhanced Micro Rheology, HEEV AYADE, MARCEL BREMERICH, HIROSHI ARIMATSU, DAISUKE MIZUNO, Kyushu University — An essential feature of the cytoskeleton is their ability to perform variety of mechanical functions in cells. The active force generation by molecular motors keeps the living cytoskeletons far from equilibrium that makes understanding of cell mechanics and behaviors particularly challenging. Here, we have investigated the non-equilibrium mechanical properties of cells using optical trapping based micro rheology, which tracks the motion of phagocytosed probe particles with high spatial and temporal resolution than video tracking micro rheology. In order to perform high resolution measurement in cells or active soft materials, the active fluctuations of the beads have to be compensated for in order to keep the beads stably in a highly focused beam spot. We achieve this by implementing a PID-controlled feedback mechanism to reposition the sample chamber with a 3D-piezo stage, for large-scale but slow motions of the probes. The stage motion is recorded as piezo-control, and the motion of the probe from the laser focus is provided as the quadrant photodiode output. Sum of those signals reconstitutes the complete bead trajectory. The method reported here is robust in accessing thermal and athermal fluctuations in active systems.

Q1.00123 Viscoelastic chiral liquid crystals: Response to heat and light, DANIEL BATEMAN, None, PETR SHIBAEV, Fordham University — Highly viscous cholesteric liquid crystals with distinctive viscoelastic properties were studied [1,2] as heat and light driven materials able to contract under light irradiation and heating. Materials are comprised of glass-forming oligomers (Wacker oligomers), low molar mass liquid crystals, and azo dyes. The latter provide sensitivity of the whole material to light irradiation. Mixtures with different azo dyes were studied and their effectiveness in terms of mechanical response (sample contraction) was determined. The optimal concentration of oligomers in terms of maximizing the elastic response and retaining high processability was found for different compositions of material. The mechanism of mechanical response is discussed in terms of the contraction of helical pitch and entropic changes in the overall structure of oligomer-liquid crystal mixture. 1] Petr V. Shibaev1, Benjamin Crooker1, Michael Manevich2, and Eckhard Handel.3 Appl. Phys. Lett. 99, 233302 (2011), [2] Peter V. Shibaev, Pierre Rivera, Dashiel Teter, Salvatore Marsico, Martin Sanzari, Veena Ramakrishnan, Eckhard Handel, Optics Express 16, 2965 (2008)

Q1.00124 Influence of curvature on the morphology of brain microvascular endothelial cells, MAO YE, ZHEN YANG, ANDREW WONG, PETER SEARSON, Johns Hopkins University, SEARSON GROUP TEAM — There are hundreds or thousands of endothelial cells around the perimeter of a single artery or vein, and hence an individual cell experiences little curvature. In contrast, a single endothelial cell may wrap around itself to form the lumen of a brain capillary. Curvature plays a key role in many biological, chemical and physical processes, however, its role in dictating the morphology and polarization of brain capillary endothelial cells has not been investigated. We hypothesize that curvature and shear flow play a key role in determining the structure and function of the blood-brain barrier (BBB). We have developed the “rod” assay to study the influence of curvature on the morphology of confluent monolayers of endothelial cells. In this assay cells are plated onto glass rods pulled down to the desired diameter in the range from 5 – 500 µm and coated with collagen. We show that curvature has a significant influence on the morphology of endothelial cells and may have an important role in blood-brain barrier function.

Q1.00125 Thermal response of a protein (H3.1) by a coarse-grained model with knowledge-based interactions, BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — The effect of temperature on the conformation of a histone (H3.1) is studied by a coarse-grained Monte Carlo simulation based on three knowledge-based contact potentials (M3[1], BT[2], BFVK[3]). We find that the histone H3.1 undergoes a systematic (possibly continuous) structural transition from a random coil to a globular conformation on reducing the temperature, a general feature from each potential. The range over which such a systematic response in variation of the radius of gyration (Rg) with the temperature (T) occurs, however, depends on the potential. Multi-scale structures of the protein are examined by analyzing the scaling of the structure functions with the wave vector. Quantitative comparison of the structure emerging from three potentials will be presented.


This work is supported by Air Force Research Laboratory.

Q1.00126 Computational model for Halorhodopsin photocurrent kinetics, JAIME BRAVO, Department of Biomedical Engineering, The Ohio State University, ROXANA STEFANESCU, Department of Pediatric Neurology, University of Florida, SACHIN TALATHI, Department of Biomedical Engineering, University of Florida — Optogenetics is a rapidly developing novel optical stimulation technique that employs light activated ion channels to excite (using channelrhodopsin (ChR)) or suppress (using halorhodopsin (HR)) impulse activity in neurons with high temporal and spatial resolution. This technique holds enormous potential to externally control activity states in neuronal networks. The channel kinetics of ChR and HR are well understood and amenable for mathematical modeling. Significant progress has been made in recent years to develop models for ChR channel kinetics. To date however, there is no model to mimic photocurrents produced by HR. Here, we report the first model developed for HR photocurrents based on a four-state model of the HR photocurrent kinetics. The model provides an excellent fit (root-mean-square error of 3.186x10^-1) to an empirical profile of experimentally measured HR photocurrents. In combination, mathematical models for ChR and HR photocurrents can provide effective means to design test light based control systems to regulate neural activity, which in turn may have implications for the development of novel light based stimulation paradigms for brain disease control.

1) This work is supported by the US Army Research Laboratory.

Q1.00127 Kinetics of inter-segmental contact in semiflexible polymers, REZA AFRA, BRIAN TODD, Dept of Physics, Purdue University — Diffusion-limited contact between polypeptide segments is an elementary step in protein folding and this process sets an upper limit on protein folding kinetics. A common theoretical approach to calculating this “speed limit” is to reduce the high-dimensional conformational search to a one-dimensional diffusion along an effective reaction coordinate. We employed Brownian dynamic simulations to test the validity of this approximation for inter-segmental contact kinetics in the semiflexible polymer model. This model is often used to describe the unfolded protein state. We find that one-dimensional diffusion models cannot capture the correct scaling between contact dynamics and either capture radius or chain length. Our findings highlights the difficulty of describing high-dimensional protein molecules with simple kinetic theories.
Q1.00128 Effect of Mutations on HP Lattice Proteins

**GUANGJIE SHI, THOMAS VOGELO, DAVID P. LANDAU**
The University of Georgia, YING WAI LI, Oak Ridge National Laboratory, THOMAS WÜST, Swiss Federal Research Institute WSL — Using Wang-Landau sampling with appropriate trial moves we investigate the effect of different types of mutations on lattice proteins in the HP model. While exact studies have been carried out for short HP protein systems, we systematically analyse the changes in structure and degeneracy of ground states of particular proteins and measure thermodynamic quantities like the stability of ground states and the specific heat, for example. Both, neutral mutations, which do not change the structure and stability of ground states, as well as critical mutations, which do change the thermodynamic behavior qualitatively, have been observed.

Research supported by NSF


Q1.00129 Nearest Neighbor Interactions Affect the Conformational Distribution in the Unfolded State of Peptides

**SIOBHAN TOAL, REINHARD SCHWEITZER-STENNING, Drexel University, KARIN RYBKA, HARDOL SCHWALBE, Johann Wolfgang Goethe University** — In order to enable structural predictions of intrinsically disordered proteins (IDPs) the intrinsic conformational propensities of amino acids must be complemented by information on nearest-neighbor interactions. To explore the influence of nearest-neighbors on conformational distributions, we preformed a joint vibrational (Infrared, Vibrational Circular Dichroism (VCD), polarized Raman) and 2D-NMR study of selected GlyG host-peptide: GDyG, GSyG, GxLG, GxVG, where x/y = (A,K,LV). D and S (L and V) were chosen at the x (y) position due to their observance to drastically change the distribution of alanine in xAy tripeptide sequences in truncated coil cylinders. The conformationally sensitive amide’ profiles of the respective spectra were analyzed in terms of a statistical ensemble described as a superposition of 2D-Gaussian functions in Ramachandran space representing sub-ensembles of p Pall, J-strand, helical, and turn-like conformations. Our analysis and simulation of the amide I’ band profiles exploits excitonic coupling between the local amide I’ vibrational modes in the tetra-peptides. The resulting distributions reveal that D and S, which themselves have high propensities for turn-structures, strongly affect the conformational distribution of their downstream neighbor. Taken together, our results indicate that Dx and Sx motifs might act as conformational randomizers in proteins, attenuating intrinsic propensities of neighboring residues. Overall, our results show that nearest neighbor interactions contribute significantly to the Gibbs energy landscape of disordered peptides and proteins.

Q1.00130 A large scale membrane-binding protein conformational change that initiates at small length scales

**TREVOR GRANDPRE, MATTHEW ANDORF, DePaul University, SRINIVAS CHAKRAVARTHY, Illinois Institute of Technology, ROBERT LAMB, TAYLOR POOR, Northwestern University, ERIC LANDAHL** — The fusion (F) protein of parainfluenza virus 5 (PIV5) is a membrane-bound, homotrimeric glycoprotein located on the surface of PIV5 viral envelopes. Upon being triggered by the receptor-binding protein (HN), F undergoes a greater than 100 nm ATP-independent refolding event. This refolding event results in the insertion of a hydrophobic fusion peptide into the membrane of the target cell, followed by the desolvation and subsequent fusion event as the two membranes are brought together. Isothermal calorimetry and hydrophobic dye incorporation experiments indicate that the soluble construct of the F protein undergoes a conformational rearrangement event at around 55 deg C. We present the results of an initial Time-Resolved Small-Angle X-Ray Scattering (TR-SAXS) study of this large scale, entropically driven conformational change using a temperature jump. Although we the measured radius of gyration of this protein changes on a 110 second timescale, we find that the x-ray scattering intensity at higher angles (corresponding to smaller length scales in the protein) changes nearly an order of magnitude faster. We believe this may be a signature of entropically-driven conformational change.

Q1.00131 Shear History Independence in Colloidal Aggregation

**WILLIAM HEINSON, AMITABHA CHAKRABARTI, CHRISTOPHER SORENSEN**, Department of Physics, Kansas State University — Stimulated by experiments, we have carried out detailed simulations of aggregation in the presence of shear in a model colloidal system with a short-range attractive potential. For weak shear rates we find that the shear enhanced the aggregation and that the long time state of the system is independent of the shear history. For strong shear rates, precipitous fragmentation occurred after the shear was turned on and after an induction period, the aggregation quickly rebounded in a stochastic manner similar to classical nucleation phenomena. However, the long-time state of the system is, once again, independent of the shear history. Thus, for both weak and strong shear cases, shear rate acts as a state variable of the aggregating system. Shear rates employed in the simulations can be attained in laboratory experiments as confirmed by computing the dimensionless Péclet numbers.

Q1.00132 Crystal-like Formation in Dilute Aqueous Media with Binary Charged Block Copolymer Micelles

**MISOOK LEE, KYUNG JEE MIN, Seoul National University, JINKEE HONG, Kyunghee University, KOOKHEON CHAR, Seoul National University** — The morphology of charged block copolymer micelle (BCM) complexes, consisting of polystyrene-block-poly(acrylic acid) (PS-b-PAA) and polystyrene-block-poly(4-vinyl pyridine) (PS-b-P4VP) micelles, was controlled by pH of aqueous solvent as well as solvent quality. To determine the effective pH range for the inter-corona combination of PAA and P4VP blocks in aqueous media, we studied the dissociation behavior of both coronas using Fourier Transform Infrared Spectroscopy. Lower pH region (pH<5.0) in aqueous media offers stronger interactions between oppositely charged corona blocks, resulting in polymeric-hexagonal prism cores. In the higher pH region (pH>5.5), they first self-assembled into hierarchical spherical states induced by the simple adsorption of small PS-b-PAA BCMs on the surfaces of PS-b-P4VP large compound micelles since the degree of ionization of P4VP blocks is relatively low. However, the core-cut BCM complex morphology with high aggregation number does not allow the hexagonal prism structure to be formed without rearranging strongly aggregated core blocks. We note that the core-cut BCM complexation in higher DMF content of a mixed solvent induces inter-corona association leading to the hexagonal prism structure due to the decrease in selectivity of water for PS blocks.

Q1.00133 Free energy change for aggregation of charged monolayer-protected gold nanoparticles

**REID VAN LEHN, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology** — Monolayer-protected gold nanoparticles (AuNPs) are an important class of nanomaterials with applications in drug delivery and biosensing. However, the utility of AuNPs is limited by the spontaneous aggregation of particles in solution, which is observed even for highly charged, water-soluble AuNPs. Such aggregation cannot be well-described by continuum theories that would predict the dominance of repulsive electrostatic interactions over weaker van der Waals interactions. In this work, we show that small AuNPs (diameter < 10 nm) protected by charged alkanethiol monolayers may aggregate due to a ligand-mediated short-range attraction that compensates for electrostatic repulsion. The short-range attraction is driven by the hydrophobic effect as the flexible ligands deform to shield hydrophobic surface area from water. We use novel simulations to calculate the free energy change for bringing two AuNPs together from infinite separation and show that the free energy change depends on particle size, monolayer composition, and the surrounding medium. This work provides insight into the key role that ligand interactions play in AuNP aggregation and suggests guidelines for the design of protecting monolayers.
Q1.00134 Direct Measurement of Diffusion of Terbium Ions Through a Silica Gel Matrix\(^1\), M. BLADES, T. IGNOTOVA, Lehigh University, J.G. DUQUE, S.K. DOORN, Los Alamos National Laboratory, S.V. RÖTKit, Lehigh University — The use of rare earth ions as optical bio-markers and for the study of complex nanoscale systems via resonant energy transfer has been suggested and successfully demonstrated. Our capability to extract reliable information from such an experiment critically depends on understanding the underlying physics of interactions in the studied material. Here we investigate the diffusion of Terbium into a silica hydrogel matrix. Diffusion rates and optical properties can be related to differences in gel morphology and rare earth ion behavior in gels prepared with and without nanotubes. Absorption mechanisms, micelle formation, and Terbium/nanotube interaction are discussed.

\(^1\)NSF Grant ECCS-1202398

Q1.00135 Mechanical characterization of diblock copolymer “armored” emulsion droplets . DAMITH P. ROZAIRO, ANDREW B. CROLL, North Dakota State University — There has been an increased interest in block copolymer vesicles due to a plethora of possible application ranging from targeted drug delivery to cosmetically active agents. In this regard, understanding the physics of the block copolymer vesicle and its morphology is critical to the rational development of these technologies. As a step towards more complex vesicle structures, we describe experiments in which we carefully examine the interface and morphology of polystyrene-b-polyethyleneoxide (PS-PEO) emulsion drops. In our study, PS-PEO acts as a surfactant and at the toluene-water interface creates a monolayer, inhibiting drop recombination and minimizing interfacial energies. Our experiments are conducted in a water cell where the buoyant force is exploited to push drops against a thin sheet of mica. The shape of the drops is measured using an upright confocal microscope and compared with a Bashforth-Adams model in order to examine the mechanical response to the buoyant force. We observe unique dynamics as the drops buckle at short timescales trapping a small pocket of fluid which slowly drains away. Furthermore, the influence of polymer concentration, changes in pH and block copolymer architecture on the morphology and dynamics of the droplets is examined.

Q1.00136 The order-to-disorder transition behavior of PS-b-P2VP thin film system . HYUNGJU AHN, DU YEOL RYU, Yonsei University — We investigated the transition behavior such as the order-to-disorder transition (ODT) for symmetric poly(styrene)-block-poly(2-vinyl pyridine) (PS-b-P2VP) using SAXS and GISAXS for block copolymer bulks and films. The bulk transition temperature of PS-b-P2VP was significantly influenced by the interfacial interactions in thin films, leading to the different transition temperature. From these results, we will discuss about the interfacial interaction effects on the phase behaviors in bulks and thin films system of PS-b-P2VP.

Q1.00137 Reactivity of End-functionalized Polymers Containing Diels-Alder Functional Groups . YUAN MENG, YUAN ZHANG, MITCHELL ANTHAMATTEN, University of Rochester — Incorporation of reversible covalent bond into macro-molecular systems has proven useful in engineering novel responsive architectures, and Diels-Alder bonding in this context is now well established. However, efficient synthesis of end-functionalized polymers is a major obstacle hindering further development of responsive and modular polymer architectures. In this current research, two immiscible polymers, poly(methyl methacrylate) (PMMA) and poly(benzyl methacrylate) (PBzMA) with controlled molecular weight, bearing terminal furan-maleimide groups, are prepared via Reversible Addition-Fragmentation chain transfer (RAFT) polymerization. The reactivity of such end-functionalized polymers is explored to expose the relationship between chain composition and their ability to undergo modular cross-coupling to form monodisperse block copolymers. To elucidate how reaction conditions affect the efficiency of the Diels-Alder reaction, Hydrogen Nuclear Magnetic Resonance (H-NMR) and Size Exclusion Chromatography (SEC) techniques are actively applied. Experimental results will be interpreted on the basis of dissimilarity between interaction energies of polymer segments and the concentration of reactive groups.

Q1.00138 Can coarse-grained force field parameters be transferable? , MALGORZATA KOWALIK, Department of Chemical Engineering, 121 Fenske Laboratory, University Park, Pennsylvania 16802, USA, JANNA K. MARANAS, Department of Chemical Engineering, 107 Fenske Laboratory, University Park, Pennsylvania 16802, USA — We present results from molecular dynamics simulations of self-assembled copolymers in explicit coarse-grained water. Our goal is to provide intermolecular potentials for coarse-grained beads that are mixture independent. With such transferable potentials, forming new combinations of copolymers and adding new polymers is relatively straightforward. In this approach, each coarse-grained bead (polymer as well as water) is assigned mixture independent Lennard-Jones parameters. We use generic combining rules, with a pair-independent scaling parameter for interactions between hydrophilic and hydrophobic beads. We succeed in describing six coarse-grained beads system using only six intermolecular parameters, to describe 15 individual interactions. We conclude that a transferable set of intermolecular parameters is possible.

Q1.00139 Diffusion of liquid polystyrene into glassy poly(phenylene oxide) characterized by DSC\(^1\), LINLING LI, XIAOLIANG WANG, DONGSHAN ZHOU, GI XUE, Department of Polymer Science and Engineering, Nanjing University — We report a diffusion study on the polystyrene/poly(phenylene oxide) (PS/PPO) mixture consisted by the PS and PPO nanoparticles. Diffusion of liquid PS into glassy PPO (l-PS/g-PPO) is promoted by annealing the PS/PPO mixture at several temperatures below Tg of the PPO. By tracing the Tgs of the PS-rich domain behind the diffusion front using DSC, we get the relationships of PS weight fractions and diffusion front advances with the elapsed diffusion times at different diffusion temperatures using the Gordon-Taylor equation and core-shell model. We find that the plots of weight fraction of PS vs. elapsed diffusion times at different temperatures can be converted to a master curve by Time-Temperature superposition, and the shift factors obey the Arrhenius equation. Besides, the diffusion front advances of l-PS into g-PPO show an excellent agreement with the 1/2 scaling law at the beginning of the diffusion process, and the diffusion coefficients of different diffusion temperature also obey the Arrhenius equation. We believe the diffusion mechanism for l-PS/g-PPO should be the Fickean law rather than the Case II, though there are departures of original linearity at longer diffusion times due to the limited liquid supply system.

\(^1\)Diffusion of liquid polystyrene into glassy poly(phenylene oxide) characterized by DSC

Q1.00140 Polymer Brush Grafted Nanoparticles and Their Impact on the Morphology Evolution of Polymer Blend Films , HYUN-JOONG CHUNG, University of Alberta, KOHI OHNO, Kyoto University, RUSSELL J. COMPOSTO, University of Pennsylvania — We present a novel pathway to control the location of nanoparticles (NPs) in phase-separating polymer blend films containing poly(methyl methacrylate) (PMMA) and poly(styrene-ran-acrylonitrile) (SAN). Because hydrophobic polymer phases have a small interfacial energy, \(\sim 1 \text{ mJ/m}^2\), subtle changes in the NP surface functionality can be used to guide NPs to either the interface between immiscible polymers or into one of the phases. Based on this idea, we designed a class of NPs grafted with PMMA brushes. These PMMA brushes were grown from the NP surface by atom transfer radical polymerization (ATRP), which results in chains terminated with chlorine atoms. The Cl end groups and shorter chain length cause an increase in surface energy of short-chained NPs can be attributed to (i) an extended brush conformation (entropic) and/or (ii) a high density of “unfavorable” end groups (entropic). Finally, the impact of NPs on the morphological evolution of the polymer blend films will be discussed. Ref: H.-J.Chung et al., ACS Macro Lett. 1(1), 252-256 (2012).
Q1.00141 Polymer Blend Emulsions Stabilized by Janus Particles , KYLE BRYSON, THOMAS RUSSELL, RYAN HAYWARD, University of Massachusetts - Amherst — Kinetic trapping of bicontinuous polymer morphologies through the interfacial segregation of nanoparticles is of interest due to the unique combination of the properties of each component provided by such structures, and their potential for use as membranes and composite materials. However, this strategy is challenging to realize in polymeric systems, due to the difficulties in preparing particles that are neutrally wetted by the two polymer phases. Janus particles afford a route to circumvent the necessity of neutral wettability. In addition, both theory and experiment have shown enhanced interfacial adsorption energies for Janus particles, as well as greater flexibility in controlling particle orientation at the interface, in comparison to homogeneous particles. Dumbbell-shaped gold-silica Janus particles were synthesized using several sizes of gold seeds. These particles were made amphiphilic by functionalization with both polymeric and small molecule silanols and thiol. Their interfacial activity was measured using pendant drop tensiometry, and their ability to stabilize bicontinuous emulsions of polymers was examined by TEM. The results elucidate the role of particle wettability on interfacial behavior and the structure of stabilized emulsions.

Q1.00142 A new method for homogeneous and uniformly dispersed nanofiber composites using electrospinning , KENTARO WATANABE, ATSUSHI HOTT A, Department of Mechanical Engineering, Keio University — A method for the fabrication of a new type of homogeneous and well-dispersed nanofiber composite was introduced. Electrospinning can fabricate unswollen polymer nanofibers (NF) by electrostatic repulsion, which can be used for nano-filters and cell scaffolds. Polymer solution was put in a syringe and a high voltage was applied to the needle tip, while the polymer solution was ejected from the syringe toward a grounded metal plate (collector) to form unswollen NF. In order to make a nanofiber composite, the NF were then sandwiched by base polymers and molded. The traditional sandwich method would produce biased and relatively inhomogeneous composites. We therefore modified the metal plate to an optimized metal container that could contain polymer solution for the base composite material. This new method resulted in homogeneous mixing of NF that were ejected from the syringe to be directly included in the polymer solution. Polyvinylalcohol (PVA) was used for NF and polydimethylsiloxane (PDMS) was used for the polymer matrix. Field emission scanning electron microscopy (FE-SEM) revealed homogeneous and well-dispersed PVA NF in PDMS. The new method for the fabrication of homogeneous composites could be used for other combinations of polymeric NF and polymer matrix.

Q1.00143 Effect of Carbon Nanotubes on Thermal Behavior of Poly(L-lactide) and Poly(D-lactide) Electrospun Fibers1 , YAZHE ZHU, MAO BIN, PEGGY CEBE, Tufts University — Thermal properties and crystallization behavior of electrospun polymer composites fibers of poly (L-lactide) (PLLA) and poly (D-lactide) (PDLLA) blended with a small amount of carbon nanotubes (0.1-4 wt%) were systemically studied by differential scanning calorimetry, wide- and small- angle X-ray scattering , and time-resolved Fourier transform infrared spectroscopy. The disordered α′-form crystal and the more stable α-form crystal in polymer composites are produced respectively at low and high crystallization temperatures (Tc). It was found that the α′- to α-crystalline phase transition occurs prior to the dominant melting in both polymer composites PLLA and PDLLA crystallized at low Tc. We compare the effect of carbon nanotubes on this transition for neat and filled samples. Moreover on increasing the content of CNTs from 0.1 to 4 wt%, the induction period for crystallization was shortened and the polymer composites' crystallization rate was enhanced. The α′- to α-crystalline phase transition of PLLA and PDLLA was better accelerated at low Tc from 80°C to 120°C. With increasing Tc, CNTs have smaller influence on the transition.

1 The authors kindly acknowledge National Science Foundation for financial support through DMR-1260610 and MRI Program under DMR-0520655 for thermal analysis instrumentation. X-ray related work was conducted at the Brookhaven National Laboratory.

Q1.00144 The investigation of the viscoelastic properties of silica/PMMA nanocomposites as a function of silica surface chemistry1 , HEATHER CONWAY, DENIZ RENDE, RAHMI OZISIK, Rensselaer Polytechnic Institute — Poly(methyl methacrylate), PMMA, has been used as an economic alternative to glass and polycarbonate in differing situations because of its lightweight, shatter resistance, and ease of processability. The uses of PMMA can be expanded if its weakness to impact force and its scratch resistance are improved. In the current study, viscoelastic properties of silica nanoparticles filled PMMA were investigated via nanindentation experiments. Silica nanoparticles are known to increase the toughness of PMMA. In the current study, silica nanoparticles were chemically modified with fluorinated alkanes to alter nanofiller-polymer interactions. Results show that viscoelastic properties are strongly affected by silica surface chemistry and silica concentration.

1 This work was partially supported by NSF CMMI-1200270 and DUE-1003574

Q1.00145 Responsive metal/polymer nanocomposites via photothermal effect1 , MERVE SEYHAN, Rensselaer Polytechnic Institute and Yeditepe University, DENIZ RENDE, LI PING HUANG, Rensselaer Polytechnic Institute, SEYDA MALTA, Yeditepe University, RAHMI OZISIK, NIHAT BAYSAL, Rensselaer Polytechnic Institute — Metal nanoparticles can efficiently generate heat when exposed to electromagnetic radiation. The amount of heat generated and the temperature increase depends on the number of nanoparticles and their shape. In the current work, gold nanoparticles (AuNPs) were used as heat sources within polyethylene oxide (600,000 g/mol) via the photothermal effect. AuNPs were synthesized through Frens method, and were characterized using TEM. A laser source with a wavelength of 532 nm was used to heat AuNPs. Raman spectroscopy data showed that irradiation of AuNPs led to increasing temperature profiles in the vicinity of AuNPs, which is a result of the surface plasmon resonance. This property of AuNPs would enable the control of viscoelastic response of the polymer by altering crystallinity and temperature of the polymer matrix, thereby, providing responsive materials.

1 This work is partially supported by NSF CMMI-1200270 and DUE-1003574. MS was supported by TUBITAK 2214 grant. NB was supported by TUBITAK 2219 grant.

Q1.00146 Simulation of heat transport in polymer nanocomposites , NING SUN, MIRIAM RAFIALOVICH, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University, NY, 11794 — The design of fire-safe materials by using flame retardants within polymers requires a fundamental understanding of the physics and dynamics of the heat transport process within the multiphase systems. We have developed a Lattice-Boltzmann model to simulate the 3-D heat transfer in a two-component system comprised of a polymer matrix and flame retardant nanocomposite fillers. By varying the volume fraction of the fillers, we compared the heat propagation phenomena before and after the percolation of the nano-fillers in the system. We also vary the size, shape, thermal conductivity and heat capacity of the nanofiller to study their effects on the heat dissipation and the time to ignition.

Q1.00147 Modified thiol-ene networks: Tuning the glass transition temperature and energy damping capabilities , DANIEL SAVIN, OLIVIA MCNAIR, DAVIS BRENT, The University of Southern Mississippi — Utilizing thiol-ene ‘click’ reactions, it is possible to produce thermoset networks that are highly homogeneous and thus exhibit enhanced energy damping capabilities. This talk will present recent results in the characterization and impact testing of modified thiol-ene networks with tunable physical properties. In particular, we synthesize ternary networks containing (1) bulky side-chain substituents, (2) isocyanate functionality, or (3) dual thiol components to improve control over the glass transition temperature and strain at break. In addition, we present results in the high-impact compression testing to demonstrate the energy damping capabilities of these materials.
Q1.00148 ABSTRACT WITHDRAWN

Q1.00149 ABSTRACT WITHDRAWN

Q1.00150 ABSTRACT WITHDRAWN

Q1.00151 ABSTRACT WITHDRAWN

Q1.00152 Solid State Charge Transport in Radical Polymers, LIZBeth ROSTo, BRYAN BOUDOURIS, School of Chemical Engineering, Purdue University — Organic electronic devices based on π-conjugated polymers have attracted increasing attention over the past decades; however, many important synthetic and structural issues (e.g., uncontrolled polymerization schemes, the presence of residual metal catalysts) currently stymie the ability of these materials to replace traditional inorganic electronic materials. Here, we present the controlled and impurity-free synthesis of a fundamentally new type of charge-conducting polymer in which a pendant stable radical group on each repeat unit allows for charge transport (i.e., radical polymers). Specifically, these molecules were synthesized using controlled radical polymerization techniques such that well-defined and easily tunable molecular weights and narrow molecular weight distributions could be had without the use of metal-based catalysts. Additionally, for the first time, we systematically characterize the charge transport ability of radical polymers and the effect of molecular weight on the transport properties of a model radical polymer, poly(2,2,6,6-tetramethylpiperidinyl)oxymethacrylate). Furthermore, we have utilized temperature-dependent transport measurements in order to suggest a mechanism for carrier transport in this emerging class of optoelectronically-active polymers.

Q1.00153 Microstructure and conductivity of in-situ polymerized poly(3,4-ethylenedioxythiophiophene) (PEDOT) crystals
d. JINGLIN LIU, LIANGQI OUYANG, Materials Science and Engineering, The University of Delaware, JINGHANG WU, Materials Science and Engineering, The University of Delaware; Macromolecular Science and Engineering Center, The University of Michigan, CHIN-CHEN Kuo, BIn WEL, DAVID MARTIN, Materials Science and Engineering, The University of Delaware — Conjugated polymers are widely used in organic solar cells, biomedical devices, and chemical sensors. Both chemical and electrochemical methods have been developed for preparing conducting polymers, but the extent of crystalline order is usually modest. Here we synthesized highly-ordered brominated (3,4-ethylenedioxythiophene) (EDOT-Br) monomer crystals via electrochemical methods. The kinetics of the synthesis was studied with a Quartz Crystal Microbalance (QCM) and Cyclic Voltammetry (CV). The chemical structure of the EDOT-Br monomer has been confirmed by Nuclear Magnetic Resonance (NMR), Ultraviolet-Visible Spectroscopy (UV-Vis), Fourier Transform Infrared Spectroscopy (FTIR), and Mass Spectrometry (MS). The EDOT-Br monomer crystals can be in-situ polymerized into highly ordered PEDOT conjugated polymer crystals by annealing at temperatures below the EDOT-Br melting point. The crystalline structure was studied by optical microscopy, electron microscopy and X-Ray analysis. The conductivity and electrochemical properties of both the EDOT-Br monomer and corresponding PEDOT polymer crystals were examined with electrochemical impedance spectroscopy (EIS) and CV.

Q1.00154 Adaptive lenses using transparent dielectric elastomer actuators, SAMUEL SHIAN, ROGER DíEBÖLD, DAVID CLARKE, School of Engineering and Applied Sciences, Harvard University — Variable focal lenses, used in a vast number of applications such as endoscope, digital camera, binoculars, information storage, communication, and machine vision, are traditionally constructed as a lens system consisting of solid lenses and actuating mechanisms. However, such lens system is complex, bulky, inefficient, and costly. Each of these shortcomings can be addressed using an adaptive lens that performs as a lens system. In this presentation, we will show how we push the boundary of adaptive lens technology through the use of a transparent electroactive polymer actuator that is integral to the optics. Detail of our concepts and lens construction will be described as well as electromechanical and optical performances. Preliminary data indicate that our adaptive lens prototype is capable of varying its focus by more than 100%, which is higher than that of human eyes. Furthermore, we will show how our approach can be used to achieve certain controls over the lens characteristics such as adaptive aberration and optical axis, which are difficult or impossible to achieve in other adaptive lens configurations.

Q1.00155 Nanostructure and Dynamics of Ionic and Non-Ionic PEO-Containing Polyureas, SUNANTA CHUAYPRAKONG, JAMES RUNT, Penn State University — A series of polyethylene oxide (PEO) - based diamines with molecular weights ranging from 250 – 6000 g/mol were polymerized in solution with 4,4’-methylene diphenyl diisocyanate (MDI). In addition, PEO soft segment diamines where modified to incorporate ionomeric species and also polymerized with MDI. The role of PEO soft segment molecular weight and the presence of ionic species on nanoscale segregation and cation conductivity were explored. The former was investigated using small-angle X-ray scattering and atomic force microscopy. Dielectric relaxation spectroscopy was used to investigate polymer and ion dynamics. Local environment and hydrogen bonding were identified by using FTIR spectroscopy.

Q1.00156 Phase Behavior and Conductivity of Block Copolymers Containing Heterocyclic Diazole-Based Ionic Liquids, ONNURI KIM, MOON JEONG PARK, POSTECH — Recently, Ionic liquids(ILs) integrated polymer electrolyte membranes(PEMs) is becoming important ingredients of diverse applications such as high temperature PEM fuel cells. In present study, we explored morphology and conductivity of sulfonated PEMs upon incorporating ILs. Instead of the use of quaternary alkyl-imidazole based ILs, we employed a set of Brønstead heterocyclic diazole-based ILs possessing protic sites in cation of ILs. A wide variety of self-assembled morphologies, i.e. lamellar, hexagonal cylinder, and gyroid, have been uncovered for the IL embedded PEMs depending on kinds of heterocyclic diazoles. It is worthwhile to note that the ring structures and alkyl substituents in diazoles are found out to play important role in determining the morphology upon manipulating the Flory-Huggins interaction parameters of block copolymers. Heating of ILs-containing PEMs results in thermo-reversible phase transitions. This leads us to investigate the morphological effects of ILs incorporated PEMs on conductivities where the data demonstrate that gyroid morphology is certainly beneficial in obtaining enhanced conductivity values. Our results showed that both molecular design of ILs and structural optimization are crucial for the achievement of the utmost ionic transport properties.

1 This work was supported by NSF, DMR- 1103027.
Q1.00157 Explicit Solvent Simulations of Friction between Brush Layers of Charged and Neutral Bottle-Brush Macromolecules1, J.-M.Y. CARRILLO, University of Connecticut, W.M. BROWN, Oak Ridge National Laboratories, A.V. DOBRYNIN, University of Connecticut — We study friction between charged and neutral brush layers of bottle-brush macromolecules using molecular dynamics simulations. The deformation of the bottle-brush macromolecules under the shear were studied as a function of the substrate separation and shear stress. For charged bottle-brush layers we study effect of the added salt on the brush lubricating properties to elucidate factors responsible for energy dissipation in charged and neutral brush systems. Our simulations have shown that for both charged and neutral brush systems the main deformation mode of the bottle-brush macromolecule is associated with the backbone deformation. This deformation mode manifests itself in the backbone deformation ratio, \( \alpha \), and shear viscosity, \( \eta_s \), to be universal functions of the Weissenberg number \( W \). The value of the friction coefficient, \( \mu \), and viscosity, \( \eta_s \), are larger for the charged bottle-brush coatings in comparison with those for neutral brushes at the same separation distance, \( D \), between substrates. The additional energy dissipation generated by brush sliding in charged bottle-brush systems is due to electrostatic coupling between bottle-brush and counterion motion. This coupling weakens as salt concentration, \( c_s \), increases resulting in values of the viscosity, \( \eta_s \), and friction coefficient, \( \mu \), approaching corresponding values obtained for neutral brush systems.

1 NSF DMR-1004576

Q1.00158 Influence of Ion Content, Cation Size and Polymerization Method on Ion Association States of Poly(ethylene oxide)-based Ionomers, HANQING MASSER, JING-HAN HELEN WANG, RALPH COLBY, PAUL PAINTER, JAMES RUNT, Penn State University — The effects of ion content, cation size and polymerization method on ion association states are systematically studied using FTIR spectroscopy in a series of ionomers with short ethylene oxide and ionic sulfonated styrene side chains. Ion content is controlled by the ratio of these side chains. When comparing similar ionomers with different ion content, there are more free ions at higher ion content. Free radical and RAFT polymerizations yield ionomers with different molecular weights, polydispersity and ionic side chain distributions. FTIR spectroscopy demonstrates that the ionomers synthesized via free radical polymerization have more free ions compared to their RAFT analogs. The ionomers with larger cations, such as tetramethylammonium, have higher free ion contents. Information on ion association states is then related to ion conductivity and crystallinity characterized by dielectric relaxation spectroscopy and wide angle X-ray scattering, respectively.

Q1.00159 Melt State Morphology Evolution in Precise Acid Copolymers as a Function of Strain1, LURI MIDDLETON, University of Pennsylvania, JOSEPH CORDARO, Sanida National Laboratories, KAREN WINEY, University of Pennsylvania — Acid- and ion-containing polymers have specific interactions that produce complex and hierarchical morphologies that provide a remarkable combination of mechanical properties. Historically, correlating the hierarchical structure and the mechanical properties of these polymers has been challenging because (1) the polymers have random arrangements of the acid or ionic groups along the backbone and (2) structural characterization is typically performed ex situ relative to mechanical testing. We addresses both of these challenges through in situ deformation of PRECISE acid copolymers. PRECISE acid copolymers were synthesized by from well-defined macromonomers via acyclic diene metathesis (ADMET). The precision of the molecular structure imposes uniformity in the polymer morphologies through precise separation between acid groups leading to better defined lamellae thickness and well-defined interaggregate spacings. Here, we report the first results from simultaneous synchrotron X-ray scattering and melt state uniaxial extensional flow of precise acid copolymers. These in situ studies will be discussed alongside ex situ studies of the mechanical properties.

1 Acknowledgements: Erica McCready and Dr. Wesley Burghardt at Northwestern University. Sunsgik Lee and Benjamin Reinhart at Argonne National Laboratories

Q1.00160 Polysiloxane-graft-PEG/Phosphonium Ionomer Morphology and Ion Transport, MICHAEL O’REILLY, University of Pennsylvania, SIWEI LIANG, JOSHUA BARTELS, JAMES RUNT, RALPH COLBY, Pennsylvania State University, KAREN WINEY, University of Pennsylvania — A series of random polysiloxane-based copolymer single ion conductors with phosphonium and polyethylene glycol side chains have been synthesized at various compositions and counterions. Morphology is investigated via X-ray scattering, and reveals microphase separation on extremely small length scales. Despite the low molecular weight of the PEG side chain, polysiloxane and PEG assemble into microdomains with covalently bound phosphonium cations at the interface. Exceptionally low glass transition temperatures in these microphase separated ionomers allow for high ionic mobility for both bulky, charge delocalized counterions as well as small, electronegative counterions. Morphology interpretation is complemented by measurement of ion transport properties via dielectric relaxation spectroscopy.

Q1.00161 Li+ transport in poly(ethylene oxide) based electrolyte: A combined study of neutron scattering, dielectric spectroscopy, and MD simulation, CHANGWOO DO, Oak Ridge National Laboratory, PETER LUNKENHEIMER, Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany, DIDDO DIEDENS, Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany, MARION GÖTZ, MATTHIAS WIEß, ALOIS LOIDL, Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany, XIAO-GUANG SUN, Oak Ridge National Laboratory, JÜRGEN ALLGAIER, MICHAEL OHL, Jülich Centre for Neutron Science, Forschungszentrum Jülich, 52425 Jülich, Germany — Dynamics of Li+ transport in polyethylene oxide (PEO) and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) mixtures are investigated by combining various experimental techniques [neutron spin-echo and dielectric spectroscopy] with molecular dynamics (MD) simulations. Our results suggest that the characteristic live times within the cages formed by oxygens are mainly determined by the alpha-relaxation which corresponds to local segmental motions of polymers, to a large extent, by the beta-relaxation which is associated with local motions of the ion pairs, to a small extent, and by the alpha-relaxation which is associated with the backbone motions. The characteristic alpha-relaxation is then determined by the characteristic alpha-relaxation of the solvent, which is associated with the backbone motions of the polymer, and by the characteristic alpha-relaxation of the ion pairs, which is associated with the motions of the ions and their solvation shells.

Q1.00162 Nonlinear Elasticity of Biological and Polymeric Networks and Gels1, A.J. OYER, J.-M.Y. CARRILLO, A.V. DOBRYNIN, University of Connecticut, F.C. MACKINTOSH, Vrije Universiteit — Biological and polymeric networks show remarkably high deformability at relatively small stresses and can sustain reversible deformations up to ten times of their initial size. Using theoretical analysis and molecular dynamics simulations we propose and test a theory that describes nonlinear mechanical properties of a broad variety of biological and polymeric networks and gels by relating their macroscopic strain-hardening behavior with molecular parameters of the network strands. This theory provides a universal relationship between the strain-dependent network modulus and the network deformation as a function of the first invariant, \( I_1 \), of the network deformation matrix. Our analysis shows that depending on the rigidity of the polymeric strands between cross-links there are two different nonlinear network deformation regimes. Networks made of polymer chains with bending constant \( K > 1 \) behave as polymeric network made of a worm-like chains in the interval of network deformations \( \frac{\Delta L}{L} < 1 - (K^2 + 2)^{-1/2} \) and as networks made of freely-jointed chains for \( \frac{\Delta L}{L} > 1 - (K^2 + 2)^{1/2} \). Here, \( I_1 \) is a strand extensibility ratio of the mean-square value of the undeformed strand size, \( \langle R_s^2 \rangle \), to the square of the fully extended strand size, \( \langle R_{max}^2 \rangle \). However, networks made of flexible chains with \( K < 1 \) have only one nonlinear deformation regime.

1 NSF DMR-1004576
Q1.00163 Mechanical similarities observed between polypropylene gels and molten polypropylenes, TETSU OUCHI, MISUZU YAMAZAKI, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — The gelation of syndiotactic and isotactic polypropylenes (sPP and iPP) was found when PPs were dissolved in 1,2,4,5-tetraphenylbenzene (tetralin). Interestingly, it was found that the storage modulus of sPP-gel became higher than that of iPP-gel when PPs were dissolved in tetralin at low PP concentration (<40 wt%). The result was distinctly different from the result of the neat PPs without solvent, as it is widely known that the modulus of sPP is significantly lower than that of iPP. Moreover, by measuring the storage moduli of solid sPP and iPP as a function of temperature, it was found that, above the melting points of PP, the storage modulus of PP became higher than that of iPP, which was similar to the behavior of the storage modulus observed in the dilute PP-gels. Such mechanical similarity between PP-gels and PP-melts was also observed within iPP samples with different molecular weights. From these experimental results, it was considered that the amorphous phase of PP had profound influence on the mechanical properties of PP-gels at low PP concentration (<40 wt%), while the crystalline phase of PP had a major impact on the mechanical properties of PP-gels at relatively higher PP concentration (>40 wt%).

Q1.00164 Dynamics of Surface Reorganization of Poly(methyl methacrylate) in Contact with Water, AYANOBU HORINOUCHI, Department of Applied Chemistry and International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, HIRONORI ATARASHI, YOSHIHISA FUJI, KEIJI TANAKA, Department of Applied Chemistry, Kyushu University — New tools for tailor-made diagnostics, such as DNA arrays and tips for micro-total-analysis systems, are generally made from polymers. In these applications, the polymer surface is in contact with a water phase. However, despite the importance of detailed knowledge of the fundamental interactions of polymer interfaces with liquids, such studies are very limited. As an initial benchmark for designing and constructing specialized biomedical surfaces containing polymer, aggregate states and dynamics of chains at the water interface should be systematically examined. We here apply time-resolved contact angle measurement to study the dynamics of the surface reorganization of poly(methyl methacrylate) (PMMA) in contact with water. By doing the measurements at various temperatures, it is possible to discuss the surface dynamics of PMMA based on the apparent activation energy. Also, sum-frequency generation spectroscopy revealed that the surface reorganization involves the conformational changes in the main chain part as well as the side chains. Hence, the dynamics observed here may reflect the segmental motion at the outermost region of the PMMA film, in which water plays as a plasticizer.

Q1.00165 Observation of Birefringence of an Electrosprinning Jet in Flight, KAIYI LIU, DARRELL RENEKER, The University of Akron — Solutions of polystyrene in N,N-dimethylformamide, polyacrylonitrile in N,N-dimethylformamide, and polyethylene oxide in water were electrospun. The charged liquid jets in flight were illuminated with polarized light converged on the jets by a Fresnel lens with a black background at the center, and were observed using a high speed camera, coaxial with the Fresnel lens, behind an analyzer which was crossed with a polarizer in front of the light source. The first several turns of coiled jet after the onset of electrical bending instability showed birefringence for all solutions, while no obvious birefringence was observed in the straight segments of the jets. This indicated that molecular chains in the coiled jet were aligned under elongation to a higher extent than those in the thicker straight jet.

Q1.00166 Explicit Proof of the Tube Concept in Polymer Dynamics, MAX KOLB, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, F-6936 Lyon, France, MONIQUE A.V. AXELOS, Biopolymères, Interactions, Assemblages, INRA, F-44300 Nantes, France — The key to the understanding of the dynamics of strongly entangled polymers is the tube concept and the reptation theory. For the lack of a mathematically unambiguous definition these concepts have been supported mostly by indirect evidence, such as crossover phenomena in various time correlation functions. Here we formulate the tube in a mathematically precise way and use this definition to explicitly calculate the predicted properties of reptation tube. Dynamic Monte Carlo simulations show that for strongly entangled polymers the tube does exist with the expected properties, most notably with a finite tube width. At the same time, slower than predicted early time Rouse dynamics and unexpectedly fast disentanglement effects due to finite chain lengths are responsible that the reptation limit can only be seen clearly for polymers whose contour length well exceeds one hundred tube widths. This is an explanation for the generally observed deviations from the asymptotic scaling predictions, both in experiments and in simulations. Effects such as dynamic tube shortening and tube dilution can be explicitly monitored in the present approach.

Q1.00167 Anisotropy Analysis of Polymer Chains upon Uniaxial Extension, HOWARD WANG, Institute for Material Research, State University of New York, Binghamton, HAO SUN, SHI-QING WANG, Department of Polymer Science, University of Akron, YANG-YANG WANG, Department of Chemistry, University of Tennessee, Knoxville — Small angle neutron scattering has been used to measure entangled chains in polymer melts upon uniaxial stretching. The scattering anisotropy strongly depends on neutron moment transfer vector, revealing chain relaxation at different length scales. Such analysis allows for the comparison of various model predictions.

Q1.00168 Structure and Dynamics of Polymer/Ionic Liquid Systems Studied by In-Situ Electron Microscopy, PAUL KIM, THOMAS RUSSELL, DAVID HOAGLAND, Polymer Science and Engineering Department, University of Massachusetts — Ionic liquids (ILs) have extremely low vapor pressures and high conductivities, which taken together, make many IL-soft matter systems suitable for investigating by electron microscopy. Polymer crystallization in ultrathin film has attracted increasing attention as it provides (i) new clues on the nature of polymer crystallization and (ii) opportunity for enhancing the performance of polymer thin film devices. Exploiting ILs as crystallizing solvents, the evolving morphologies of several semi-crystalline polymers were investigated in-situ by optical microscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). To understand polymer dynamics in ILs, nanoparticles dispersed in ILs were investigated as model dynamical systems. Spatial and temporal imaging information affords insight into polymer-IL interactions.

Q1.00169 Crystallization Control in Crystalline-Crystalline PEO-b-PCL Diblock Copolymers, RYAN M. VAN HORN, ELLIOTT HASENKOPF, CHRISTINA MUCCI, Allegheny College — Understanding the crystallization behavior of crystalline-crystalline (CC) diblock copolymers is crucial in tailoring their macroscopic properties. The order of crystallization and structure of the phase-separated CC material is dependent on many factors including, but not limited to, the concentration of the individual blocks, $T_C$, $T_m$, $M_0$, and domain size. PEO-b-PCL copolymers are unique in that their $T_c$ values are similar. As such, manipulation of the crystallization sequence or overall crystallinity of each block is more difficult. Using DSC and FTIR analysis, work has been done to observe the effects of thermal history and solvent interactions on the crystallization of PEO-b-PCL copolymers with differing $M_0$ ratios. Preliminary results indicate that the mechanism, crystallinity, and eventually macroscopic properties may be tuned using different crystallization conditions.

Q1.00170 SAXS/WAXS studies of flow-induced crystallization of poly(1-butene) in uniaxial extensional flow, ERICA MCCREADY, WESLEY BURGHARDT, Northwestern University — We report studies of flow-induced crystallization of poly(1-butene) in uniaxial extensional flow. Flow was produced using an SER extensional flow fixture housed in a custom built convection oven designed to provide x-ray access for in situ studies of polymer structure using synchrotron x-ray scattering techniques. Samples were loaded into the SER fixture, heated well into the melt, and then cooled to a temperature at which quiescent crystallization would be prohibitively slow. A short interval of uniaxial extensional flow was then applied, after which simultaneous wide- and small-angle x-ray scattering (SAXS and WAXS) patterns were collected to study the phase transformation kinetics and morphology of the subsequent accelerated crystallization. The impact of both deformation rate and total applied strain on the crystallization process were examined.
Q1.00171 SAXS/WAXS studies of flow-induced crystallization of poly(1-butene) in shear flow, BINBIN LUO, WESLEY BURCHARDT, Northwestern University — Flow-induced crystallization of poly(1-butene) was studied in shear flow. Flow was produced using a Linkam shear cell that has been modified to allow x-ray access for in situ studies of polymer structure using synchrotron x-ray scattering techniques. After loading in the shear cell samples were first heated well into the melt, and then cooled to a crystallization temperature selected such that negligible quiescent crystallization would occur on reasonable time scales. A short burst of shear flow was then applied at various rates, after which simultaneous wide-angle and small-angle x-ray scattering (SAXS and WAXS) data were collected to study the resulting accelerated crystallization kinetics, as well as the morphology of the resulting crystallites (e.g., degree of crystallite orientation). The impact of both deformation rate and total applied strain on the crystallization process were examined.

Q1.00172 Statistics of single molecule rotation driven by electrons, CHARLES SYKES, Tufts University — In stark contrast to nature, current manmade devices, with the exception of liquid crystals, make no use of nanoscale molecular motion. In order for molecules to be used as components in molecular machines, methods are required to couple individual molecules to external energy sources and to selectively excite motion in a given direction. Recently a new, stable and robust system of molecular rotors consisting of thioether molecules bound to metal surfaces has offered a method with which to study the rotation of individual molecules as a function of temperature, molecular chemistry, proximity of neighboring molecules, and surface structure [1, 2]. Arrehnius plots for the rotation of dibutyl sulfide yielded a rotational barrier of 1.2 kJ per mol. While these results reveal that small amounts of thermal energy are capable of inducing rotation, thermodynamics dictates that thermal energy alone cannot be used to perform useful work in the absence of a temperature gradient. Electrical excitation of individual thioether molecular rotors is performed using with electrons from a scanning tunneling microscope tip. Experimental data for the electrically excited motion of asymmetric thioether molecules is presented and the statistics of and mechanism for directed motion is discussed [1, 2].


Q1.00173 Active contractility and motor-driven effective interactions in a model cytoskeleton, SHENSHEN WANG, Massachusetts Institute of Technology, PETER WOLYNES, Rice University — Contractile forces are essential for many developmental processes involving cell shape change and tissue deformation. Recent experiments on reconstituted actomyosin network, the major component of the contractile machinery, have shown that active contractility occurs above a threshold motor concentration and within a window of cross-link concentration. We present a microscopic dynamic model that incorporates two essential aspects of actomyosin self-organization: the asymmetric load response of individual actin filaments and the correlated motor-driven events mimicking myosin-induced filament sliding. Using computer simulations, we examine how the concentration and susceptibility of motors contribute to their collective behavior and interplay with the network connectivity to regulate macroscopic contractility. Our model is shown to capture the formation and dynamics of contractile structures and agree with the observed dependence of active contractility on microscopic parameters. We further provide a theoretical framework to investigate the intricate interplay between local force generation, network connectivity and collective action of molecular motors. This framework is capable of accommodating both regular and heterogeneous pattern formation, arrested coarsening and macroscopic contraction in a unified manner.

1 This work is supported by NSF via Grant PHY-0822283 and the Bullard-Welch Chair at Rice University.

Q1.00174 Generalized formulation of Brownian Vortices, HENRIQUE W. MOYES, ROSS BAUER, DAVID G. GRIER, Department of Physics and Center for Soft Matter Research, New York University — Brownian vortices are stochastic noise driven machines that arise from the motion of particles subjected to static non conservative force fields. This motion is characterized by a toroidal circulation in the probability flux whose direction can be tuned by changing the temperature of the system. A discrete minimal model for Brownian Vortices were described by previous work done by B. Sun, D. G. Grier and A. Y. Grosberg. Here we theoretically look for a continuous model in the form of a generalization of the equilibrium Boltzmann relation for the probability density in the case where the driven forces have a non conservative solenoidal component. This generalized relation features the temperature induced probability flux reversal. We further extend our theory to time dependent force fields and study the possibility of stochastic resonance in the characteristic frequency of circulation of the driven particle. This model is experimentally applied to investigate the motion of colloidal spheres in an optical trap whose intensity is oscillatory in time.

Q1.00175 Electric control interfacial jamming and dynamics, MENGMENG CUI, CAROLINE MIESCH, IREM KOSIF, HUARONG NIE, TODD EMRICK, THOMAS RUSSELL, University of Massachusetts Amherst — Particles, partially wetted by two immiscible fluids, can adsorb at the interface and interfacially jammed when the interfacial area is decreased. Here, electric fields were used to change the interfacial area by distorting or merging fluid droplets suspended in an immiscible liquid. To get the desired interfacial jamming, ligand exchange was used to enhance the binding energy of the particles at the interface. Jamming nanoparticles at the interface arrests the dynamics so as to kinetically trap morphologies in highly non-equilibrium states. Morphologies hitherto inaccessible using conventional routes were obtained by the interfacial jamming. The hyper-diffusive dynamics of interfacial jamming and its dependence on nanoparticle concentration, size and shape were observed by X-ray photo correlation spectroscopy (XPCS). Kinetics were studied by tensiometer and optical microscopy.

Q1.00176 SOFT CONDENSED MATTER —

Q1.00177 Modeling the tuning of lasing in liquid crystal based one-dimensional Photonic Crystal using the Finite Difference Time-Domain Method, PAOLA CASTRO-GARAY, Departamento de Física, Universidad de Sonora, Blvd. Luis Encina y Rosales, Hermosillo, Sonora 83180, Mexico. JESUS MANZANARES-MARTINEZ, Departamento de Investigacion en Fisica, Universidad de Sonora, Apartado Postal 5-088, Hermosillo, Sonora 83180, Mexico, YOHAN JASDID RODRIGUEZ-VIVEROS, DAMIAN MOCTEZUMA-ENRIQUEZ, Departamento de Fisica, Universidad de Sonora, Blvd. Luis Encina y Rosales, Hermosillo, Sonora 83180, Mexico. — In this work, a numerical study based on the Finite Difference Time-Domain Method is presented to determine the lasing from a finite one-dimensional Photonic Crystal composed by Porous Silicon and Liquid Crystal is proposed. As a consequence of the zero energy states in the Band Gap and the high Density of States at its edges, the emission is inhibited in the Gap and stimulated in its edges. We investigate the conditions where light emitted by a Gaussian source embedded in the Photonic Crystal can be switched into a monochromatic emission. We present the tuning of the lasing by changing the Density of States due to the tunability of the liquid crystal dielectric function.
Q1.00178 On the variation of Differential Polarizability in polarized Raman Scattering measurements, KARTHIK NAYANI, OK PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology — Jones et al recently developed a framework to measure P2 and P4 using PRS[1]. The method requires the measurement of the angular dependence of the depolarization ratio. While the agreement of the results of P2 and P4 with theory is satisfactory there are some aspects to the methodology that need further scrutiny. The differential polarizability ratio (r) is used as a fitting parameter to the depolarization profile. The value of r so calculated from the method of Jones et al. has a sharp discontinuity at the phase transition from the nematic to the isotropic phase (TNI) and also the variation of r in the nematic phase is not well understood. Further we show that when values of r as obtained by data fitting are used in the expression of the original method of Jen et al. values of P2 and P4 are in excellent agreement with theoretical predictions, raising the premise that a better understanding of the variation of r needs to be developed more accurate experiments using PRS.


Q1.00179 Effect of protein (Myoglobin) on the isotropic to nematic phase transitions, GERMANO IANNACCHIONE, PARVATHALU KALAKONDA, JOHN ARNOLD, SHAUN MARSHALL, IZABELA STROE, Worcester Polytechnic Institute — High-resolution calorimetry and broad-band dielectric spectroscopy have been performed on colloidal dispersions of myoglobin protein in a nematic liquid crystal as a function of protein content. The myoglobin protein was uniformly dispersed in the dry state in pentaerythritol (5CB) liquid crystal with weight fraction from 0 to 100 wt%, and cover the temperature range of 180 to 420 K under near equilibrium conditions. Such colloidal systems may be attractive to isolate the behavior of the protein as it interacts with the desired liquid crystal property as well as probing the effect of functional/active nano-particles on LC behavior.

Q1.00180 Elastic constants and material properties of novel shaped liquid crystals, M. SCHMITTHENNER, The College of Wooster, Wooster OH 44691, P.K. CHALLA, J.T. GLEESON, Kent State University, Kent OH 44240, SHILA GARG, The College of Wooster, Wooster OH 44691 — We studied the entanglement and relaxation of V-shaped, U-shaped, and rod-shaped granular media. Our experiment was modeled after Gravish et al.’s work [1]. A clear understanding on how these particles interact with each other on a macroscopic scale can help us model how microscopic liquid crystal molecules with similar shapes behave. In order to entangle the granular media, the particles were subjected to a sinusoidal acceleration within a confined cylinder. Once entangled the cylinder was removed to leave a freestanding column, which was then accelerated at various ‘g forces’ to entangle and cause a collapse. Video recordings of the experiment were used to analyze the dynamics of packing and collapse. The U-shaped granular media took a longer time to relax in comparison with the rod-shaped and V-shaped granular media. We conclude that this is because the U-shaped granular media had 90◦ angles, which allowed the particles to latch on to each other better than the rod-shaped and the V-shaped particles. [1] N. Gravish, S. Franklin, D. Hu, D. Goldman, Phys. Rev. Lett., 108, 208001 (2012).

1This work was supported by NSF DMR 0964765.

Q1.00181 Entanglement and Relaxation of Liquid Crystal Shaped Granular Media1, THERESA ALBON, The College of Wooster, Wooster OH 44691, WILDER IGLESIAS, ANTAI JAKLI, Kent State University, Kent OH 44240, SHILA GARG, The College of Wooster, Wooster OH 44691 — We studied the entanglement and relaxation of V-shaped, U-shaped, and rod-shaped granular media. Our experiment was modeled after Gravish et al.’s work [1]. A clear understanding on how these particles interact with each other on a macroscopic scale can help us model how microscopic liquid crystal molecules with similar shapes behave. In order to entangle the granular media, the particles were subjected to a sinusoidal acceleration within a confined cylinder. Once entangled the cylinder was removed to leave a freestanding column, which was then accelerated at various ‘g forces’ to entangle and cause a collapse. Video recordings of the experiment were used to analyze the dynamics of packing and collapse. The U-shaped granular media took a longer time to relax in comparison with the rod-shaped and V-shaped granular media. We conclude that this is because the U-shaped granular media had 90◦ angles, which allowed the particles to latch on to each other better than the rod-shaped and the V-shaped particles. [1] N. Gravish, S. Franklin, D. Hu, D. Goldman, Phys. Rev. Lett., 108, 208001 (2012).

1This work was supported by NSF DMR 0964765.

Q1.00182 Optical Investigation of Novel Liquid Crystals, CHRISTOPHER WECKERLY, CHANDRA PRAYAGA, AARON WADE, University of West Florida, Physics Department — We present our research on the optical investigation of the phase transitions of novel, optically active liquid crystals (LC’s) fabricated at the UWF Chemistry Department. As liquid crystals transition from the isotropic to the nematic to the smectic phases, they have different levels of alignment. This results in a change in the fluorescence spectra and transmitted optical properties as a function of temperature. Sample preparation consists of spin coating the LC, forming an optical cell. The sample is then exposed to a laser beam and the fluorescence is measured with a spectrograph. Simultaneously, the transmission is measured with a photodiode. The results show significant changes in the fluorescence and transmitted optical properties as a function of temperature.

Q1.00183 Novel chiral dopants: Light and environmental sensitivity, SETH BOURG, SHANNON ROSARIO, PETR SHIBAEV, Fordham University, Department of Physics — The effectiveness of novel chiral dopants based on compounds able to form hydrogen bonds is studied for the compounds themselves, their hydrogen-bonded associates with non-chiral light sensitive molecules and with other chiral dopants. The effect of association is discussed in terms of the chemical structure and the shape of the substitute. Light irradiation of chiral hydrogen-bonded associates based on light sensitive azo-derivatives leads to changes of twisting power of the latter. This change is compared to that produced by chemical bonding between chiral dopants and associates. The behavior of chiral dopants in different liquid crystalline matrices is studied, and the response of liquid crystals to environmental changes, manifested not only in changes of helical pitch [1] but also in structural changes, is discussed.

Q1.00185 Vesicles sensing using resistive-pulse method\textsuperscript{1} \ 1YAUHENI RUDZEVICh, YUQING LIN, LEE CHOW, University of Central Florida — Here we present a “resistive-pulse” method that allows translocations, counting and measuring size distribution liposomes with radii from 25 nm to 125 nm. This technique is based on using two chambers filled with electrolyte solution and separated by a partition with a nanopore between electrodes. It was found that ionic current drops when nanoparticle entering sensing nanopore of a pulled glass micropipette, producing a clear translocation signal. Pulled borosilicate micropipette with opening 50 – 150 nm was used as a sensing instrument. This method provides a direct, fast and inexpensive way to characterize inorganic and organic nanoparticles in a solution.

\textsuperscript{1}LC acknowledges the financial support of National Science Foundation through Grant ECCS 0901361.

Q1.00186 Different Transition Mechanisms and Tunable Wall Thicknesses of Block Copolymer Vesicles \ 1MENGYING XIAO, RONG WANG, DAIQIAN XIE, School of Chemistry and Chemical Engineering, Nanjing University — By using dissipative particle dynamics, we studied how to control the two pathways for vesicle-formation mechanism considering the hydrophobic/hydrophilic block ratio, polymer-solvent interaction, and polymer concentration. A crucial balance between the segregation of inner-hydrophobic beads and the attraction of outer-hydrophilic beads drastically affects the self-assembly pathways of amphiphilic block copolymer into vesicles from one mechanism over the other. And during the transition period between these two pathways, vesicles are formed through an in-between pathway. In addition, we have evaluated the thickness of the hydrophobic layer and observed two types of dependence on the vesicle size. Our results indicate that as the degree of hydrophobicity of the blocks increases, from the whole strong behavior to the whole weak behavior relationship, the transformation is observed in large sized vesicles first and then in small sized vesicles. Two characteristics, the chain compaction of the vesicles and the area densities of inner corona, are thought to be important in controlling the membrane thickness. Acknowledgments. This work has been supported by NNSFC (Nos. 20874046, 21074053 and 21133006) and NBRPC (No. 2010CB923303).

Q1.00187 Hyper-branched Structures via Flow Coating \ 1YUJE LIU, DONG YUN LEE, University of Massachusetts-Amherst, CÉCILE MONTEUX, CNRS-ESPCI-Université Pierre et Marie Curie, ESPCI, ALFRED J. CROSBY, University of Massachusetts-Amherst — Evaporative self-assembly has been shown to be a scalable method for organizing non-volatile solutes, e.g., nanoparticles; however, the influence of substrate surface energy in this technique has not been studied extensively. In this work, we utilize an evaporative self-assembly process based upon flexible blade flow coating to fabricate organic structures on substrates that have been modified to systematically vary surface energy. We focus on the patterning of polystyrene. We observe a variety of polystyrene structures including dots, hyper-branched patterns, stripes and lines that can be deposited on substrates with a range of wetting properties. We explain the mechanism for these structural formations based on the competition between Marangoni flow, adsorption, friction and viscosity. The development of this fundamental knowledge is important for controlling hierarchical manufacturing of nanoscale objects with different surface chemistries and compositions.

Q1.00188 Synthesis of high complexity Janus particles in chemical and physical anisotropy and their assembly \ 1JONGMIN KIM, CHANG-HYUNG CHOI, SUNG-MIN KANG, CHANG-SOO LEE\textsuperscript{1}, Chungnam National University — Self-assembly has been explored as a novel strategy for making new functional materials with unique physical, chemical, and mechanical properties in various fields. To date, many assembly building blocks and techniques has been introduced from molecular to meso-scale, which rely on chemical and physical driving forces. Janus particles are considered as a favorable building block to make various structures. However, to achieve complex 3D structure in self-assembly, it still requires further complexity in particle shapes. Several techniques have been reported in literatures providing variety in shapes but, it is still difficult to make 3D shapes such convex or concave particles. Herein, we present a simple micromolding method for synthesis of complex Janus particles and its self-assembly via 2D orbital shaking. The synthetic method allows for both chemical and physical anisotropy such as the length of hydrophobic block and 3D shapes with high controllability. We also demonstrated that the shape induced by shape complexity, aspect ratio and solvent polarity which results in various assembled structures including simple dimer, linear polymer like structure, and ring like structure.

\textsuperscript{1}corresponding author

Q1.00189 Using Light to Create Nanogrids in Polymer/Nanoparticles Composites \ 1YA LIU, OLGA KUKSENOK, ANNA BALAZS, University of Pittsburgh — One of the challenges in creating high-performance polymeric nanocomposites is establishing effective routes for controlling the morphology of both the polymeric components and the nanoparticles, which impart the desirable optical, electrical and mechanical properties to the material. Using computational modeling, we design an effective method to control assembly of polymeric nanocomposites comprising nanorods and a photosensitive binary blend. We focus on scenarios where the composites can be organized into variety of nanogrids with well defined structural features. We harness spatial light illumination with the background illumination of the entire composite and secondary, higher intensity light sources that are rastered over the sample. We show that our system displays an essentially defect-free morphology, with the nanoparticles localized in the energetically favorable domains. Furthermore, we demonstrate that by controlling the length and a chemical nature of nanorods (such as their wetting properties), one can order both polymeric components and nanoparticles into variety of complex nanogrid structures. The ability to control morphology provides a means of tailoring the properties and ultimate performance of these hybrid materials.

\textsuperscript{1}The work was funded by DOE

Q1.00190 Supramolecular Assembly of Organic-Inorganic Hybrid Polyoxometalate Nanoclusters at Solid-liquid Interface \ 1NA QI, BENXIN JING, YINGXI ZHU, Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN 46556 — Polyoxometalate (POM) inorganic nanoclusters have recently emerged as building blocks for the design and synthesis of novel functional materials for broad applications ranging from catalysis to nanomedicines. Rather than taking the slow self-assembly of POMs in aqueous solutions, we have investigated the assembly of hybrid Anderson-type Mo-based POMs with organic ligands at a solid surface by Langmuir-Blodgett (LB) deposition and characterized the films by AFM, TEM, and X-ray diffraction. We have observed the formation of well-ordered monolayer or bilayer consisting of periodic arrangement of hybrid POM nanoclusters, showing a strong dependence on substrate chemistry and LB compression pressure. The controlled assembly of hybrid POM nanocluster films by LB deposition could be used as a template with stoichiometric crystalline nanostructure to the programmed assembly of novel multi-functional supramolecular complexes.

Q1.00191 Mechanical Behavior of Randomly Packed Nanoellipsoid Films \ 1DAEYEON LEE, University of Pennsylvania, LEI ZHANG, University of Pennsylvania, GANG FENG, Villanova University — We investigate the mechanical behavior of films composed of randomly packed nanoellipsoids with varying aspect ratio using nanoindentation. The packing fraction of nanoellipsoids, determined using gravimetric analysis, is found to have excellent agreement with previously reported results based on simulations. Our study shows that the volume fraction of the films rather than the aspect ratio of the particles is the primary factor that determines the modulus and hardness of nanoellipsoid films. We show, however, that the aspect ratio of the nanoellipsoids has a significant impact on the toughness and the failure mechanism of nanoellipsoid films. While short aspect ratio nanoellipsoid films develop shear bands under nanoindentation, films with high aspect ratio nanoellipsoids do not exhibit shear band formation. We will discuss the potential relevance of our results to other types of random packings such as granular materials and bulk metallic glasses.
Q1.00192 Evaporation induced ordering in polymer-colloid suspensions, ERKAN SENSES, Stevens Institute of Technology, MATTHEW BLACK, University of Maryland at College Park, THOMAS CUNNINGHAM, PINAR AKCORA, Stevens Institute of Technology — When evaporated from aqueous solutions, colloidal particles tend to deposit non-uniformly on hydrophilic substrates due to capillary flow from the center of droplet to the pinned contact line. The so called “coffee-ring” deposition has been extensively studied in polymer solutions and colloidal suspensions; however, the behavior of the mixtures of polymer-colloid suspensions under evaporation remains unexplored. The competition between the homogenous fluid phase and the depletion induced phase separation offers rich phase behavior to these three component systems over a wide range of size ratios and concentrations. In this work, we present the formation of long-range, ordered colloid-rich and polymer-rich phases with a well-defined periodicity from homogenous mixture of colloids and polymer via solvent evaporation. The kinetics of the phase separation, studied by video microscopy and Fourier transform analysis of the images obtained at different times, suggests that the early growth of the phases can be quantitatively described by spinodal decomposition kinetics. The effect of particle and polymer concentrations, polymer and particle size ratios, interparticle bridging and substrate on microscopic phase separation will be discussed.

Q1.00193 Controlling the scattering properties of thin, particle-doped coatings, WILLIAM ROGERS, MADELEINE CORBETT, Harvard SEAS, VINOTHAN MANOHARAN, Harvard SEAS and Physics — Coatings and thin films of small particles suspended in a matrix possess optical properties that are important in several industries from cosmetics and paints to polymer composites. Many of the most interesting applications require coatings that produce several bulk effects simultaneously, but it is often difficult to rationally formulate materials with these desired optical properties. Here, we focus on the specific challenge of designing a thin colloidal film that maximizes both diffuse and total hemispherical transmission. We demonstrate that these bulk optical properties follow a simple scaling with two microscopic length scales: the scattering and transport mean free paths. Using these length scales and Mie scattering calculations, we generate basic design rules that relate scattering at the single particle level to the film’s bulk optical properties. These ideas will be useful in the rational design of future optically active coatings.

Q1.00194 Local strain fields in two-dimensional colloidal crystals with bond strength disorder, MATTHEW GRATALE, YE XU, TIM STILL, ARJUN YODHI, Department of Physics and Astronomy, University of Pennsylvania — We study the local strain fields of two-dimensional colloidal crystals consisting of random distributions of hard polystyrene particles and soft microgel particles. Using standard video microscopy and particle tracking techniques, we analyze the variations of local configurations around each particle due to thermal motion. With this information we derive the best-fit affine strain tensor and the non-affinity for each particle in the sample, which allow us to study the mechanical properties of our colloidal crystals. We then observe the changes in these properties as we transition from a predominately hard-sphere crystal to predominately soft-sphere crystal, that is we explore how the mechanical properties are affected by replacing hard inter-particle bonds with soft inter-particle bonds.

Q1.00195 Structural and Dynamical Studies of Concentrated Micrometer-Sized Colloidal Suspensions, FAN ZHANG, ANDREW ALLEN, LYLE LEVINE, National Institute of Standards and Technology, JAN ILAVSKY, GABRIELLE LONG, Argonne National Laboratory — It is a well-documented challenge to quantify the dynamic behaviors of concentrated, optically opaque micrometer-sized colloidal suspensions with laser scattering techniques due to the complications introduced by multiple scattering events. In order to overcome this limit, we have developed an ultra-small angle X-ray scattering (USAXS) based X-ray photon correlation spectroscopy (XPCS) technique to probe the equilibrium dynamics of such materials. With this technique as well as USAXS, we have tracked the structural and dynamical properties of concentrated monodisperse suspensions of different sized polystyrene (PS) microspheres in glycerol. For these PS suspensions, we found their static structures display a hard-sphere like behavior. Furthermore, by analyzing the intensity autocorrelation functions, we found the inverse of the effective diffusion coefficients display a peak with respect to the scattering vector that resembles the peaks in the static structure factors, a signature of de-Gennes narrowing. We also identified evidence supporting a collective motion of the microspheres.

Q1.00196 Transient Memories in Experiments on Sheared Non-Brownian Suspensions, JOSEPH PAULSEN, SIDNEY NAGEL, University of Chicago — A novel kind of memory has been observed in simulations of cyclically sheared non-Brownian suspensions [1]. Here we report on experiments designed to see these effects in the lab. In this type of memory, a system remembers a set of shear amplitudes but forgets most of them later on, even as they are continually applied. If noise is added, the system can store all memories indefinitely. While exceedingly counterintuitive, these properties can be understood from simple considerations, and the phenomenon is expected to be generic—the same effect is seen in simulations and experiments on traveling charge-density waves [2]. We perform experiments on a non-Brownian suspension at low Reynolds number, motivated by previous work with this system [3]. In our experiments, we form multiple memories that appear to forget in the same fashion. The final and crucial point is whether the forgetting is sufficiently gradual, so that one memory erodes away as another takes over. This key point distinguishes multiple transient memories from other classes of memory, where forgetting is immediate and unforgiving.

2 S.N. Coppersmith et al., PRL 78, 3983 (1997).

Q1.00197 Extensional rheology of a two dimensional foam, NICHOLAS HAGANS, KLEBERT FEITOSA, James Madison University Department of Physics and Astronomy — We report on changes in the packing structure and flow properties of a two dimensional bubble raft of slightly polydisperse bubbles. High resolution image video is used to track the collective motion of the bubbles as the foam is subjected to an oscillatory stretching field. The foam displays both elastic and plastic behavior under varying stress, with sudden collective rearrangements occurring along slip lines separating semi-crystalline domains. Measurements of local bubble rearrangements show that the events are temporally correlated, but not spatially correlated.

Q1.00198 Formation of a quasi-two dimensional bubble pile, DANIEL SHORTS, James Madison University Student, KLEBERT FEITOSA, James Madison University Professor — We investigate the formative stages of a bubble pile at a liquid interface before the foam reaches steady-state. The pile is produced by a continuous bubbling of air into a soapy solution in a container of rectangular cross section. We find that above a critical flow rate, the bubbling produces a crater at the interface whose diameter is proportional to the flow rate. Extending from the borders of the crater, we observe a gentle slope at the water-foam interface whose angle with the horizontal is weakly dependent on the flow rate. As the pile is formed, the slope above the interface develops a dome-like profile that grows in diameter until it reaches the boundaries of the container. We show that the slope and the foam profile are a result of an isotropic pressure exerted by the arriving bubbles at the interface.
Q1.00199 Creating Reconfigurable Materials Using "Colonies" of Oscillating Polymer Gels. DEBABRATA DEB, University of Pittsburgh; PRATYUSH DAYAL, Indian Institute of Technology Gandhinagar, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh — Species ranging from single-cell organisms to social insects can undergo auto-chemotaxis, where the entities move towards a chemo-attractant that they emit themselves. This mode of signaling allows the organisms to form large-scale structures. Using computational modeling, we show that millimeter-sized polymer gels can display similar auto-chemotaxis. In particular, we demonstrate that gels undergoing the self-oscillating Belousov-Zhabotinsky (BZ) reaction not only respond to a chemical signal from the surrounding solution, but also emit this signal and thus, multiple gel pieces can spontaneously self-aggregate. We focus on the collective behavior of "colonies" of BZ gels and show that communication between the individual pieces critically depends on all the neighboring gels. We isolate the conditions at which the BZ gels can undergo a type of self-recombining: if a larger gel is cut into distinct pieces that are moved relatively far apart, then their auto-chemotactic behavior drives them to move and autonomously recombine into a structure resembling the original, uncut sample. These findings reveal that the BZ gels can be used as autonomously moving building blocks to construct multiple structures and thus, provide a new route for creating dynamically reconfigurable materials.

Q1.00200 The conformations of cyclic polymers in bidisperse blends of cyclic polymers. MICHAEL LANG, Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany — The size of cyclic polymers in bidisperse blends of chemically identical molecules is analyzed by computer simulations. The compression of entangled rings can be explained by the changes in the penetrable fraction of the surface bounded by the ring. Corrections for small rings can be approximated by a concatenation probability 1 – P_{DO} that a cyclic polymer entraps at least one other cyclic polymer. Both results are in line with a previous work [1] on the compression of entangled cyclic polymers in monodisperse melts. For entangled cyclic polymers, the backbone of a polymer chain is free to pass through an entire chain of another polymer in the melt. In this work, we investigate the glissile dynamics of microlayers of variable stiffness in dense aqueous suspensions using confocal microscopy. Poly(N-isopropylacrylamide) (PNIPAM) microparticles of variable stiffness in aqueous media are synthesized by free radical polymerization with varied cross-linking density. We investigate five separate crosslinking densities to fully encompass the transition from "soft" to "stiff" glasses. We have observed that the dynamic heterogeneity is more pronounced as stiffness increases, indicating the effect of fragility on glassy dynamics of dense colloidal liquids. Furthermore, when the "soft" glasses are confined between two solid surfaces at a gap spacing of several particle diameters, particle motions become arrested with notably increasing dynamic length scales at smaller volume fractions, suggesting the enhanced fragility by special confinement.

Q1.00201 Disorder-assisted melting and the glass transition in amorphous solids. ALESSIO ZACCONE, EUGENE TERENTJEV, Cavendish Laboratory, University of Cambridge — The mechanical response of solids depends on temperature because the way atoms and molecules respond collectively to deformation is affected at various levels by thermal motion. This is a fundamental problem of solid state science and plays a crucial role in metallurgy, aerospace engineering, energy. In disordered solids (glass, amorphous semiconductors, ceramics, metallic glass, polymers) the vanishing of rigidity as a function of temperature is not well understood because continuum elasticity is inapplicable due to the disorder leading to nontrivial (nonaffine) components in the atomic displacements. Our theory explains the basic mechanism of the melting transition of amorphous solids in terms of the lattice energy lost to nonaffine motion, compared to which thermal vibrations turn out to play a negligible role. The theory is in good agreement with data on melting of amorphous polymers (where no alternative theory can be found in the literature) and offers new opportunities in materials science.

Q1.00202 Development of a multi-resolution simulation approach. ANU NAGARAJAN, SILVINA MATSYIKA, University of Maryland, College Park, MD — The accurate representation of the aqueous environment in molecular dynamics simulations of medium to large systems poses a challenge in terms of simulation time scale and computational power. Multi-resolution simulation technique can be used to represent the solvent environment for simulating very large systems by splitting the system into nested regions. The different resolutions are combined to represent the solvent environment based on its physical relevance so that important regions of the solvent environment are in full atomistic representation and rest are in coarse-grained representation. Our method aims to represent the correct electrostatic properties in different representations and enable smooth transitions across the various resolutions. The ultimate goal of this work is to develop a multi-scale simulation method, for simulating bio-molecules in a multi-resolution solvent environment. This will allow us to gain the speed up necessary to simulate big macromolecular systems.

Q1.00203 Elastic Constants of Indium Arsenide at Room Temperature by Resonant Ultrasound Spectroscopy. FOUIZ ARAMMASI, MING YIN, Benedict College — The three independent elastic constants, C_{11}, C_{12}, and C_{44} of indium arsenide (InAs) single crystal were determined at room temperature using resonant ultrasound spectroscopy (RUS) technique. We will present and compare our results with those obtained from more conventional measurement techniques. We also compare our results to those of other III-V compound semiconductors such as gallium arsenide (GaAs).
Q1.00206 The role of substrate pre-compression on post-wrinkling bifurcations. ANESIA AUGUSTE, University of Massachusetts - Amherst, LIHUA JIN, ZHICANG SUO, Harvard University, RYAN HAYWARD, University of Massachusetts - Amherst — Surface instabilities play key roles in a variety of contexts including flexible electronics, surfaces with switchable properties, tissue engineering and biosensors. Wrinkles for elastic bilayers are well known to result from a balance between the bending energy of the stiffer skin layer and the stretching/compression of the softer substrate. Previous work has also shown that due to non-linearity in the substrate elasticity, post-wrinkling bifurcations can also occur, corresponding to emergence of sub-harmonic modes and eventual formation of self-contacting folds. To further elucidate the role of substrate elasticity in this process, we developed an experimental system that allows independent variation of the degree of compression in the substrate and in the thin film. We found that adding pre-compression to the substrate not only substantially reduces the critical strain for emergence of sub-harmonic modes, but also qualitatively changes the evolution of post-wrinkled structures. Our findings highlight the critical importance of substrate elasticity in determining the nature of post-wrinkling bifurcation modes.

Q1.00207 Non-linear responses of glass formers under temperature modulation. TAKASHI ODAGAKI, TAKAHIRO UENO, Tokyo Denki University, YASUO SARUYAMA, Kyoto Institute of Technology — The free energy landscape (FEL) approach to non-equilibrium systems has been shown to explain, in a unified manner, dynamic and thermodynamic characteristics observed in the vitrification process of supercooled liquids, and it is important to devise experiments which give information on the structure of the FEL. Here, we present a theoretical analysis of a new experimental technique which measures nonlinear responses under temperature modulation. Exploiting a simple model for glass formers, we first investigate dielectric relaxation when the temperature is subjected to a sudden change. We also report that three characteristic temperatures related to the glass transition can be determined from the analysis of the non-linear dielectric responses under oscillating temperature. Finally we discuss characteristic behavior of the frequency dependent diffusion constant, the intermediate scattering function and the generalized susceptibility under oscillating temperature.

Q1.00209 Thermal Conductivity in Supercooled Water1. JOHN BIDDLE, VINCENT HOLTEN, JAN SENGERS, MIKHAIL ANISIMOV, University of Maryland, College Park — The heat capacity of supercooled water, measured down to ~37 C, shows an anomalous increase as temperature decreases. The thermal diffusivity, the ratio of thermal conductivity and the heat capacity per unit volume, shows a decrease. These anomalies may be associated with a hypothetical liquid-liquid critical point in metastable water below the line of homogeneous nucleation. The data suggest that the thermal conductivity does not show a significant critical enhancement, in contrast to what is observed near the vapor-liquid critical point. We have used mode-coupling theory to investigate the possible effect of critical fluctuations on the thermal conductivity of supercooled water, and shown that indeed this effect would be too small to be measurable at experimentally accessible temperatures. We discuss physical reasons for the striking difference between the vapor-liquid and liquid-liquid critical points of thermal conductivity in water. We also discuss the discrepancy between the thermal conductivity calculated from experimental data and that obtained by computer simulations of the TIPSP water-like model.

1 American Chemical Society Petroleum Research Fund Grant No. 52666-ND6

Q1.00210 Mechanical output of myosin II motors is regulated by myosin filament size and actin network mechanics. SAMANTHA STAM, Biophysics Graduate Program, University of Chicago, Chicago, IL, JONATHAN ALBERTS, Center for Cell Dynamics, University of Washington, Friday Harbor, Washington, MARGARET GARDEL, Department of Physics, University of Chicago, Chicago, IL, EDWIN MUNRO, Department of Molecular Genetics and Cell Biology, University of Chicago, Chicago, IL — The interactions of bipolar myosin II filaments with actin arrays are a predominant means of generating forces in numerous physiological processes including muscle contraction and cell migration. However, the spatiotemporal regulation of these forces depends on motor mechanochemistry, bipolar filament size, and local actin mechanics is unknown. Here, we simulate myosin II motors with an agent-based model in which the motors have been benchmarked against experimental measurements. Force generation occurs in two distinct regimes characterized either by stable tension maintenance or by stochastic buildup and release; transitions between these regimes occur by changes to duty ratio and myosin filament size. The time required for building force to stall scales inversely with the stiffness of a network and the actin gliding speed of a motor. Finally, myosin motors are predicted to contract a network toward stiffer regions, which is consistent with experimental observations. Our representation of myosin motors can be used to understand how their mechanical and biochemical properties influence their observed behavior in a variety of in vitro and in vivo contexts.

Q1.00211 Development of a Polarizable Protein-like Coarse Grained Model. SAI JANANI GANESAN, SUDI JAWAHERY, SILVINA MATYSIAK, University of Maryland, College Park — The use of coarse grained simulations to explore larger biological systems and longer timescales has become increasingly popular. One of the major drawbacks of most coarse grained protein models is the absence of polarization effects and hence the inability to reproduce accurate electrostatic screening. The inclusion of polarization effects to amino acids will allow us to characterize the role of dipole-charge interactions in driving secondary structural preferences. We have formulated a polarizable coarse-grained protein-like model using the Drude oscillator approach. The root of the model is based on the coarse-grained MARTINI force field. We apply the new model to polyalanine peptides and observe secondary structure changes in different solvent environments, caused due to changes in dipole interactions. We also explore the effects of adding charged amino acids like Lysines, on conformational preferences of the polyalanine system. Extensions of the current model to more complex systems will also be presented.

Q1.00212 Highly scalable many-GPU simulations of soft matter systems using HOOMD-blue. JENS GLÄSER, Dept. of Chemical Engineering and Materials Science, University of Minnesota, JOSHUA ANDERSON, SHARON CLOTZER, Department of Chemical Engineering, University of Michigan, Ann Arbor, DAVID MORSE, Dept. of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis — We present a new version of the highly optimized, versatile and easy to use molecular dynamics software HOOMD-blue [1] running on tens to hundreds of GPUs. By taking advantage of a refined version of Plimpton’s communication scheme [2] fully implemented on the GPU and of standard MPI software, we demonstrate excellent strong scaling in simulations that have as few as 20,000 particles per GPU. This opens up the possibility of carrying out extremely performant multi-million particle simulations on GPU-based clusters and supercomputers, which are becoming increasingly available to the scientific community.


Q1.00213 Application of Zwanzig-Mori projection in model coarse-graining. JIANHUA XING, ABHISHEK MUKHOPADHYAY, Virginia Tech — Reconstruction of equations of motion from incomplete or noisy data and dimension reduction are two fundamental problems in the study of dynamical systems with many degrees of freedom. We generalize the Zwanzig–Mori projection formalism, originally developed for Hamiltonian systems close to thermodynamic equilibrium, to general non-Hamiltonian systems lacking detailed balance. Then we develop a numerical algorithm to extract dynamic information for constructing the generalized Langevin equation. Numerical tests show that the formalism works remarkably.
Q1.00214 Molecular Simulations of The Formation of Gold-Molecule-Gold Junctions, HUAUCHAN WANG, The George Washington University — We perform classical molecular simulations by combining grand canonical Monte Carlo (GCMC) sampling with molecular dynamics (MD) simulation to explore the dynamic gold nanojunctions in an Alkenedithiol (ADT) solvent. With the aid of a simple driving-spring model, which can reasonably represent the long-range elasticity of the gold electrode, the spring forces are obtained during the dynamic stretching procedure. A specific multi-time-scale double reversible reference system propagator (double-RESPA) algorithm has been designed for the metal-organic complex in MD simulations to identify the detailed metal-molecule bonding geometry at metal-molecule-metal interface. We investigate the variations of bonding sites of ADT molecules on gold nanojunctions at Au (111) surface at a constant chemical potential. Simulation results show that an Au–ADT–Au interface is formed on Au nanojunctions, bond-breaking intersection is at 1–1 bond of the monatomic chain of the cross-section, instead of at the Au–Au bond. Breaking force is around 1.5 nN. These are consistent with the experimental measurements.

Q1.00215 Computational NMR, IR/RAMAN calculations in sodium pravastatin: Investigation of the Self-Assembled Nanostructure of Pravastatin-LDH (Layered Double Hydroxides) Systems1, PHILIPPE PETERSEN, VANESSA CUNHA, MARCOS GONCALVES, HELENA PETRILLI, VERA CONSTANTINO, Universidade de Sao Paulo, INSTITUTO DE FISICA, DEPARTAMENTO DE FISICA DE MATERIAIS E MECANICA TEAM, INSTITUTO DE QUIMICA, DEPARTAMENTO DE QUIMICA FUNDAMENTAL TEAM — Layered double hydroxides (LDH) can be used as nanocarriers for immobilization of Pravastatin, in order to obtain suitable drug carriers. The material’s structure and spectroscopic properties were analyzed by NMR, IR/RAMAN and supported by theoretical calculations. Density Functional Theory (DFT) calculations were performed using the Gaussian03 package [1]. The geometry optimizations were performed considering the single crystal X-ray diffraction data of tert-octylammonium salt of Pravastatin [2]. Tetramethylsilane (TMS), obtained with the same basis set, was used as reference for calculating the chemical shift of 13C. A factor was used to compare theoretical and experimental harmonic vibrational frequencies. Through the NMR and IR/RAMAN spectra, we were able to make precise assignments of the NMR and IR/RAMAN of Sodium Pravastatin.


1We acknowledge support from CAPES, INEO and CNPQ.

Q1.00216 Electric-Field Induced Structural Evolution of Water Clusters (H$_2$O)$_n$ [n = 9 - 20]: Ab initio Density Functional Approach1, RAJEЕV PATHAK2, Department of Physics, University of Pune, Pune, Maharashtra, India — Response of neutral water clusters (H$_2$O)$_n$, n = 9 through 20, to external electrostatic fields (0 to 1V/A), is studied for the lowest-energy conformers within in the energy band ~2 kcal/mol, for each “n,” employing the versatile B3LYP hybrid prescription of density functional theory in conjunction with the polarized basis 6-311+G(2d, 2p). Increase in the field elongates and weakens hydrogen-bond networks; “opening up” three-dimensional cluster morphologies to complex net-like structures culminating into their disintegration at specific threshold values. All conformations are stable: they manifest as local minima on their potential energy surfaces. Field-induced structural transitions are invariably accompanied by an abrupt increase in the electric dipole moment, which is marked at breakdown, where the highest-occupied and lowest-unoccupied molecular orbital energy gap diminishes to zero. Remarkably, as a consequence of their zero or very small electric dipole moments, certain conformers endowed with molecular symmetry exceptionally exhibit a peculiar behavior: they either remain completely robust to increase in the field, or break up into smaller, identical, robust building units with tetramer, pentamer and hexamer ring- or cubic-geometries.

1BCU Research Grant from University of Pune is gratefully acknowledged.

2Work carried out by: Rajeev K. Pathak, Dhurba Rai, Anant D. Kulkarni, Shridhar P. Gejji, and Libero J. Bartolotti

Q1.00217 Promote Water Photosplitting via Tuning Quantum Well States in Supported Metal Clusters, ZIJING DING, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, ZI LI, GANG LIU, Department of Physics and Astronomy, California State University, Northridge, California 91330-8266, USA, SHENG MENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — In an effort to facilitate water photosplitting at surfaces, we identify quantum well states of magic gold clusters supported on ultrathin MgO/Ag(001) as the key to favor sunlight absorption and photocatalytic reactions. Based on density functional theory (DFT) and time-dependent DFT calculated ons, the adsorption geometry, electronic structures, and excited state properties of supported metal nanoparticles can be precisely controlled. By decreasing the thickness of MgO film, charge transfer to supported gold clusters, and therefore the occupation and energy spacings of quantum well states, can be gradually tuned, leading to redshifted and enhanced plasmonic excitations and optimized energy levels for water splitting. Using nudged elastic band (NEB) and constraint DFT, we further calculate the barriers for water splitting in the ground state as well as in excited states. The barriers are found correlated with adsorption sites of water on the gold cluster. Surface hopping calculations indicate the lifetime of excited states is long enough to induce water photo-dissociation.

Q1.00218 Helical inversion reaction pathway for π/π stacking in aromatic compounds, AZUSA MURAOKA, Meiji University, CREST, HIROSHI USHIYAMA, KOICHI YAMASHITA, University of Tokyo, CREST — Polyaromatics have the π/π stacking interaction, which shows that two aromatic units preferentially interact in a parallel-displaced orientation, such as the crystal packing of organic molecules. Recently, π/π stacking compounds have become of interest in the photocatalysis solar energy transformational materials. In particular, the stable configurations of neutral and cationic π-phenylenes have helical tightly packed π-phenylenes with π/π stacking interactions. To investigate helical inversion pathways, we have studied theoretically the stable and transition-state geometries of neutral and cationic π-phenylenes using the density functional theory method. We have found that π-phenylenes follow an inversion reaction pathway with three transition-states in which the configuration of each phenylene is inverted. This means that π-phenylenes cannot convert from right- to left-handed geometry at once; however, we suggest a step-by-step reaction pathway through the three transition-state structures.

Q1.00219 Cathode Luminescence Spectroscopy of Gold Nanoparticle Catalyst in CO and O$_2$ Environments, TAKAYUKI TANAKA, NAOKI YAMAMOTO, KUNIO TAKAYANAGI, Tokyo Institute of Technology, CREST, JST — Gold nanoparticle catalysts for low-temperature CO oxidation (2CO + O$_2$ $\rightarrow$ 2CO$_2$) [1] are especially attractive for applications in air purification. It is proposed that the resonance state of O$_2$ (2π* → 1π*) activated oxidation of CO and hydrogenation in and gold nanoparticle on TiO$_2$ (Au/TiO$_2$) [1, 2] and TiO$_2$ photocatalyst [3]. The TiO$_2$ is prepared by cleavage and annealing of rutile single crystal. Gold nanoparticles were deposited at vacuum. The Au/TiO$_2$ catalyst was observed by scanning transmission electron microcopy (STEM). Cathode luminescence spectra were acquired, when the electron probe were scanned in Au/TiO$_2$. A CL peak is detected in spectra of vacuum. The peak energy depended on specimen and its location, e.g. 3.10 and 3.15 eV. The energies were close to band gap energy (3.0 eV). The CL peak of vacuum is attributed to electron-hole recombination of TiO$_2$. The peak energy shifts because of interference effects. Cathode luminescence spectra change by O$_2$ exposure of 3x10$^{-4}$ Pa. The differential spectra from vacuum to O$_2$ show new peaks, which have larger energies than band gap energy, 3.1 to 3.6 eV. The new peaks by O$_2$ exposure are the resonance state of O$_2$ adsorption. We will report the results of CL experiments of O$_2$. CO exposure and co-exposure of CO and O$_2$ and propose mechanism of CO oxidation in Au/TiO$_2$. [1] M. Haruta et al., J. Catal. 144 (1999) 175. [2] T. Tanaka, et al., Surf. Sci. 604 (2010) L75. [3] H. Irie et al., J. Phys. Chem. C 113, 10761 (2009).
the hydrotreating of LCO gas oils and to the hydrocracking of vacuum residues from different origins (e.g. Athabasca).

adjusts the molar fractions of the generated molecules in order to further improve the properties of the mixture. In the second step, a kinetic Monte Carlo set of molecules with the appropriate analytical properties via a Monte Carlo method. The second algorithm, called reconstruction by entropy maximization, of the process is generated via two successive molecular reconstruction algorithms. The first algorithm, termed stochastic reconstruction, generates an equimolar OLIVEIRA, Luis.Pereiradeoliveira@gmail.com, JAN J. VERSTRAETE, IFP Energies nouvelles, BP 3, 69360 Solaize, France — A novel kinetic modeling strategy MAX KOLB, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, F-69364 Lyon, France, LUIS PEREIRA DE LUNA, IFP Energies nouvelles, BP 3, 69360 Solaize, France — A novel kinetic modeling strategy for refining processes for heavy petroleum molecular reconstruction algorithms. The first algorithm, termed stochastic reconstruction, generates an equimolar set of molecules with the appropriate analytical properties via a Monte Carlo method. The second algorithm, called reconstruction by entropy maximization, adjusts the molar fractions of the generated molecules in order to further improve the properties of the mixture. In the second step, a kinetic Monte Carlo method is used to simulate the effect of the refining reactions on the previously generated set of molecules. The full two-step methodology has been applied to the hydrotreating of LCO gas oils and to the hydrocracking of vacuum residues from different origins (e.g. Athabasca).

Molecule-based kinetic Monte Carlo modeling of hydrotreating processes applied to Light Cycle Oil gas oils, MAX KOLB, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, F-69364 Lyon, France, LUIS PEREIRA DE LUNA, IFP Energies nouvelles, BP 3, 69360 Solaize, France — A novel kinetic modeling strategy for refining processes for heavy petroleum molecular reconstruction algorithms. The first algorithm, termed stochastic reconstruction, generates an equimolar set of molecules with the appropriate analytical properties via a Monte Carlo method. The second algorithm, called reconstruction by entropy maximization, adjusts the molar fractions of the generated molecules in order to further improve the properties of the mixture. In the second step, a kinetic Monte Carlo method is used to simulate the effect of the refining reactions on the previously generated set of molecules. The full two-step methodology has been applied to the hydrotreating of LCO gas oils and to the hydrocracking of vacuum residues from different origins (e.g. Athabasca).

Q1.00222 Characterization of Self-Assembly Processes in Ionic Liquids, MICHAEL McCUTCHEON, SILVINA MATYSIAK, University of Maryland, College Park — Surfactants are commonly used in a large number of industrial applications because of their remarkable ability to influence the properties of surfaces and interfaces. The spontaneous self-assembly of surfactants into micelles in an aqueous environment has been very well characterized. With the emergence of room-temperature ionic liquids (ILs), there is a clear need to revisit the driving forces behind the aggregation of surfactants in IL. This project aims to obtain a mechanistic description of the self-assembly of anionic surfactants (SO$_4$H and SO$_4^{2-}$) in an ionic liquid (EMM[EtSO$_4$]). We are exploring the evolution of aggregates with time and the stability of micelle-like aggregates using atomistic simulations. The structural phase behavior is also characterized to explore morphological modifications. In addition, structural properties of the ionic liquid close to the aggregates are evaluated to characterize the link between aggregated structure and changes in the solvent structure.

Q1.00223 Probing the interface of Charged Surfactants in Ionic Liquids by XPS1, LANG CHEN, HARRY BERMUDEZ, Department of Polymer Science and Engineering, University of Massachusetts Amherst — Room-temperature ionic liquids (ILs) are playing increasingly vital roles in many processes of both fundamental and applied natures such as separations and catalysis. It is therefore critical to obtain a better understanding of their interfacial properties such as surface charge and composition. Here we examine the influence of positively-charged surfactants on IL interfaces by X-ray photoelectron spectroscopy (XPS). The roles of surfactant alkyl chain length, concentration, and information depth on interfacial properties are investigated. Depending on the chain length and concentration, the surfactants can alter the IL interface to varying extents, highlighting a simple route to manipulate interfacial properties. XPS also reveals that surfactant counterions predominantly dissociate into the bulk. As a consequence, ion exchange occurs between surfactant and like-charged IL ion. Our results are a further demonstration of the ability of XPS to give insights into the surface activity and aggregation behavior in multi-component ionic liquid systems.

Q1.00224 Physiosorption, Diffusion, Adsorption/Desorption of Molecular Hydrogen on Graphene, MAJID KARIMI, Indiana University of PA, JUSTIN PETucci, Indiana University of PA, GIANFRANCO VIDALI, Syracuse University — The interaction of a H$_2$ molecule with a graphene surface is studied using AIREBO bond-order potential. Adsorption potential, desorption potential, and diffusion barriers of H$_2$ on graphene are obtained and compared with the corresponding results from the first-principles. The massively parallel molecular dynamics codes (lammps) and nudged elastic band (NEB) method are employed to do these calculations.

Q1.00225 Experimental study of Ar-CH$_4$ gas mixture adsorption over exfoliated graphite: kinetic reversal of adsorption selectivity1, MATIAS RAFTI, Instituto de Investigaciones Fisicoquímicas Teoricas y Aplicadas, (INIFTA-CONICET), Universidad Nacional de La Plata, VAIVA KRUNGLEVICIUTE2, ALDO MIGONE, Southern Illinois University Carbondale — Adsorption is one of the processes used for achieving the separation of gas mixtures. In this poster we present the results of a combined gas composition and adsorption isotherm study performed to investigate how a mixture of two gases with different binding energies adsorbs on exfoliated graphite at temperatures between 70 and 90 K. In our experiments we observed a very interesting phenomenon: adsorption overshoot. This is a phenomenon that occurs in the initial stages of adsorption when the lower binding energy species adsorbs onto the substrate in a greater proportion than the stronger binding species. As time elapses and adsorption equilibrium is approached, this stronger species starts replacing the weaker species in the adsorbed phase. In such a principle, this phenomenon would allow the possibility of achieving gas mixture separation by controlling the adsorption time. Our results will be compared with those from recent numerical simulations that predicted similar behavior on a one dimensional uniform substrate.

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2Present address: UPenn/NIST, 100 Bureau Drive, Gaithersburg, MD.
Q1.00227 Phases transitions and interfaces in temperature-sensitive colloidal systems . DUC NGUYEN, PhD, PETER SCHALL, Dr. — Colloids are widely used because of their exceptional properties. Beside their own applications in food, petrol, cosmetics and drug industries, photonic, optical filters and chemical sensor, they are also known as powerful model systems to study molecular phase behavior. Here, we examine both aspects of colloids using temperature-sensitive colloidal systems to fully investigate colloidal phase behavior and colloidal assembly.

Q1.00228 Dynamics of concentration fluctuations in nanocolloidal suspensions . ALEXIS PAYNE, ANA OPRISAN, College of Charleston — We studied the dynamics of concentration fluctuations in nanocolloidal suspensions using the shadowgraph visualization technique. The set up involved a CCD camera capturing the fluctuations occurring in a sample cell undergoing a free diffusion process. We performed three experiments with different gold, silver, and silica colloidal suspensions. For each trial, the colloids power spectrum, structure factor, and correlation time were found using a dynamic structure method. Each experiment’s fluctuations varied significantly from the others. This was due to variations in particle size, concentration and possible plasmonic interactions. All the nanocolloidal suspensions’ structure factors and correlation times followed the expected power laws. From the correlation time, the diffusion coefficient for all three colloidal suspensions was calculated which coincided with expected results.

Q1.00229 Active Microrheology Using Optical Tweezers to Characterize Viscoelastic Properties of Entangled DNA . COLE D. CHAPMAN, UCSD, KENT LEE, DEAN HENZE, University of San Diego, DOUGLAS E. SMITH, UCSD, RAE M. ANDERSON, University of San Diego — We use active microrheology techniques to investigate the frequency-dependent linear elastic and viscous moduli (G’, G”) of entangled DNA. Utilizing optical tweezers, single microphores, embedded within solutions of entangled DNA of varying molecular lengths and solution concentrations, are driven sinusoidally over a frequency range of 0.6 - 95 Hz, while fluorescence microscopy is used to simultaneously visualize the deformation of a sparse number of DNA molecules entangled in the solution. DNA lengths of 11 kbp – 115 kbp and solution concentrations of 1.0 – 2.5 mg/ml are probed to determine the dependence of the viscoelasticity of entangled DNA on solution concentration and, for the first time, molecular length. Results are compared to theoretical predictions for entangled polymers, as well as previously reported microrheology results.

Q1.00230 Structure of high-PT water and mineral interface with high-resolution x-ray reflectivity . HONGPING YAN, CHANGYONG PARK, Carnegie Institution of Washington — Hydration and chemistry at mineral-water interface are fundamental to control mineral dissolution and growth at microscopic level. The structure is crucial to describe the interfacial processes such as electrical double layer and ion exchange. Density profiles across various mineral-water interfaces revealed characteristic water orderings in accordance with the termination and morphology of mineral surfaces [1]. The previous observations, however, have been limited to ambient pressure conditions due to the lack of proper instrument to handle extreme conditions (e.g., high-pressures). Here, we developed a high-pressure and high-temperature (high-PT) aqueous interface cell specifically designed for high-resolution x-ray reflectivity measurement from mineral-water interface under pressure up to 40 MPa and a temperature up to 770K. The first demonstration is presented with a few examples including olivine (010)-water interface. Observation of structure and reactivity of hydrothermal fluids on mafic and/or ultramafic mineral surfaces can provide a fundamental basis of our understanding of the hydration process of mineral surface in deep-sea environment.

Q1.00231 The role of rare earth oxide nanoparticles in suppressing the photobleaching of fluorescent organic dyes , ANUBHAV GUHA, Horace Greeley High School, ANINDITA BASU, University of Pennsylvania — Organic dyes are widely used for both industrial as well as in scientific applications such as the fluorescent tagging of materials. However the process of photobleaching can rapidly degrade dye fluorescence rendering the material non-functional. Thus exploring novel methods for preventing photobleaching can have widespread benefits. In this work we show that the addition of minute quantities of rare earth (RE) oxide nanoparticles can significantly suppress the photobleaching of dyes. The fluorescence of Rhodamine and AlexaFluor dyes was measured as a function of time with and without the addition of CeO2 nanoparticle additives (two RE oxides that contain an oxygen vacancy based defect structure), as well as with FeO nanoparticles (which has an oxygen excess stoichiometry). We find that the rare earth oxides significantly prolonged the lifetimes of the dyes. The results allow us to develop a model based upon the presence of oxygen vacancies defects that allow the RE oxides to act as oxygen scavengers. This enables the RE oxide particles to effectively remove reactive oxygen free radicals generated in the dye solutions during the photosorption process.

Q1.00232 Quantum Chemistry based Coupled Electron Nuclei Dynamics Simulation . TOMOTAKA KUNISADA, HIROSHI USHIYAMA, KOICHI YAMASHITA, The University of Tokyo — Electron dynamics with classical nuclei motion was performed to study electron-nuclei coupled (non-adiabatic) process of molecular system. Non-adiabatic transition from one adiabatic state from another adiabatic state occurred during the simulation, which was confirmed by monitoring adiabatic state populations. The change of charge distribution and dipole moment in the molecule was analyzed in order to study electron dynamics. To see electron dynamics more clearly, the change of the electronic character of the electronic wave function was examined in terms of configuration functions. These results show that, not only the population of each adiabatic state but also the coherence between adiabatic states plays important roles in such ultrafast electron dynamics induced by non-adiabatic transition.

Q1.00233 Strain effects on electron transport through ds-DNA molecules . SADEQ MALAKOOTI, ERIC HEDIN, YONG JOE, Ball State University — Molecular electronics of a double stranded poly(G)-poly(C) DNA molecule under axial mechanical strain is examined with a tight binding scheme. Slater-Koster theory is implemented to describe electronic coupling constants in terms of inter-orbital distances. Electronic structure of an infinite-length DNA model, including band structure and total density of states, is studied for both stretching and compressional cases. In addition, electronic transmission spectra as well as current-voltage characteristics under application of mechanical strain for a 30 base-pair DNA molecule coupled between two semi-infinite electrodes are investigated. Results demonstrate a very sensitive strain dependency for DNA electronics.

Q1.00234 Quantification of crumpling in graphene oxide and other sheet-like nanostructures . PETER BEAUCAGE, DURGESH RAI, GREGORY BEAUCAGE, University of Cincinnati, SIDDHARTH PRADHAN, University of Tennessee Knoxville — Two-dimensional sheet-like nanostructures have garnered significant scientific interest in recent decade, particularly due to their inherent high specific surface areas (SSAs). Such large SSAs also result in an intrinsic tendency to crumple or fold based on surface interactions under ambient conditions. An understanding of the topological details of such structures has revealed various qualitative features driven by thermodynamics and interfacial chemistry. A scaling model based methodology will be presented which can be utilized to do quantitative analysis using small angle scattering data. A wide range of materials like graphene oxide, membrane layers as well exfoliated sheets of molybdenum oxide and tungsten oxide have been investigated to understand how such quantification may yield a general classification of such materials based on crumpling behavior.
Q1.00235 Electrical properties of the α-pyrochlore Bi$_2$-$\gamma$Sr$_3$Ir$_2$O$_7$ solid solution. PABLO DE LA MORA, Facultad de Ciencias, CARLOS COSIO CASTÁNEDA, Facultad de Química, FRANCISCO MORALES LEAL, Instituto de Investigación en Materiales, GUSTAWO TAVIZON, Facultad de Química, Universidad Nacional Autónoma de México — To study the electrical properties of the Bi$_2$-$\gamma$Sr$_3$Ir$_2$O$_7$ ($\{\text{Ir}_2\text{O}_4\}$) solid solution ab-initio DFT (WIEN2k) calculations were done. In this compound, when $\gamma$ is reduced, the resistivity increases and the $\rho$/T slope also increases. In this system the Bi$_2$-$\gamma$Sr$_3$Ir$_2$O$_7$ substructure has little contribution to the conductivity, even so, it is indirectly responsible to the conductivity modifications, since it affects the other substructure; Ir$_2$O$_4$, which is conducting. When Bi is substituted by Sr, it pushes O, shortening the In-O bond and the resistivity is supposed to decrease; instead a small increment is found. What is found is that this increment is due to the relaxation time, $\tau$. There are two contributions to $\tau$; a) static, the random replacement of Bi by Sr introduces ‘impurities’, shortening $\tau$, therefore increasing the resistivity, b) dynamic, due to the thermal oscillations of the atoms. What is found is that the effect of the oscillations in the compound with Sr has a larger impact on the electronic structure, thus increasing the $\rho$/T slope.

Q1.00236 Micellization behavior of Poly[2,7-(9,9-dihexylfluorene)]-b-Poly(2-vinylpyridine) in MeOH/THF Mixed Solvents via a Combination of Coarse-Grained and All-Atom Molecular Dynamics Methods. CHIN-WEN CHEN, JING-SAIN LIN, WEN-CHANG CHEN, CHING-HUANG, National Taiwan University, CHEN-WENCHEANG COLLABORATION — Coarse-grained (CG) and all-atom (AA) molecular dynamics (MD) methods are proposed to investigate the micellar behavior of a semiconducting conjugated diblock polymer, poly[2,7-(9,9-dihexylfluorene)]-b-poly(2-vinylpyridine) (PF-b-P2VP) in MeOH/THF. We adopt the iterative Boltzmann inversion method to obtain CG force filed through mapping route with AA MD data. In order to compare experimental result [1], we first choose PF$_x$-b-P2VP$_{11}$ with $\theta=0.1$ and varying ratio of MeOH/THF. When MeOH/THF = 0/100, due to the fact the THF is a common solvent. We observe no micellar formation with increasing ratio of P2VP selective solvent in MeOH/THF. When MeOH/THF = 100/0, the PF-b-P2VP$_{11}$ is a nearly lattice-matched substrate for growth of GaN film. The non-polar gallium nitride (GaN) film is a potential candidate for high-quality due to its narrowest FWHM at 3.4eV. According to these analytic results, we found that thermal annealing treatment could improve the quality of free-standing GaN. Our study indicates that metal domain LiGaO$_2$-plane GaN disappeared for higher $\alpha$-plane GaN sample. When the growth direction of GaN is [100] oriented ($\alpha$-plane) instead of [0001] oriented ($\gamma$-plane). It was found that the $\gamma$-plane GaN disappeared for higher growth temperature and the zinc-blende GaN appeared. The band gap was changed when we tuned III/V ratio. The crystal characteristics of GaN films for different growth parameters were studied by scanning electron microscopy (SEM), transmission electron microscopy (TEM), photoluminescence (PL), X-ray diffraction (XRD), and reflection high-energy electron diffraction (RHEED).

Q1.00237 SEMICONDUCTORS —

Q1.00238 Characterization of free-standing GaN with thermal treatment. CHEN-CHI YANG, IKAI LO, CHENG-HUNG SHIH, CHIA-HUAN HU, YING-CHIEH WANG, YU-CHIAO LIN, CHENG-DA TASI, SHUO-TING YOU, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, R. O. C.; WEI-HAN LEE, ELECTROPHYSICS, NATIONAL CHIAO TUNG UNIVERSITY, 1001 UNIVERSITY ROAD, HSINCHU 30010, TAIWAN, R. O. C. — We have grown free-standing GaN by hydride vapor phase epitaxy. The free-standing GaN samples were annealed by rapid thermal annealing for 3 minutes at 600, 650, 700, 750, and 800°C in vacuum. The crystal structure and quality of GaN samples were characterized by X-ray diffraction. We found that the full width half maximum of the (0002) and (10-12) of GaN samples are decreased significantly after thermal annealing. The (0002) rocking curve of GaN sample was 218.8 arcsec without thermal annealing, and it became 49.5 arcsec after annealing at 800°C. The FWHM of the (10-12) rocking curve was 113.5 arcsec without thermal annealing, and it reduced to 58.3 arcsec after annealing at 800°C. According to the observation of atomic force microscopy, we found that the dislocation density of annealed GaN samples (7.0x10$^6$/cm$^2$) is smaller than that of pre-annealed GaN samples (1.0x10$^7$/cm$^2$). The optical properties of the samples by photoluminescence measurement which showed that the sample annealed at 650°C had the best quality due to its narrowest FWHM at 3.4 eV. According to these analytic results, we found that thermal annealing treatment could improve the quality of free-standing GaN.

Q1.00239 GaN Grown on Sputtering AlN Buffer Layer with Sapphire Substrate by Plasma-Assisted Molecular-Beam Epitaxy. YU-CHIAO LIN, IKAI LO, WEN-YUAN PANG, CHENG-HUNG SHIH, CHEN-CHI YANG, CHENG-DA TASI, SHUO-TING YOU, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan, SEAN WU, Department of Electronics Engineering and Computer Sciences, Tung-Fang Institute of Technology, Kaohsiung, Taiwan. — The non-polar gallium nitride (GaN) film is a potential candidate for high-efficient optoelectronic devices. This study reports the characterization of GaN grown on aluminum nitride (AIN) buffer layer by plasma-assisted molecular-beam epitaxy (PA-MBE). The AIN buffer layer containing both $\gamma$-plane and $\alpha$-plane AIN was grown by RF magnetron sputter on a sapphire substrate before growing GaN. The growth direction of GaN is [100] oriented ($\alpha$-plane) instead of [0001] oriented ($\gamma$-plane). It was found that the $\gamma$-plane GaN disappeared for higher growth temperature and the zinc-blende GaN appeared. The band gap was changed when we tuned III/V ratio. The crystal characteristics of GaN films for different growth parameters were studied by scanning electron microscopy (SEM), transmission electron microscopy (TEM), photoluminescence (PL), X-ray diffraction (XRD), and reflection high-energy electron diffraction (RHEED).

Q1.00240 Characterization of $\gamma$-plane GaN epi-film Grown on LiGaO$_2$ substrate by Plasma-Assisted Molecular Beam Epitaxy. SHUO-TING YOU, CHENG-HUNG SHIH, IKAI LO, YING-CHIEH WANG, CHEN-CHI YANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, R. O. C; MITCH CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, R. O. C; LIGAO O$_2$ (001) is a nearly lattice-matched substrate for growth of $\gamma$-plane GaN film. However, GaN single crystal has multi-domains defect on LiGaO$_2$ (001), i.e. metal domain and oxygen domain. In this work, we have studied the growth mechanism of $\gamma$-plane GaN on two domain areas by plasma-assisted molecular beam epitaxy. We found that the growth mechanism of $\gamma$-plane GaN on LiGaO$_2$ was in the form from 3D to 2D evaluated by the observation of in-situ reflection high energy electron diffraction (RHEED). According to RHEED and TEM analyses, we found that zinc-blend GaN islands were formed at early growth stage. The surface morphology of GaN grown on two domains was observed by AFM image which showed that the GaN grown on the metal domain was flat. The luminescence properties of the GaN grown on two-domain LiGaO$_2$ were also analyzed by photoluminescence and cathodoluminescence, which also showed that the $\gamma$-plane GaN grown on metal domain has better luminescence property than that grown on oxygen domain. Our study indicates that metal domain LiGaO$_2$ (001) is suitable to grow high quality $\gamma$-plane GaN.

1 This project is supported by National science council of Taiwan(NSC 101-2112-M-002-009). Prof. Monica Olvera de la Cruz, Dr. Rastko Sknepnek and Ms. Ting I.N.G. Li, Northwestern University.

2 This project is supported by National science council of Taiwan(NSC 101-2112-M-110-006-MY3).

3 This project is supported by National science council of Taiwan(NSC 101-2112-M-110-006-MY3).
Q1.00241 Characterization of textit{M-plane GaN thin film grown on pre-annealing $\beta$-LiGaO$_2$ (100) substrate}$^1$. CHENG-DA TSAI, CHENG-HUNG SHIH, IKAI LO, YING-CHIEH WANG, CHEN-CHI YANG, YU-CHIAO LIN, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan, R.O.C.; MITCH M.C. CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung, Taiwan, R.O.C. — We used the plasma-assisted molecular-beam epitaxy to grow the M-plane GaN thin films on $\beta$-lithium gallate, $\beta$-LiGaO$_2$, which had been annealed in vacuum and in air ambient. With the X-ray diffraction analysis, different azimuth angles ($0^\circ$ and $90^\circ$) were applied in $\omega - 2\theta$ scanning measurement. The signal of M-plane GaN was deviated from the normal value to be $-0.147$ in vacuum and $-0.048$ in air ambient, which showed that LGO substrate pre-annealed in air can reduce the compressive strains in the growing sample effectively. The same result was confirmed by the Raman scattering analysis. It showed that the sample pre-annealed in vacuum had $E_2$ phonon frequency which was shifted to 574.35 cm$^{-1}$ due to the stress and the sample pre-annealed in air had $E_2$ phonon frequency which was shifted only to 568.73 cm$^{-1}$. In conclusion, thermal annealing of $\beta$-LiGaO$_2$ substrate in air can improve the quality of growing M-plane GaN and effectively suppresses the formation of lithium-rich surface for the growth M-plane GaN thin films on $\beta$-LiGaO$_2$ substrate.

$^1$This project is support by National Science Council of Taiwan (NSC 101-2112-M-100-006-MY3).

Q1.00242 Hubbard $U$ Calculations for Dilute Magnetic Semiconductors$^1$. TETSUYA FUKUSHIMA, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO COLLABORATION, GUSTAV BILHMAYER COLLABORATION, PETER DERDECHS COLLABORATION, PHIVOS. MAVROPOULOS COLLABORATION, RUDOLF ZELLER COLLABORATION — Based on constrained density functional theory, we present ab initio calculations for the Hubbard $U$ parameter of transition metal impurities in dilute magnetic semiconductors, by choosing Mn in GaN as an example. The calculations are performed by two methods: (i) the Korringa-Kohn-Rosker (KKR) Green function method for a single Mn impurity in GaN and (ii) the Full-potential Linear Augmented Plane Wave (FLAPW) method for large supercell of GaN with a single Mn impurity in each cell. By changing the occupancy of the majority $t_2$ gap state of Mn, we determine the $U$ parameter either from the total energy differences $E(N + 1)$ and $E(N − 1)$ of the $N + 1$ and $N − 1$ excited states with respect to the ground state $E(n)$, or by using the single particle energies for $N + 1/2$ and $N − 1/2$ occupancies (Janak’s transition state model). Both methods give nearly identical results. Moreover the values calculated by the Green function technique and the supercell method agree quite well.

$^1$The authors acknowledge the financial support from the JSPS Core-to-Core Program.

Q1.00243 Spin-polarized transmission through multiple, series-coupled Aharonov-Bohm rings. ERIC HEDIN, YONG JOE, JAMES CUTRIGHT, Ball State University, Dept. of Physics & Astronomy — Multiple, series-coupled nanoscale Aharonov-Bohm rings with a quantum dot (QD) embedded in each arm are analyzed for their transmission and current-voltage (I-V) characteristics. A tight-binding model is used to obtain the electron transmission as a function of energy. Application of an external magnetic field is shown to produce spin-polarized transmission bands as a result of Zeeman-splitting of the QD energy levels. The band structure of the multiple-ring device is studied as a function of Zeeman splitting energy, QD energy levels, and inter-dot coupling. I-V calculations correlating to the band structure demonstrate that this device can produce highly spin-polarized current with either ohmic or semiconductor behavior, depending on the Fermi energy and the Zeeman splitting energy of the system.

Q1.00244 Enhancement of the Spin Conductance of a Magnetic Superlattice$^1$. NAMMEE KIM, HEESANG KIM KIM, Department of Physics, Soongsil University, JINWOO KIM, Research Center for Integrative Basic Science, Soongsil University — For a spin device application of a magnetic superlattice, we investigate the optimal condition to get a fully spin-polarized current with sizable ballistic conductance. We consider a quasi-one dimensional magnetic superlattice, formed by a periodic magnetic field and a split gate technique on a two dimensional electron gas system. We obtain such a condition by analyzing an energy miniband dispersion and a spin dependent transmission probability for each channel. The transfer matrix theory and Bloch’s theorem are used in the detailed calculation. From the results, we propose an optimized aspect ratio of size parameters of a quasi-one dimensional magnetic superlattice as a spin filter to generate currents having simultaneous full spin-polarization and sizable ballistic conductance.

$^1$The Korea Research Foundation (NRF, grant No. 20120007534)

Q1.00245 The optical, electronic and magnetic properties of Fe based binaries and diluted alloys. AHMAD ALSAAD, Department of Physics, Jordan University of Science & Technology, ISSAM ALQATTAN. DEPARTMENT OF APPLIED MATHEMATICS AND SCIENCES TEAM — The optical, electronic, and magnetic properties of binaries and alloys containing small amount of iron (Fe) have been presented. In particular, diluted Fe alloys have been examined by several experimental techniques such as magnetization measurements, nuclear magnetic resonance or neutron scattering. Theoretically, the understanding of diluted Fe alloys has not been yet satisfactorily studied. We present ab initio calculations based on Local Density Approximation of Density Functional Theory for Fe based binaries and Fe lightly doped alloys (not to exceed 10%) with 3d and 4d transition elements. Results on the densities of states, the local magnetic moments, and the electronic specific heat around the 3d and 4d impurities have been reported. Contrary to the case of Co, Mn, and Ni alloys. Our density of states results indicate that most of the optical, electronic and magnetic properties of Fe alloys is attributed to the majority-spin states rather than the minority-spin states. This arises from the fact that the Fermi energy falls into the minimum of the minority-spin density of states rather than the minimum of the majority-spin states. The mechanism behind this very complicated magnetic behavior of Fe based binaries and alloys have been addressed and explained. The comparison between our theoretical results and the available experimental results will be presented.

Q1.00246 Electronic Structures of the Doped Cesium Niobate Cs$_2$Nb$_2$O$_{11}$. JIANJUN LIU, ROBERT SMITH, Department of Chemistry, University of Nebraska Omaha, Lincoln, NE 68182, LIU WANG, WAI-NING MEI, RENAT SABIRIANOV, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, HSIN-YI HSU, HSIAO-LIN LIU, Department of Physics, National Taiwan Normal University, Taipei 11677, Taiwan — Samples of the photocatalyst cesium niobate (Cs$_2$Nb$_2$O$_{11}$) have been prepared with various amounts tantalam and sulfur doped onto the niobium and oxygen sites, respectively. Tantalum doping was effected by solid-state reactions at very high temperatures. Sulfur substitution was effected by passing gaseous carbon dioxilide over pure or tantalam-doped samples at elevated temperatures. The amount of sulfur substitution was controlled by varying the time and temperature of the reaction, with higher temperatures and longer reaction times affording greater substitution. Band-gap values varied in accordance with composition are compared with the density functional theory calculations and experimental techniques such as the optical reflectance spectroscopy and spectroscopic ellipsometry, and the agreement is impressive.
Q1.00247 Dielectric Polarization 1/f Noise: a signature of defect-free oxides at nanotransistors interface, NICOLAS CLEMENT, IEMN-CNRS (France), KATSUKIHIKO NISHIGUCHI, NTT Basic Research Labs (Japan), DOMINIQUE VUILLAUME, IEMN-CNRS (France), AKIRA FUJIWARA, NTT Basic Research Labs (Japan) — Low frequency 1/f noise has been a well-studied method for evaluation of materials quality for devices operation. The two main sources of 1/f noise have been identified as the mobility noise (Hooge's equation) related to defects in the channel and the trapping-detrapping noise (Mc Whorter equation) related to defects in oxide at semiconductor interface. Here we show that for a 0D nanotransistor (typically 15 nm diameter and 40 nm length), dielectric polarization 1/f noise is observed at room temperature when there is no defect at interface. Such noise, derived from the fluctuation-dissipation theorem and related to the imaginary part of the capacitance (fluctuation of dipoles in oxide), has been measured in capacitors but never reported in field-effect transistors due to its lower amplitude compared to trapping-detrapping noise inducing almost 1/f curve with only 2 active traps. Since in 0D transistors the Debye screening length is larger than devices dimensions at room temperature, trapping-detrapping noise amplitude is easily determined and distinguished from DP noise. Therefore, we believe that such noise is a non-invasive and direct method for claiming the absence of defects at semiconductor-oxide interface in nanodevices and probe the dynamics of dipoles in materials at nanoscale.

Q1.00248 Physical Insight into III-Nitride Material Quality for RF Transistors Based on Delay Time Analysis, PANKAJ SHAH, TONY IVANOV, FRANK CROWNE, TERRANCE O'REGAN, ANTHONY BIRDWELL, EDWARD VIVEIROS, US Army Research Laboratory — A delay time analysis provides valuable guidance on optimizing III-nitride high electron mobility transistors (HEMTs). The procedure involves extracting an RF lumped element compact model with parasitics. We will present trends observed for different III-nitride HEMTs. One case indicated an AlGaN/GaN structure with a thin GaN channel layer on a thicker low aluminum AlGaN buffer exhibited lower total carrier delays (2.48 ps) in the saturation region of operation (Vds between 4V and 9V) compared to a structure with a single thick GaN buffer (3.14 ps). This is related to the former structure's lower total transit time (1.88 ps vs. 2.21 ps). This result may be due to fewer defects in the thin GaN channel region grown on a thicker AlGaN buffer compare to using a single somewhat thicker GaN buffer on a thin AlGaN buffer, and a different electrostatic potential distribution due to the AlGaN acting as a back barrier. The former has a maximum intrinsic current cutoff frequency of 67 GHz vs 56 GHz for the latter. The influence of temperature which can affect carrier transport (intrinsic delay) and series resistances (charging delay) will be discussed. In-house pulsed current-voltage analysis and impedance analyzer based conductance measurements provide related information to confirm our results.

Q1.00249 Density functional calculations of point defects in InAs1, JONATHAN MOUSSA, PETER SCHULTZ, Sandia National Laboratories — Standard semilocal density functional methods do not generate a gap in the Kohn-Sham eigenvalues for InAs, a semiconductor with an experimental gap of 0.4 eV. Without a theoretical band gap, it becomes difficult to identify, specify and characterize pure localized states of point defects with energy levels within the experimental band gap. The bulk band gap problem can be alleviated with screened hybrid density functionals, such as the Heyd-Scuseria-Ernzerhof (HSE) functional, that open the generalized Kohn-Sham eigenvalue gap of InAs to near the experimental value. However, even without a Kohn-Sham gap, the local moment chargecounter (LMCC) method [Phys. Rev. Lett. 96, 246401 (2006)] is able to predict charge transition energy levels of localized defect states, using standard semi-local functionals. We present an LMCC-based study of standard point defects in InAs using semilocal density functionals and compare the results to HSE-based calculations to assess the validity of LMCC calculations in this situation.

1Sandia 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. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Q1.00250 Electron relaxation via interaction with optical phonons in disordered metals and semiconductors, ANDREI SERGEEV, MICHAEL REIZER, VLADIMIR MITIN, University at Buffalo — Using the Green function formalism we study the energy transfer from hot electrons to phonons due to interference between inelastic electron scattering on optical phonons and elastic scattering from imperfections and defects. We calculated the electron-phonon relaxation time and the electron-phonon thermal conductance as a function of the electron mean free path with respect to elastic electron scattering. We also investigate concentration dependencies of the relaxation processes. The results show that in semiconductors and in semiconductor structures the relaxation is enhanced by disorder, in metals and metallic structures the interference effect is strongly depends on vibrations of impurities and defects.

Q1.00251 Large Area Synthesis of WS2 Crystalline Sheets Directly on SiO2 and Their Transfer to Other Substrates, ANA LAURA ELIAS, NESTOR PEREA-LOPEZ, The Pennsylvania State University, ANDRES CASTRO-BELTRAN, Universidad Autonoma de Nuevo Leon, AYSE BERKDEMIR, SIMIN FENG, RUITAO LV, AARON LONG, The Pennsylvania State University, TAKUYA HAYASHI, YOONG AHM KIM, MORINOBU ENDO, Shinshu University, HUMBERTO R. GUTIERREZ, University of Louisville, SUJOY GHOSH, SAIKAT TALAPATRA, Southern Illinois University Carbondale, NIKHAR R. PRADHAN, LUIS BAILCAS, Florida State University, FLORENTO LOPEZ-URIAS, HUMBERTO TERRONES, MAURICIO TERRONES2. The Pennsylvania State University — Metal dichalcogenides (e.g. MoS2, WS2, NbS2) have attracted attention because they are layered materials that could exhibit either semiconducting or metallic properties. These materials could be significantly modified when these materials become monolayers. Here we report for the first time the synthesis of large area few-layer WS2 by a two step method. WO3 thin films were first grown on a Si/SiO2 substrate and these films were sulfurized in a second step. Furthermore, we have developed an efficient route to transfer these WS2 films onto different substrates. WS2 films of different thicknesses have been analyzed by Raman spectroscopy, HRTEM and AFM. Characterization techniques demonstrate the presence of mono-, bi- and few-layered WS2 in the as-grown samples. The novel photoluminescence properties of the films will also be discussed.

1on leave from IPICYT
2Shinshu University

Q1.00252 RuO2/Graphene composites for super-capacitor electrodes, FATIMA AMIR, TARIQ RAMALL. St John's University, REBECCA FOREST, University Of Houston — Metal oxides/graphene composites show significant improvement in their electrochemical properties compared to their individual constituents, such as high capacity, high rate capability and excellent cycling stability. Ruthenium dioxide (RuO2) has been recognized as an important electrode material for water electrolysis, oxygen reduction, and super-capacitors. A crucial aspect of all these applications is their structural, morphological and electrical properties. We have synthesized RuO2 from hydrolysis and oxidation of ruthenium tri-chloride RuCl3, which we physically mixed to graphene and used to coat tungsten substrates. For comparison, we also have deposited commercial RuO2 hydrate mixed with graphene on tungsten. The samples were then annealed at different temperatures. The effect of temperature has been studied in detail. Surface morphology analysis using a scanning electron microscope (SEM) shows smaller grain size at temperatures higher than 180 C. Structural properties obtained by using x-ray diffraction revealed an amorphous structure at temperatures lower than 180 C. The supercapacitance of the RuO2/graphene electrode is found to be dependent on the surface morphology.

1This project was supported by the Clare Booth Luce Foundation
Q1.00253 Diameter Control of HP-Ge Crystal Growth, HAO MEI, Univ. of South Dakota — Large single crystals of germanium are being grown using the Czochralski technique, in which a precisely cut seed crystal is dipped into the molten germanium and then withdrawn slowly, while maintaining the temperature of the melt just above the freezing point. Typically the seed is rotated while the crystal is being formed. The resulting crystal is typically oriented with a (100) crystal axis parallel to the growth direction. The crystal growth process is conducted in a hydrogen (H₂) atmosphere, with the H₂ flowing inside a quartz envelope. High purity germanium (HP-Ge) crystals with diameter 3 ~ 9 cm are grown on weekly basis at university of South Dakota. As Czochralski growth is a dynamic process, the thermal geometry in the furnace undergoes a considerable change during the crystal growth process. A load cell was introduced to control the crystal growth process. Growing crystals with automation system is studied. In order to grow crystal automatically, the relationship between input power and crystal weight or crystal diameter is investigated. We show that HP-Ge crystal growth could be controlled automatically using software with feedback system.

Q1.00254 Surface passivation effects on the performance of p-planar HPGe radiation detector, MUHAMMAD KHIZAR, GUOJIAN WANG, DONGMING MEI, University of South Dakota, South Dakota, USA — Surface passivation of HPGe detectors are always critical to reduce or eliminate the surface effects responsible for limiting both the leakage current and breakdown voltages of these devices. Among the critical part of any HPGe detector is the intrinsic surface, where the full bias voltage is applied at 77K. Typically, in order to make these surfaces electrically passive, and to avoid surface leakage currents, a thick layer of SiO₂ is deposited by using different high temperature dry/wet deposition techniques. However, surface passivation using such techniques can result modifying the electrical field, by compromising the charge collection in the volume near the contact surfaces. Another option is the amorphous germanium (a-Ge), which acts as a passivant as well as bi-polar blocking contacts. In this study, we have designed a controlled experiment to use Ge oxidation contact as a passivation layer by testing the electrical behavior of the crystal after each oxidation treatment. For this, a high quality a-Ge layer (~100 nm to 150 nm) is deposited at 1.5x10⁶ torr using low temperature RF plasma sputtering deposition technique. Among the key characteristics of the deposited passivation layer includes the depositions rates, the precursors (pre-mixed (H₂:15% and Ar) flow rates, plasma power, chamber pressure, and target to-substrate distance. We show the results from our study using home grown HPGe crystals at USD.

Q1.00255 Performance optimization of c-Si1-xGex/Si heterostructure thin film solar cells with step-graded bandgap profile, MUHAMMAD KHIZAR, MD. AMINUAL EHSAN, JAYESH GOVANI, DONGMING MEI, University of South Dakota, South Dakota, USA — In this paper, the performance optimization of c-Si1-xGex/Si heterostructure thin film solar cells along with the effect of step-graded absorber layer is discussed by modeling and simulation. Different cells with 1, 3, 5, and 7µm thick step-graded layers of p-type c-Si1-xGex on top of 20µm p-Si buffer layer are simulated. A comparative study of the thin film solar cell structures with and without a step-graded absorption layer is also performed. Some of the key characteristics such as short-circuit current density (Jsc), open circuit voltage (VOC), and fill factor (FF) are calculated for varying concentration of Germanium (Ge) in c-Si1-xGex graded layer. With the optimized Ge concentration in the step-graded layer, significant enhancement in the overall efficiency of the solar cells has been calculated. The effect of thickness variation of alloyed layer for varying Ge composition ~ 0.1—10% has also been carried out. Finally, the cell performance is calculated on the bases of current density–voltage characteristics curves and external quantum efficiency. We found that the optimized graded cell structure with larger Ge fraction was responsible for a higher magnitude and smaller thickness dependence of the short circuit current density. This is attributed to the larger absorption coefficient that increases optical carrier generation in the near surface region for larger Ge contents. Further studies for the band-gap engineering of this step-graded absorber layer is still being performed.

Q1.00256 Magneto-transport measurement in BiTeI single crystal, CHANG-RAN WANG, Institute of Physics, Academia Sinica, CHIA-TSO HSIEH, Institute of Physics, Academia Sinica, Department of Physics, National Taiwan University, RAMAN SANKAR, Center for Condensed Matter Sciences, National Taiwan University, WEI-LI LEE, Institute of Physics, Academia Sinica, GUANG-YU GUO, Graduate Institute of Applied Physics, National Chengchi University, Department of Physics, National Taiwan University, FANG-CHENG CHOU, Center for Condensed Matter Sciences, National Taiwan University. INSTITUTE OF PHYSICS, ACADEMIA SINICA TEAM, DEPARTMENT OF PHYSICS, NATIONAL TAIWAN UNIVERSITY COLLABORATION. CENTER OF NONLINEAR SCIENCE AND TECHNOLOGY OF CHINA TEAM — TiO₂ is a large band gap semiconductor with a wide range of applications including in photocatalysis, decontamination, and solar-energy conversion. Conversion to the well studied rutile phase, the anatase phase appears more common in nanocrystals and shows higher activity in photocatalysis. However, only a few literatures investigated the surface structure of anatase(001), which is assumed to be the origin of anatase's high reactivity, due to its thermodynamic instability and the difficulty in obtaining high quality samples. In the present work, reconstructed anatase TiO₂(001)(1×4) surface has been investigated by atomic resolved STM together with the first-principles calculations. Two types of defects were found on the surface, which appear as dark spots and bright spots. The adsorption behavior of H₂O, O₂, and CO₂ molecules were studied. Surprisingly, it was found that all the molecules only adsorbed on the defect sites, which is against to the current understanding of the high activity of anatase (001) surface. Based on first-principles calculations we provide a new structure model of O saturated TiO₂(001) (1×4) surface, which behaves inactive in photocatalysis.

Q1.00257 Surface Reconstruction and Molecular Adsorption on Anatase TiO₂(001)-(1×4), HUJUJIAN SUN, BING WANG, JIN ZHAO, BING WANG, JINLONG YANG, JIANGUO HOU, University of Science and Technology of China, UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA TEAM — TiO₂ is a large band gap semiconductor with a wide range of applications including in photocatalysis, decontamination, and solar-energy conversion. Conversion to the well studied rutile phase, the anatase phase appears more common in nanocrystals and shows higher activity in photocatalysis. However, only a few literatures investigated the surface structure of anatase(001), which is assumed to be the origin of anatase's high reactivity, due to its thermodynamic instability and the difficulty in obtaining high quality samples. In the present work, reconstructed anatase TiO₂(001)(1×4) surface has been investigated by atomic resolved STM together with the first-principles calculations. Two types of defects were found on the surface, which appear as dark spots and bright spots. The adsorption behavior of H₂O, O₂, and CO₂ molecules were studied. Surprisingly, it was found that all the molecules only adsorbed on the defect sites, which is against to the current understanding of the high activity of anatase (001) surface. Based on first-principles calculations we provide a new structure model of O saturated TiO₂(001) (1×4) surface, which behaves inactive in photocatalysis.

Q1.00258 Characterization of Terminal Hydroxyl on TiO₂(110) Surface, QIUNG ZHENG, HAO FENG, SHIJING TAN, JIN ZHAO, BING WANG, JINLONG YANG, JIANGUO HOU, University of Science & Technology of China, UNIVERSITY OF SCIENCE & TECHNOLOGY OF CHINA TEAM — TiO₂ is important in a wide variety of applications, among which is the water splitting and hydrogen production. However, as an important intermediate product of H₂O splitting, terminal hydroxyl has not been well studied. In the present work, we have used STM together with first-principles calculations to investigate the electronic and structural properties of terminal hydroxyl on the calculated TiO₂(110) (1×2) surface, which is associated with a high conductance and a low conductance state in the I-V spectral. Based on the first-principles calculations, we assign this feature to proton hopping between bridge oxygen and terminal oxygen with a hopping barrier of 0.29 eV. The hopping rate under various applied biases and the current follow a power-law: R ~ I², which implies an inelastic electron tunneling process. Moreover, the hopping rate increased exponentially with increasing biases, reminiscent of thermal excited Arrhenius relation, while in our case it is hot electron excitation.
Q1.00255 Ultrafast coherent acoustic and optical phonon dynamics of amorphous Ge$_2$Sb$_2$Te$_5$ thin films. MIN JU SHIN, DONG HAK KIM, DAEYOUNG LIM, Kyung Hee University — The coherent acoustic and optical phonon dynamics of Ge$_2$Sb$_2$Te$_5$ (GST) thin films are investigated by pump-probe spectroscopy. The transient reflectivity changes with oscillation period on the order of sub-picosecond and tens of picoseconds were observed. The longer oscillation with oscillation period and dephasing time on a time-scale of tens of picoseconds hasn’t been reported previously and can be consistently explained by coherent acoustic phonon generation in the form of a stain pulse propagating into substrate. The shorter period oscillations correspond to coherent optical phonon $A_1$ mode by displacive excitation of coherent phonon mechanism. Its temperature dependent frequency shift was due to a three-phonon anharmonic decay, while its dephasing was dominated by temperature independent phonon-defect scattering. Laser fluence-dependent coherent optical phonon $A_1$ mode softening and a dephasing rate increase were observed and attributed to the high density electrons and accompanying lattice distortion as well as to the lattice heating.

Q1.00260 Observation of amorphous InGaZnO by aberration corrected transmission electron microscope. TAIKHIRO SUZUKI, KUNIO TAKAYANAGI, Tokyo Institute of Technology; Crest, JST — Transparent amorphous oxide semiconductors (TAOSs) such as amorphous InGaZnO (a-IGZO) have been receiving a good deal of attention [1,2]. High conductivity of TAOSs is understood by the overlap between metal s-orbitals, where metals locate at oxygen octahedral sites. We investigated local order of metals by transmission electron microscopy in which electron phases are well adjusted using aberration correctors up to the wave vector of $2\pi/50$ pm. Auto correlation of high resolution electron micrographs of a-IGZO thin films showed the first nearest neighbor metal-metal distance. Metal-metal distance depends on the overlapping between the s-orbitals, so that such structural information helps characterization of electron mobility of TAOSs.

Q1.00261 Zero-point motion and temperature effects on the band gap of semiconductor nanoclusters. GABRIEL BESTER, P. HAN, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — We calculate the band gap renormalization of semiconductor nanoclusters, avoiding the high computational costs associated with the calculations of the self-energy (Fan) and the Debye-Waller terms. This approach allows us to address clusters with a few hundred atoms. For Silicon nanoclusters, we obtain a band gap reduction of hundreds of meV associated with the quantum zero point motion. This reduction rapidly increases with decreasing cluster size. Based on the Bose-Einstein distribution, we further study the temperature dependence of the band gap in semiconductor nanoclusters and find a band gap shift of -580 meV and -270 meV when going from $T = 0$ to room temperature for silicon clusters with radii of 9.6 and 11.9 Å, respectively. Furthermore, we find that the band gap renormalization of semiconductor nanoclusters is dominated by the optic-like vibrational modes with $\Gamma_4$ point group symmetry.

Q1.00262 Calculation of Energy States for Multi-Layer GaAs-AlGaAs Semiconductor Laser. CHIN-SHENG WU, Yuan Ze University — Semiconductor laser operation requires high frequency performance. Multi-layer Quantum wells are effective prameters in semiconductor lasers because they allow some extra degree of freedom in the design of the desired emitted wavelength through adjustment of the wells numbers in addition to width $w$ around 15 nm and barrier height $V'$ around 300 meV. Those wells are to provide the potential term of the Shrödinger equation. Dispersion relation between the energy and wave number increases the first term of the Shrödinger equation, which is the kinetic energy. Hence dispersion relations in conduction band and valence band are available for the effective mass approximation. We also add the exchange-correlation energy into the Shrödinger equation. Alternating GaAs-AlGaAs layers produce a variety of energy states. Transitions among states are related to laser frequencies. Because of the presence of multi-layer quantum wells the electrons have discrete energies and these appear as peak in the absorption measurements.

Q1.00263 Tunable Band Gap of Boron Nitride Interfaces under Uniaxial Pressure. ELIZANE MORAES, TAISE MANHABOSCO, ALAN DE OLIVEIRA, RONALDO BATISTA, Federal University of Ouro Preto — In this work we show, by means of a density functional theory formalism, that the interaction between hydrogen terminated boron nitride surfaces gives rise to a metallic interface with free carries of opposite sign at each surface. A band gap can be induced by decreasing the surface separation. The size of the band gap changes continuously from zero up to 4.4 eV with decreasing separation, which is understood in terms of the interaction between surface states. Due to the high thermal conductivity of cubic boron nitride and the coupling between band gap and applied pressure, such tunable band gap interfaces may be used in high stable electronic and electromechanical devices. In addition, the spacial separation of charge carries at the interface may lead to photovoltaic applications.

Q1.00264 Bending strain induced exciton fine-structure splitting and shift in bent ZnO microcrystallines. XUEWEN FU, QIANG FU, ZHIMIN LIAO, XINLI ZHU, JUN XU. School of physics, Peking University, Beijing, China, HANCHUN WU, CRANN School of Physics, Trinity College Dublin, Dublin, Ireland, ZHUHUA ZHANG, WANLIN GUO, Institute of Nano Science, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P. R. China, Nanjing, China, DAEWON MIN, School of physics, Peking University, Beijing, China — Bend Strain causes rich physical phenomena, such turning the mechanical energy into electricity in nanowire nano-generators by Z. L. Wang, significant modification of the emission energy of semiconductor micro/nanowire materials up to 100 meV, and enhancement of the light emission intensity up to 17 times of the LEDs etc. Here, we investigate for the first time the exciton spectra evolution in bent ZnO microcrystallines along the radial direction via high spatial/energy resolution cathodoluminescence (C-CL) spectroscopy. Our experiments show that the exciton peak splits into many fine peaks towards the compressive part while retains one peak in the tensile part and the emission peak displays a continuous blue-shift from tensile to compressive edges. In combination with first-principles calculations, we show that the observed near-band-edge emission splitting in compressive side is due to the valence band splitting by compressive strain and the absence of peak splitting in the tensile part may be due to the highly localized holes in the A band and the carrier density distribution across the microwire by piezoelectric effect induced electric field. Our studies may pave the way to design nanophotonic and electronic devices using bent ZnO nanowires.

Q1.00265 Applications of the Reduced-Density-Matrix Description to Electronic Relaxations in Solids and Nanostructures Due to Scattering by Phonons. ALEX KUTANA, Rice University, VERNE JACOBS, Naval Research Laboratory — We show some examples of the application of our reduced-density-matrix description to electronic relaxations in solids and nanostructures. In this work, we apply the theory to study the behavior of electrons and holes in the bulk phase as well as at the interface between two nanoscale materials. We evaluate carrier lifetimes and quantify charge and energy transfer in these systems. We also calculate line widths and shifts that are then used to construct theoretical linear absorption spectra, which are compared with experimental results.

Work supported by the Office of Naval Research. A portion of this work was performed under the ASEE post doc program at NRL.
Q1.00266 Reduced-Density-Matrix Approach for the Spectral Description of Multi-Photon Processes in Quantized Many-Electron Systems. VERNE JACOBS, Naval Research Laboratory, ALEX KUTANA, Rice University. — A reduced-density-matrix description is developed for the evaluation of the frequency-dependent transition rates for multi-photon processes in quantized many-electron systems. Our objective is to provide a fundamental foundation for systematic spectral simulations for atomic, molecular, and solid-state systems. A perturbation expansion of the frequency-domain Liouville-space self-energy operator is employed to evaluate the spectral-line widths and shifts in the isolated-line and short-memory-time (Markov) approximations. The lowest-order contributions from environmental electron-photon and electron-phonon interactions are systematically taken into account. The proposed description is directly applicable to dynamical processes in a variety of systems, including semiconductor, photochemical, and biological, without further approximations. In particular, our description can be applied to investigate the dynamical behavior of electrons in bulk and nanoscale semiconductor materials entirely from first principles, using the density functional formalism and existing electronic structure codes.

1Work supported by the Office of Naval Research. A portion of this work was performed under the ASEE post doc program at NRL.

Q1.00267 Microscopic charge fluctuations in hexagonal boron nitride. ADRIA NICOLAEV, University of Bucharest, Faculty of Physics, Materials and Devices for Electronics and Optoelectronics Research Center, CLAUDIA RODL, GIULIA PEGOLOTTI, RALF HAMBACH, LUCIA REINING, Laboratoire des Solides Irradiés, UMR 7642, CNRS-CEA, Ecole Polytechnique, F-91128 Palaiseau, France and European Theoretical Spectroscopy Facility, STEFAN ANTOKE, University of Bucharest, Faculty of Physics, Materials and Devices for Electronics and Optoelectronics Research Center — We present an ab initio approach to the electron dynamics through the calculation of the total polarizability matrix, including the off-diagonal elements. The charge density induced in a system by an external perturbation is computed in real space and time, following the idea of Abbamonte et al. The difference between our approach and the one from Ref. [1] is that we can calculate not only the diagonal response $\chi(q,\omega)$, but also the off-diagonal elements of the matrix $\chi_{\alpha\beta}(q,\omega)$. Hence, we have access to the microscopic charge oscillations which are induced by the local-field effects. We have studied these charge oscillations at various frequencies comprising interband-transition and plasmon-excitation energies. The real-space approach allows us to see which electrons (or orbitals) contribute to which kind of excitation. The final goal is to offer theoretical support and benchmark to future inelastic x-ray scattering experiments that may measure also the off-diagonal elements of the polarizability. The method is applied to hexagonal boron nitride (h-BN) which is the most stable of the three existing structures (hexagonal, cubic, and wurtzite) at room temperature and ambient pressure.

2Support from the ESF through the project POSDRU 107/1.5/S/80765 is acknowledged.

Q1.00268 Infrared optical properties of Mn1.56Co0.96Ni0.48O4 thin films prepared by chemical solution deposition. YANQING GAO, ZHIMING HUANG, YUN HOI, JING WI, WEI ZHOU, LEI FANG, ZHUHAI CHU, Shanghai Institute of Technical Physics — Mn1.56Co0.96Ni0.48O4 (MCN) films have been prepared on Al2O3 substrate by chemical solution deposition method. X-ray diffraction and microstructure analyses show a cubic spinel structure and the thickness of the films is 2.12 μm. Mid-infrared optical properties of MCN films have been investigated using transmission spectra and infrared spectroscopic ellipsometry. The transmission spectra can roughly be divided in two regions: a transparent oscillating one at longer wavelength and a strongly absorbing one for wavelength less than 2.2 μm. The optical band gap of the MCN film has been derived to be 0.64 eV by assuming a direct transition between valence and conduction bands. The optical constants and thickness of the thin films have been obtained by fitting the measured ellipsometric parameter data with classical infrared model. The refractive index n of the MCN films decreases as the wavelength increases, but the extinction coefficient k monotonously increases in the wavelength range of 2-7 μm. The maximal n value is 2.63, and the maximal k value is only 0.024. The above results are instructive for the applications of MCN films in infrared detecting.

Q1.00269 Carrier recombination in m-plane GaN thin films. ZHI-XUAN TZENG, Department of Physics, National Kaohsiung Normal University, YAN-ZHI TZENG, Department of Physics, National Sun Yat-sen University, MENF-EN LEE, Department of Physics, National Kaohsiung Normal University, DER-JUN JANG, Department of Physics, National Sun Yat-sen University — The radiative and nonradiative recombination of InGaN/GaN multi-quantum well light emitting diode was studied by a time-correlated single-photon counting apparatus with temporal resolution of 150 ps using laser pulses of energy 4.5 eV from a Ti:sapphire laser. Two major PL peaks were found in all the three GaN samples with different N/Ga ratios. The PL contributed by the bandgap recombination was found first blue-shift below 100 K and become red-shift with increasing temperature. The carrier localization, for both holes and electrons, is responsible for the blue-shift in PL spectra and constant of radiative rates below 100 K. The temperature dependence of radiative recombination time is consistent with theoretical prediction. The carrier localization, for both holes and electrons, is responsible for the blue-shift in PL spectra and constant of radiative rates below 100 K.

Q1.00270 The carrier recombination of InGaN/GaN MQW LED. CHING-LIANG LIN, SHAN-FU WANG, ZHI-XUAN CHEN, DER-JUN JANG, Department of Physics, National Sun Yat-sen University, MENF-EN LEE, Department of Physics, National Kaohsiung Normal University — The radiative and nonradiative recombination of InGaN/GaN multi-quantum well light emitting diode was studied by a time-correlated single-photon counting apparatus with temporal resolution of 150 ps using laser pulses of energy 4.5 eV from a Ti:sapphire laser. The energy of the PL peak intensity was found to be blue-shift below 100 K and become red-shift with increasing temperature. Activation energies of 11 and 109 meV were found by single-photon counting apparatus with temporal resolution of 150 ps using laser pulses of energy 4.5 eV from a Ti:sapphire laser. Two major PL peaks were found in all the three GaN samples with different N/Ga ratios. The PL contributed by the bandgap recombination was found first blue-shift below 100 K and then red-shift as temperature increases. We found that the internal quantum efficiency as well as the nonradiative recombination rate decreased with N/Ga ratio may be due to the large defect concentration in high N/Ga ratio. The radiative recombination rate was constant below 100 K in all samples and was dependent on temperature with $T^{-3/2}$. The temperature dependence of radiative recombination time is consistent with theoretical prediction. The carrier localization, for both holes and electrons, is responsible for the blue-shift in PL spectra and constant of radiative rates below 100 K.

Q1.00271 Electronic and optical properties of hexagonal boron nitride thin films. Y. CHEN, B. CAI, M.L. NAKAKAMI, Department of Physics, Graduate Center and Brooklyn College - CUNY, R.C. RAI, Department of Physics, SUNY College at Buffalo — We report the surface, structural, electronic, and optical properties of hexagonal boron nitride (h-BN) thin films grown on (0001) sapphire substrate by an electron-beam deposition technique. The h-BN thin films have been deposited in nitrogen environment and post-deposition annealed to improve the stoichiometry and the crystalline quality. Atomic force microscopy, x-ray diffraction, optical spectroscopy, and Hall-effect measurement were employed to characterize the h-BN thin films. We carried out temperature dependent transmittance measurements (78 – 450 K and 190 – 3000 nm) on the h-BN thin films in order to investigate the optical properties and the temperature dependence of the energy band gap. The optical data below the energy band gap have been modeled with the Urbach effect and a free exciton. We present the temperature dependence of the free exciton and the energy gap of undoped h-BN thin films. The results will be compared with photoluminescence measurements. We will also present the results of Mg-doped h-BN thin films in an effort to make p-type h-BN.
Q1.0027 Calculation of the gap in Ce$_{1/2}$NbO$_3$. PABLO DE LA MORA, Facultad de Ciencias, JOSE FRANCISCO GOMEZ GARCIA, Facultad de Quimica, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Nacional Autonoma de Mexico — With experimental measurements, Ce$_{1/2}$NbO$_3$ was found to have a small gap of 0.25-0.78eV. In order to find whether this gap is due to electronic origin ab-initio DFT (WIEN2k) calculations were done. To find the correct gap, the calculations were done using a modified Becke-Johnson (mBJ) potential. A ‘conducting’ Nb-O gap with a Ce:4f peak in the middle was found. In the convergence process, due to the nature of the mBJ potential, this Ce:4f interfered with the Fermi energy $E_F$. To avoid this problem a Hubbard $U_{ff}$ was added to the Ce atom, then it was possible to extrapolate back and obtain the correct ‘conducting’ Nb-O gap of 2eV with the Ce:4f peak at 1.36eV from the lower end of the gap. With this it can be confirmed that the conduction is not of electronic nature.

Q1.00273 Ab-Initio Study of Excitonic Absorption for Layered LaCuChO and BaCuChF (Ch= {S,Se,Te}) Structures, JASON VIELMA, GUENTER SCHNEIDER, Oregon State University — Layered oxychalcogenides LnCuChO (Ln = {La,Pr,Nd}, Ch = {S,Se,Te}) and isostructural layered fluorochalcogenides BaCuChF have drawn much interest in recent years as p-type wide bandgap semiconductors with applications in transparent electronics and photovoltaics. Members of both materials show strong excitonic absorption, which is observable at room temperature. However, recent studies disagree on the origin and nature of the room temperature excitons in the respective families of materials, with Ueda et al. [1] attributing the room temperature excitonic absorption in LaCuSeF to 2 dimensional quantum confinement of hole carriers in the layered structure, while Zakutayev et al. [2] argue that the room temperature excitonic absorption in BaCuChF is well described by a 3 dimensional Wannier-Mott exciton model. We report an ab-initio computational study of the optical properties including the excitonic effects for both families of materials. The optical properties are calculated using the Bethe-Salpeter equation in the GW approximation.


Q1.00274 Monovacancy in hcp-Zirconium. A. ZAKUTAYEV, et al. Phys. Rev. B (Ln = {monovacancy of hcp-Zirconium under various strains by examining the vacancy formation energy through density functional theory calculations. There is a monopolistic strain dependence on the formation energy, the formation energy decreases with respect to the increment of volumetric strain. The formation energy as a function of pressure was also examining, with a minimum value of 2.00 eV at zero pressure. The formation volume decreases with respect to the pressure, with a value of 0.6 unit-atom-volume at zero pressure particularly. The formation enthalpy increases monotonically as the pressure increases. At a pressure of ~5 GPa, the formation enthalpy becomes negative and thus the system fails.

Q1.00275 The rare earth 4f hybridization with the GaN valence band. LU WANG, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, STEVE MCHALE, JOHN MCCLOY, JAMES PETROSKY, Department of Engineering Physics, Air Force Institute of Technology, OH 45433, J. WUL, RATNARAK PALAI, Department of Physics and Institute for Functional Nanomaterials, University of Puerto Rico, San Juan, Puerto Rico 00931, YAROSLAV LOSOVYJ, The J. Bennett Johnston Sr. Center for Advanced Microstructures and Devices, Louisiana State University, Baton Rouge, LA 70806, PETER DOWBEN, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588 — The placement of the Gd, Er, and Yb 4f states within the GaN valence band has been explored by both experiment and theory. The 4f → 4f photoemission resonances for various rare earth GaN thin films (RE = Gd, Er, Yb) provide an accurate depiction of the occupied 4f state placement within the GaN. The resonant photoemission show that the major Er and Gd rare earth 4f weight is at about 5-6 eV below the valence band maximum, similar to the 4f weights in the valence band of many other rare earth doped semiconductors. For Yb, there is very little resonant enhancement of the valence band of Yb doped GaN, consistent with a largely 4f$^{14-8}$ occupancy. The placement of the rare earth 4f levels is in qualitative agreement with theoretical expectations.

Q1.00276 MAGNETISM —

Q1.00277 Competition between the screening effect and exchange interactions in the system CeCu$_{1-x}$Al$_x$Ge$^6$. W.H. LEE, J.R. LEE, H.H. SUNG, K.J. SYU, S.C. CHEN, Department of Physics, National Chung Cheng University, W. H. LEE TEAM — As revealed in the powder x-ray diffraction and crystallographic data, the single phase sample in the series CeCu$_{1-x}$Al$_x$Ge (0.1<x<0.5) crystallizes in the PoGa$_2$-type structure with space group P6/mmm. The substitution of Cu by Al in CeCu$_{1-x}$Al$_x$Ge, which increases the average conduction electron density, was found to be able to attenuate the localized Ce 4f moments. As determined from the electrical-resistivity and magnetic susceptibility measurements, both the ferromagnetic transition temperature $T_c$ value and the magnitude of the saturation moment in the series CeCu$_{1-x}$Al$_x$Ge reflect the decreasing strength of exchange interactions with the Al concentration. These results suggest that the screening effect surpasses the RKKY interactions in this system.


Q1.00278 Measuring nontrivial fusion rule of Majorana fermions in inhomogeneous transverse Ising chain, YAN CHEN, YINCHEN HE, Fudan University, China — We describe various dynamical processes aimed to create and fuse Majorana fermions in an inhomogeneous Kitaev’s wire. We show that, with the undesired excitations suppressed by inhomogeneity, fusion of Majorana fermions will result in universal measurable excitations, which can serve as a direct verification of Majorana fermions fusion rule. Moreover, we design a protocol to detect the oscillatory tunneling between two unpaired Majorana fermions. Most remarkably, our proposal is valid for transverse Ising chain, which provides a promising way to test nontrivial properties of Majorana fermions experimentally.

Q1.00279 Magnetic structure of BiFeO$_3$, V. KIRYUKHIN, M. RAMAZANOGLU, S. LEE, S-W. CHEONG, Rutgers University, W. RATCLIFF, M. LAVER, NIST, J.G. PARK, Seoul Natl. Univ. — Neutron scattering studies of the magnetic structure of single-crystalline BiFeO$_3$ are presented. Temperature dependence of the magnetic order parameter, the anharmonicity of the magnetic cycloid, and the small tilt of the spins out of the cycloid plane (local weak ferromagnetism) are discussed. Inelastic neutron scattering measurements of the microscopic magnetic coupling constants are also presented.

Q1.00280 Dynamic decay of single vortex into vortex-antivortex tuples, SHIKHA JAIN, VALENTYN NOVOSAD, Materials Science Division, Argonne National Laboratory — A variety of metastable states, including vortices, antivortices, and their combinations is typical for magnetically soft-thin films and patterned structures. Physics of individual spin vortices in patterned structures has been rather extensively explored. In contrast, there are only few studies of vortex – antivortex – vortex (v-av-v) system, in a part because v-av-v is rather difficult to obtain in experimental samples. In this work we will demonstrate how a recently proposed resonant-spin-ordering technique can be used to induce the dynamic decay of a single vortex into vortex-antivortex states in elongated elements. The approach is based on driving the system from the linear regime of constant vortex gyrotations to the non-linear regime of vortex-core reversals at a fixed excitation frequency. Subsequently reducing the excitation field to the linear regime stabilizes the system into v-av-v state that is completely decoupled from the initialization excitation frequency. Newly acquired v-av-v state is a stable state in remanence, is characterized by a number of collective excitation modes, depending on the combination of the vortex core polarities, and/or the excitation field direction.
Q1.00281 Percolation transition in quantum Ising and rotor models with sub-Ohmic dissipation. MANAL AL-ALI, Missouri University of Science and Technology, JOSE HOYOS, Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, THOMAS VOLTA, Missouri University of Science and Technology — We investigate the influence of sub-Ohmic dissipation on randomly diluted quantum Ising and rotor models. The dissipation causes the quantum dynamics of sufficiently large percolation clusters to freeze completely. As a result, the zero-temperature quantum phase transition across the lattice percolation threshold separates an unusual super-paramagnetic cluster phase from an inhomogeneous ferromagnetic phase. We determine the low-temperature thermodynamic behavior in both phases which is dominated by large frozen and slowly fluctuating percolation clusters. We relate our results to the smeared transition scenario for disordered quantum phase transitions, and we compare the cases of sub-Ohmic, Ohmic, and super-Ohmic dissipation.

1This work has been supported in part by the NSF under grant no. DMR-0906566, by FAPESP under Grant No. 2010/ 03749-4, and by CNPq under grants No. 590903/2011-8 and No. 302301/2009-7.

Q1.00282 Effect of Crystal Fields in $H_{O1-x}D_{2h}N_{12}B_{2}C$ , W.C. LEE, Dept. of Physics, Sookmyung Women’s Univ., Seoul 140-742, Korea — From the anisotropy and the temperature dependence of magnetic susceptibilities of $H_{O1-x}D_{2h}N_{12}B_{2}C$ system with magnetic field H perpendicular or parallel to c-axis, the crystalline electric field (CEF) effect has been studied and the magnetic exchange interaction constant $J_{ex}$ of rare-earth ions perpendicular to the c-axis estimated for $0 \leq x \leq 1$. The crystalline electric field parameter, $B_{Q2}$, the first Steven parameter and the most dominant term in this system, are determined from the high-temperature-limit anisotropic Weiss temperatures of the magnetic susceptibilities and there is a broad minimum around $x \sim 0.3$, where superconducting transition temperature, $T_{c}$, and Neel temperature, $T_{N}$, are almost same.

Q1.00283 A mean-field study of the Hubbard model on the anisotropic kagomé lattice, MATTHEW ENJALRAN, Southern Connecticut State University — The study of material and model systems with the kagomé lattice structure has been an active area in the field of frustrated magnetism for decades. Formed from a 2D network of corner sharing triangles, the kagomé lattice can be realized as well separated planes in materials with large moments [3] or quantum spin systems (herbertsmithite, $S=1/2$) or as a derived lattice structure, for example in pyrochlore spin ice materials in the presence of a external field along the [111] crystallographic direction. Numerous magnetic model Hamiltonians have been applied to the kagomé lattice and studied via a range of theoretical and numerical techniques. Much has been learned about new phases of matter from these works, and interest in these systems continues to grow. However, comparatively less is known about the possible low temperature phases of correlated electrons on the kagomé lattice. Hence, we study the single band Hubbard model on the kagomé lattice using mean-field theory. We allow for anisotropically hopping in order to study the effects of variable frustration on the low temperature phases of the model and for comparison to materials with distorted kagomé structures. We present preliminary results from our work.

Q1.00284 Entanglement Entropy of zig-zag spin chains with Ring Exchange, JON SPALDING, California State University, Northridge — In the study of interacting quantum spin chains, the ground state wavefunction carries information about the phases of matter that occur for different interaction parameters. In this case, a spin-1/2 chain with 3 interaction terms in the Hamiltonian–nearest neighbor, next nearest neighbor, and ring exchange, is investigated using entanglement entropy to map out a ground state phase diagram. In addition, further information can be obtained from the entanglement spectrum. Finally, preliminary investigations of the effects of an impurity on this triangular Heisenberg ladder are reported.

Q1.00285 Theoretical Study of Anisotropic Magnetoresistance Effect: Magnetization Direction Dependence in Ferromagnet with Crystal Field of Cubic Symmetry, SATOSHI KOKADO, Faculty of Engineering, Shizuoka University, MASAKIYO TSUNODA, Graduate School of Engineering, Tohoku University, FUJUN YANG, Faculty of Physics and Electronic Technology, Hubei University, YUYA SAKURABA, KOKI TAKANASHI, Institute for Materials Research, Tohoku University, KIKUO HARIGAYA, Nanosystem Research Institute, AIST, AKIMASA SAKUMA, Graduate School of Engineering, Tohoku University — We theoretically study the magnetization direction dependence of anisotropic magnetoresistance (AMR) effect of a ferromagnet with a crystal field of cubic symmetry. We first extend our theoretical model [1] to a model including the crystal field effect. Using the model, we next obtain an analytical expression of the AMR ratio, that is, $\text{AMR}(\theta) = C_2 \cos(2\theta) + C_4 \cos(4\theta)$, where $\theta$ is the relative angle between the magnetization direction and the electric current direction. The coefficients $C_2$, $C_4$, and $C_6$ are expressed by a spin-orbit coupling constant, an exchange field, a crystal field, and s-s and s-d scattering resistivities. Using this expression, we analyze the following experimental results for FeNi [2] and Co2MnSi Heusler alloy [3]: As for FeNi [2], $|C_2|$ and $|C_4|$ increase with decreasing temperature. In contrast, Co2MnSi Heusler alloy [3] has a small temperature dependence of $C_2$ and $C_4 \approx 0$.


Q1.00286 ABSTRACT WITHDRAWN

Q1.00287 High-field magnetization studies of spin-dimer systems on low-dimensional spin systems, LiCu$_2$xZn$_x$O$_2$ and FeTe$_3$O$_7$X (X = Cl, Br), J.L. HER, Division of Natural Science, Chang Gung University, Taiwan, H.C. HSU, Institute of Physics, Academia Sinica, Taiwan, Y.H. MATSUDA, K. KINDO, Institute for Solid State Physics, The University of Tokyo, Japan, C.C. CHOU, H.D. YANG, Department of Physics, National Sun Yat-Sen University, Taiwan, H. BERGER, Institutes of Physics of Complex Matter, EPFL, Lausanne, Switzerland, F.C. CHOU, Center for Condensed Matter Sciences, National Taiwan University, Taiwan — High-field magnetization of two kinds of low-dimensional spin system was studied in pulsed magnets. Several anomalies were observed in $\frac{dM}{dT}$ curves of doped LiCu$_2$xZn$_x$O$_2$ ($x = 0.07$) at low temperatures (1.3 K $T < 20$ K). When temperature decreases, the anomalies sharpens or splits at certain critical temperatures which are related to the formation of isolated spin-dimer and spin freezing state. A field-induced spin density wave state was suggested to exist at high magnetic fields. The doping of Zn$^{2+}$ ions breaks the spin-chain of Cu$^{2+}$ ions, leading to the formation of isolated spin-dimers and lowering the critical field of formation of spin density state. The magnetization process were preformed on another series of samples, FeTe$_3$O$_7$X (X = Cl, Br), which has spin-dimer, formed by Fe$^{3+}$ ions, at low temperatures and magnetic fields up to 100 T. At low temperatures, the magnetization process show four step-like structures, which have nearly equal spaces of 25 T. Both samples show similar behavior. These steps are considered to be the magnetic excitation of the antiferromagnetic spin-dimers.

Q1.00288 Giant magnetic moment in Mn11Si19 microparticles at room temperature, KIYOTAKA HAMMURA, Hitachi Cambridge Laboratory, University of Cambridge, HARRUKIKO UDONO, TOMOSUKE AONO, Ibaraki University — Following our previous paper reporting enhancement of magnetic moment in powder Mn11Si19 (∼30 microns in diameter), we report here on magnetic moment for smaller particles (∼5 microns in diameter) at 5 K to 300 K. Apart from the larger particles case, magnetisation curves against field exhibit distinctive features of soft magnetic materials over the whole range of temperatures. We observed a sort of superparamagnetism in non-microparticles.
Q1.00289 Thermal-magnetic-electric oscillator based on spin-valve effect. HEE CHUL PARK, Korea Institute for Advanced Study, Seoul, Korea, ANATOLY M. KADIGROBOV, Theoretische Physik III, Ruhr-Universitat Bochum, Germany, S. ANDERSSON, Nanostructure Physics, Royal Institute of Technology, Stockholm, Sweden, DANKO RADIC, Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia, ROBERT I. SHEKHTER, MAT JONSON, Department of Physics, University of Gothenburg, Goteborg, Sweden, V. KORENIVSKI, Nanostructure Physics, Royal Institute of Technology, Stockholm, Sweden — A thermal-magnetic-electric valve with the free layer of exchange-spring type and inverse magnetoresistance is investigated. The structure has S-shaped current-voltage characteristics and can exhibit spontaneous oscillations when integrated with a conventional capacitor within a resonator circuit. The frequency of the oscillations can be controlled from essentially dc to the GHz range by the circuit capacitance.

Q1.00290 Resonant-spin-ordering: a new approach to dynamic control of excitation bands in interacting mesomagnets. VALENTYN NOVOSAD, SHIKHA JAIN, FRANK FRADIN, JOHN PEARSON, Materials Science Division, Argonne National Laboratory, VASIL TIBERKEVICH, ANDREI SLAVIN, Department of Physics, Oakland University, SAMUEL BADER, Materials Science Division and Center for Nanoscale Materials, Argonne National Laboratory — Two interacting vortices were used as a model system to demonstrate the resonant-spin-ordering technique for effectively controlling its magnetic states and excitation bands. This is achieved by driving the system from the linear regime of constant vortex gyrotations to the non-linear regime of vortex-core reversals at a fixed excitation frequency of one of the coupled modes. Subsequently reducing the excitation field to the linear regime, stabilizes the system to a polarity combination whose resonant frequency is decoupled from the initialization frequency. The transition of the state from one polarity combination to the other is clearly evident from the contrast in the microwave absorption amplitude obtained by gradually increasing the rf-field to higher magnitudes at the resonant frequency of one of the modes and subsequently decreasing it. Hysteresis is observed in the forward and backward trace of the rf-field sweep which gives a clear signature of the mode transition. Finally, a phase diagram is built to identify the conditions necessary to choose a particular ground state configuration with respect to the amplitude and the frequency of the in-plane oscillating field.

Q1.00291 Singular behavior of plasmon and magnetostatic resonances in samples with corners1. RODRIGO ARIAS, Universidad de Chile — The plasmon resonances of dielectric-metallic nano-particles is a subject of interest, given their potential optical applications. Localized electrostatic fields can attain large magnitudes at specific locations and frequencies. The possibility to engineer the geometry of the particles as well as their positions in eventual arrays, may lead to meta-materials with desired optical properties. Also, we explore magnetostatic modes in the same geometry (in this geometry plasmon modes are formally special cases of magnetostatic modes). This work explores the nature of long wavelength plasmon and magnetostatic modes of nano wires with rectangular cross sections: their frequencies and shapes in this effectively 2D geometry are obtained. We use a method based on singular integral equations for the potentials in order to determine the eigenmodes and their frequencies. The modes can be classified into corner modes, and modes that oscillate inside the sample. The fields associated with the corner modes have power law singularities at the corner regions, while the modes with spatial oscillations have logarithmic singularities there. We find that numerically the eigenfrequencies are very sensitive to the right determination of the singular behavior of the fields at the corners.

Q1.00292 Study of statistics of magnetization reversal in permalloy(Ni$_80$Fe$_{20}$) microwires using planar Hall effect. ARNAB ROY, P. S. ANIL KUMAR, Department of Physics, Indian Institute of Science, Bangalore 560012, India — Planar Hall effect was used to study the switching behaviour of 1mm*100micron*15nm permalloy Hall bars grown in (110) orientation on Si(100). Reversal model was

\[ p(H) = \frac{2e}{B + D} \]  

The model proposed by M.P.Sharrock : 

\[ \Delta E(H) = KV (1 - \frac{H}{H_c})^{m} \]  

with $H_c = 2kT/M$ was used to find the shape of the energy landscape for the bar undergoing reversal in an applied field. Multiple reversal paths were observed for a given wire under the same conditions, each distribution in very good agreement with the above model, allowing the calculation of : 1. Temperature dependence of the effective anisotropy constant for the bar; $K(T)$ = $(1/2)^x H_c M(T)$ ($x=1$ for applied field at 0$^0$C). 2. Energy barrier landscape: An exponent m = 1.5 to 2 is expected to leading order in the expansion of the energy barrier according to the Stoner Wolfarth model, however, our results give an exponent of 2.8 to 3 for all angles (out of plane) of the applied field for the principal reversal path, pointing to mechanisms other than coherent rotation at work. If domain wall propagation and pinning is the mechanism of reversal, this study determines the energy landscape around the pinning field.

Q1.00293 Magnetic and structural anisotropies in laser ablated epitaxial thin films of full-Heusler alloy Co$_2$MnSi on SrTiO$_3$1. HIMANSHU PANDEY, P.K. ROUT, R.C. BUDHANI2, Indian Institute of Technology Kanpur, India — We present the thickness dependent magnetic properties of laser ablated epitaxial Co$_2$MnSi (CMS)Heusler alloy thin films grown on (001) oriented SrTiO$_3$ substrate. In order to study the intrinsic magnetic anisotropy, a highly ordered single crystal thin film of Heusler alloys is necessary. This provides a unique opportunity to determine the behavior of magnetization reversal, and affect important properties such as the coercive field and remanence. The two important sources of the magnetic anisotropy are the magnetic dipolar interaction and the spin-orbit interaction. The strain in films due to the lattice mismatch with the substrate affects the shape anisotropy while spin-orbit coupling changes magneto-crystalline anisotropy. We have observed an in-plane compressive strain in the films which relaxes with increasing film thickness. Although the hysteresis loops show an in-plane easy axis for all films, the single-domain phase diagram reveals a gradual transition from in-plane to out-of-plane transition of magnetization as the film thickness is decreased. The magnetization starts to cant as film thickness start to decrease and we found a canting angle of $\approx 31.8^0$ with respect to the film plane for our thinnest 5 nm CMS films.

Q1.00294 Fabrication of fully dense nanostructured MnBi magnet by hot compaction of cryo-milled powders1. GEORGE HADJIPANAYIS, VENKATA RAMARAO NEELAM, ALEX GABAY, WANG LI, University of Delaware — Recently, rare-earth-free permanent magnets (REFPMs) have attracted much attention globally owing to rare-earth metal crisis and high cost. Among the REFPMs, MnBi is a potential candidate due to its unusual large magnetocrystalline anisotropy ($K \approx 10^{7}$ erg/cc) and positive temperature coefficient of coercivity. In this work, we report for the first time a novel processing method that combines the cryo-milling with hot compaction to produce fully dense bulk nanostructured MnBi magnet. The effect of cryo-milling on particle size, phase formation, and magnetic properties of MnBi has been studied in detail. Also, the microstructural and magnetic properties of bulk nanostructured MnBi magnet were investigated. Adoption of cryo-milling results in nanocrystalline powders with particle size of 400-500 nm. Large coercivity ($H_c$) values of 18.5 kOe, and 12.9 kOe were obtained in cryo-milled powders and hot compacted magnet respectively. The MnBi magnet shows a large positive temperature coefficient of $H_c$ and the $H_c$ reaches a value of more than 30 kOe above 450 K.

1. The work was supported by Siemens.

Q1.00295 Magnetic and structural anisotropies in laser ablated epitaxial thin films of full-Heusler alloy Co$_2$MnSi on SrTiO$_3$. HIMANSHU PANDEY, P.K. ROUT, R.C. BUDHANI, Indian Institute of Technology Kanpur, India — We present the thickness dependent magnetic properties of laser ablated epitaxial Co$_2$MnSi (CMS)Heusler alloy thin films grown on (001) oriented SrTiO$_3$ substrate. In order to study the intrinsic magnetic anisotropy, a highly ordered single crystal thin film of Heusler alloys is necessary. This provides a unique opportunity to determine the behavior of magnetization reversal, and affect important properties such as the coercive field and remanence. The two important sources of the magnetic anisotropy are the magnetic dipolar interaction and the spin-orbit interaction. The strain in films due to the lattice mismatch with the substrate affects the shape anisotropy while spin-orbit coupling changes magneto-crystalline anisotropy. We have observed an in-plane compressive strain in the films which relaxes with increasing film thickness. Although the hysteresis loops show an in-plane easy axis for all films, the single-domain phase diagram reveals a gradual transition from in-plane to out-of-plane transition of magnetization as the film thickness is decreased. The magnetization starts to cant as film thickness start to decrease and we found a canting angle of $\approx 31.8^0$ with respect to the film plane for our thinnest 5 nm CMS films.

1 We acknowledge support from DIT, DST, CSIR and IIT Kanpur.

2 also at National Physical Laboratory, India.
Q1.00295 Interfacial magnetic anisotropy in Ta/CoFe$_2$O$_{4-δ}$/MgO films for Co compositions. SUNG-MIN AHN, GEOFFREY BEACH, Massachusetts Institute of Technology. To realize promising devices for high tunnel magnetoresistance and high-efficiency current-driven domain wall (DW) motion, it is crucial to optimize perpendicular magnetic anisotropy (PMA) for Ta/CoFe/MO$_x$ trilayers where M is a metal such as Al, Mg, Ta, etc. Here, the PMA in Ta/CoFe$_{100-x}$/CoFe/MgO films for alloy compositions spanning pure Co to pure Fe has been studied in order to investigate the role of chemical composition in the onset of perpendicular magnetic anisotropy at the CoFe/MgO interface. Out-of-plane magnetization is not observed in Ta/Fe/MgO ($x=0$) and Ta/Co/MgO ($x=100$), for all ranges of CoFe thickness ($t$), but a t-dependent crossover between in-plane and out-of-plane anisotropy is found for $x=20$, 50, and 80. Interestingly, effective magnetic anisotropy $K_e$ as well as interfacial anisotropy $K_i$ are maximized for Co$_{97.5}$Fe$_{2.5}$O$_{4-δ}$ at a fixed $t=0.8$ nm. The results suggest that the degree of filling of valence bands in the CoFe adjacent to the interface, which determines the relative population of the anisotropic d-bands, plays an important role in the interfacial anisotropy brought on by CoFe-O hybridization at the metal/oXide interface.

Q1.00296 Langmuir Monolayers of Superparamagnetic Nanoparticles. GORAN DOJCINOSKI, PATRICK TRUITT, Montclair State University. The surfactant coating of the superparamagnetic nanoparticles found in ferrofluids enable them to form monolayers at the air/water interface. These monolayers can be considered quasi-two-dimensional systems where the particles are confined to a surface while their magnetizations are free to rotate in all directions. Confining the nanoparticles to a surface allows observation of structure formation that is difficult to see in a bulk, opaque ferrofluid. We investigate how different surfactants affect monolayer formation. We measure pressure-area isotherms of such systems under lateral compression in a Langmuir trough and find monolayers of oleic acid coated iron nanoparticles collapse at a surface pressure between 65-70 mN/m, while dodecanoic acid coated iron nanoparticles collapse around 50 mN/m. Other surfactants with varying lengths and structure are also investigated. Studies of monolayer stability and formation in the presence of an applied magnetic will also be presented. Finally, we transfer monolayers to solid substrates and examine their morphology via atomic force microscopy.

Q1.00297 Monodisperse Magneto-Fluorescent Bifunctional Nanopropes for Bioapplications. HONGWANG ZHANG, HENG HUANG, ARND PRALLE, HAO ZENG, SUNY at Buffalo. We present the work on the synthesis of dye-doped monodisperse Fe$_3$SiO$_2$ core/shell nanoparticles as bifunctional probes for bioapplications. Magnetic nanoparticles (NP) have been widely studied as nano-probes for bio-imaging, sensing as well as for cancer therapy. Among all the NPs, Fe NPs have been the focus because they have very high magnetization. However, Fe NPs are usually not stable in ambient due to the fast surface oxidation of the NPs. On the other hand, dye molecules have long been used as probes for bio-imaging. But they are sensitive to environmental conditions. It requires passivation for both so that they can be stable for applications. In this work, monodisperse Fe NPs with sizes ranging from 13-20 nm have been synthesized through the chemical thermal-decomposition in a solution. Silica shells were then coated on the Fe NPs by a two-phase oil-in-water method. Dye molecules were first bonded to a silica precursor and then encapsulated into the silica shell during the coating process. The silica shells protect both the Fe NPs and dye molecules, which makes them as robust probes. The dye doped Fe$_3$SiO$_2$ core/shell NPs remain both highly magnetic and highly fluorescent. The stable dye doped Fe$_3$SiO$_2$NPs have been used as a dual functional probe for both magnetic heating and local nanoscale temperature sending, and their performance will be reported.

Q1.00298 Magnetic Relaxation Mechanisms in Lanthanide Single Molecule Magnets. LIVIU CHIBOTARU, LIVIU UNGUR, University of Leuven, ERIC MCINNES, RICHARD WIPENNY, University of Manchester. We present the work on the synthesis of monodisperse Fe$_3$SiO$_2$ core/shell nanoparticles as bifunctional probes for bioapplications. Magnetic nanoparticles (NP) have been widely studied as nano-probes for bio-imaging, sensing as well as for cancer therapy. Among all the NPs, Fe NPs have been the focus because they have very high magnetization. However, Fe NPs are usually not stable in ambient due to the fast surface oxidation of the NPs. On the other hand, dye molecules have long been used as probes for bio-imaging. But they are sensitive to environmental conditions. It requires passivation for both so that they can be stable for applications. In this work, monodisperse Fe NPs with sizes ranging from 13-20 nm have been synthesized through the chemical thermal-decomposition in a solution. Silica shells were then coated on the Fe NPs by a two-phase oil-in-water method. Dye molecules were first bonded to a silica precursor and then encapsulated into the silica shell during the coating process. The silica shells protect both the Fe NPs and dye molecules, which makes them as robust probes. The dye doped Fe$_3$SiO$_2$ core/shell NPs remain both highly magnetic and highly fluorescent. The stable dye doped Fe$_3$SiO$_2$NPs have been used as a dual functional probe for both magnetic heating and local nanoscale temperature sending, and their performance will be reported.

Q1.00299 Study on novel rare-earth nitride chlorides GdNCl and Gd$_2$N$_2$Cl. WANG LANG, CHEN NING, LIU XIAOLU, YANG LIU, School of Material Science and Engineering, University of Science and Technology Beijing, Beijing 100083, CHINA. YANG LI, Department of Engineering Science and Materials, University of Puerto Rico at Mayaguez, Mayaguez 00681-9044, USA. We report a joint experimental and theoretical investigation of magnetic and structural properties of novel rare-earth nitride chlorides GdNCl and Gd$_2$N$_2$Cl. By using the method of gas-solid phase reaction at high temperature, a new layered rare-earth nitride chloride GdNCl was synthesized recently. The structure and morphology were characterized by X-ray diffraction and transmission electron microscopy. The analysis results show that GdNCl compound has the same crystaline structure as the known phase CeNCl, which crystallized in a tetragonal structure with space group P4/mmm (No.129). The lattice constants are $a = b = 4.42$ nm, $c = 6.46$ nm. The layered structure of GdNCl is comprised of the double Gd-N layers and Cl layers. In addition, another new stable phase Gd$_2$N$_2$Cl was also synthesized. The Gd$_2$N$_2$Cl structure belongs to a tetragonal system with P4mm space group (No.99) and lattice constants are $a = b = 4.25$ nm and $c = 5.92$ nm. The temperature-dependent magnetic susceptibility measurements (ZFC and FC) were performed, which showed a ferromagnetic transition occurs at 70 K. The first-principle simulation based on the density functional theory was used to investigate the physical properties and structural stability of rare-earth nitride chlorides, which is consistent with the experiments.

Q1.00300 Magnetically Controlled Capacitor Membrane System. NATHAN FORTENBURY, JOHN HYDE, REGAN BECKHAM, RANDY BACK, The University of Texas at Tyler. The effects of electric fields on elastic membranes have been studied in detail in recent years. It is the purpose of this research to explore the effects of the interaction between magnetic fields and electric fields on these membranes with the addition of magnetic ferrofluid. Variables under consideration include strength and shape of magnetic field, concentration of magnetic ferrofluid, and voltage supplied to the membrane. Of particular interest are the stable state conditions for various parameters as well as maximum stable voltages for the same.
The Effect of Variation in Permittivity of Different Tissues on Induced Electric Field in the Brain during Transcranial Magnetic Stimulation, RAVI L. HADIMANI, Iowa State University. KONSTANTIN PORZIG, Ilmenau University of Technology. LAWRENCE J. CROWTHER, Iowa State University. HARTMUT BRAUER, HANNES TOEPFER, Ilmenau University of Technology. DAVID C. JILES, Iowa State University, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING, IOWA STATE UNIVERSITY TEAM, DEPARTMENT OF ADVANCED ELECTROMAGNETICS, ILMENAU UNIVERSITY OF TECHNOLOGY TEAM — Estimation of electric field in the brain during Transcranial Magnetic Stimulation (TMS) requires knowledge of the electric property of brain tissue. Grey and white matters have unusually high relative permittivities of $\sim 10^5$ at low frequencies. However, relative permittivity of cerebrospinal fluid is $\sim 10^3$. With such a variation it is necessary to consider the effect of boundaries. A model consisting of 2 hemispheres was used in the model with the properties of one hemisphere kept constant at $\varepsilon_1=0.15\text{m}^{-1}$ and $\varepsilon_2=10$ while the properties of the second hemisphere were changed kept at $\sigma_2=0.15\text{m}^{-1}$ to $2\text{m}^{-1}$ and $\varepsilon_2=10^2$ to $10^7$. A 70 mm diameter double coil was used as the source of the magnetic field. The amplitude of the current in the coil was 5488 A at a frequency of 2.9 kHz. The results show that the electric field, $E$ induced during magnetic stimulation is independent of the relative permittivity, $\varepsilon_r$ and varies with the conductivity. Thus the variation in $E$, calculated with homogeneous and heterogeneous head models was due to variation in conductivity of the tissues and not due to variation in permittivities.

**Q1.00302 Growth and Characterization of Magnetoelastic Fe$_2$TeO$_6$ Thin Films**, JUNLEI WANG, JUAN COLON SANTANA, NING WU, PETER DOWBEN, CHRISTIAN BINEK, University of Nebraska — Voltage-controlled spintronics is of vital importance in information technology where power consumption and Joule heating restrict progress through scaling. Motivated by spintronic concepts and specifically by device applications utilizing electrically controlled interface or boundary magnetization (BM) in magnetic thin film heterostructures, we report on growth, structural, magnetic and magnetoelectric (ME) characterization of the antiferromagnet Fe$_2$TeO$_6$. Magnetometry of synthesized Fe$_2$TeO$_6$ powder, in combination with ME susceptibility data reveals 3D Heisenberg criticality in striking similarity to the archetypical ME chromia. X-ray diffraction shows (110) texture of the PLD grown films. Measurements of the magnetic susceptibility of the latter confirm in-plane magnetic anisotropy. X-ray photoemission spectroscopy indicates a Te-O terminated (110) surface. We interpret it in terms of surface reconstruction. Measurements of X-ray magnetic circular dichroism combined with photoemission electron microscopy support the presence of electrically controllable BM in the PLD-grown Fe$_2$TeO$_6$ thin film.

We acknowledge financial support by NSF-MRSEC & Nanoelectronics Research Initiative.

**Q1.00303 Anomalous electron spin decoherence in an optically pumped quantum dot,** XIAOFENG SHI, University of California San Diego —

**Q1.00304 Computation of the modified magnetostriction coefficient $b'$ corresponding to different depth ranges in ferromagnetic specimens by using a frequency dependent model for magnetic Barkhausen emissions**, ORFEAS KYPRIS, Department of Electrical and Computer Engineering, Iowa State University. IKENNA NLEBEDIM, DAVID JILES, 1. Department of Electrical and Computer Engineering, Iowa State University 2. Ames Laboratory, US Department of Energy, Iowa State University — We have recently shown that a linear relationship exists between the reciprocal peak voltage envelope amplitude $1/V_{peak}$ of the magnetic Barkhausen signal and elastic stress $\varepsilon$. By applying a frequency-dependent model [1] to determine the depth of origin of the Barkhausen emissions in a uniformly stressed steel specimen, this relationship was found to be valid for different depth ranges. The linear relationship depends on a coefficient of proportionality $b'$. This was found to decrease with depth, indicating that the higher part of the frequency spectrum is less sensitive to changes in stress. In this study, the model equations have been applied at various depth ranges. It was found that the variation of $b'$ with depth can be utilized in an inversion procedure to assess the stress state in ferromagnetic specimens to give stress-depth profiles. This study is useful for non-destructive characterization of stress with depth.


**Q1.00305 ENERGY RESEARCH AND APPLICATIONS —

**Q1.00306 Fabrication of a Scalable Free Standing Single Layer Silver Nanomesh**, TIANYU SUN, CHUANFEI GUO, KRZYSZTOF KEMPA, ZHIFENG REN, Boston College — We present a method of fabricating scalable free standing single layer silver nanomeshes with uniform width. The method consists of In$_2$O$_3$/SiO$_2$ bilayer lift-off metallization, HF-H$_2$O$_2$ based catalytic etching and a chemical lift-off process. Since the linewidth and the mesh size can be well tuned by the isotropic etching of In$_2$O$_3$ islands within a broad range, this method is capable of generating nanomeshes meeting different electrical, optical, and mechanical requirements. Using this method, a 45 nm thick silver nanomesh with 20 % metallic coverage (line width $\sim 120$ nm) has an average transmittance of 65 % over the whole visible range and a sheet resistance of about 10 $\Omega$/sq. To the best of our knowledge, this is the first time that a cost-effective scalable free standing silver nanomesh with uniform linewidth was obtained. Such nanomeshes may find applications in a lot of fields where good flexibility, high transparency, and good electrical conductivity are required simultaneously, such as flexible transparent electrodes.

**Q1.00307 Theoretical Evaluation of Cu-Sn-S and Cu-Sb-S Based Solar Absorbers for Earth-Abundant Thin-Film Solar Cells**, PAWEL ZAWADZKI, HAOUEI PENG, ANDRIY ZAKUTAYEV, STEPHAN LANY, National Renewable Energy Laboratory — Current thin-film solar absorbers such as Cu(In,Ga)Se$_2$ or CdTe, although remarkably efficient, incorporate limited-supply elements like indium or tellurium. Meeting the cost competitiveness criterion necessary for a large-scale deployment of thin-film PV technologies requires development of new earth-abundant solar absorbers. In an effort to accelerate such development we combine first principles theory and high throughput experiments to explore In-free ternary copper chalcogenides. As part of the theoretical evaluation, we study the Cu$_2$SnS$_4$, Cu$_4$SnS$_4$, CuSbS$_2$ and Cu$_3$Sb$_2$ based compounds formed by isovalent alloying on Sn, Sb, and S sites. For this set of materials we predict band-structures and optical absorption coefficients and demonstrate the feasibility of achieving the optimal band gap of 1.3 eV for a single junction cell and a high optical absorption of $\sim 10^5$ cm$^{-1}$ at $E_g=0.2$ eV. We additionally perform defect studies to elucidate the doping trends within this class of materials.

The project “Rapid Development of Earth-abundant Thin Film Solar Cells” is supported as a part of the SunShot initiative by the U. S. Department of Energy, Office of Energy Efficiency and Renewable Energy under Contract No. DE-AC36-08GO28308 to NREL.

**Q1.00308 Particle scattering approach for solar concentration**, JEHAN SENEVIRATNE, MATTHEW BERG, Department of Physics and Astronomy, Mississippi State University — The focus of this work is on increasing the solar concentration ratio for Photovoltaic (PV) applications. In this work, the scattering patterns of particles with various shapes are computationally studied in the near field. The results are analyzed to develop models with high concentration ratios. Based on the results, our question: “Which particle arrangement gives the optimum solar power yield for a given physical condition?” is investigated. Our work may have an impact on solar harvesting methodologies in solar energy applications.
Q1.00309 Optical characterization of n-type conductive cuprous oxide photoanodes. JACKSON HALPIN, ROHANA GARUTHARA, Physics Department, 102 Berliner Hall, Hofstra University, Hempstead, NY 11549 — Electrodeposition technique was used to deposit chloride doped Cu2O thin films on indium tin oxide (ITO) coated glass substrates. The deposited Cu2O photoanodes were characterized by absorption, reflectance and photoluminescence spectroscopy. The effects of chloride doped photoanodes grown in different solution pH and bath temperature on the magnitude of their photocurrent are studied. The low temperature photoluminescence spectra of chloride doped Cu2O films are found to depend on the solution pH in the range 10.0-7.5. We observed two photoluminescence peaks positions at 1.45 eV and 1.65 eV for photoanodes made in pH 7.5 solution. At pH 9.6, we observed an additional photoluminescence peak around 1.8 eV. The results will be discussed with emphasis on the reflectance, absorption and photoluminescence observation.

Q1.00310 First Principal Optimization of Exciton Separation via Functional Modification of the Atomic Structure, LEVI LENTZ, ALEXIE KOLPAK, MIT — Low hole mobility and high recombination rates limit the incident photon-to-current collection efficiency (IPCE) of organic photovoltaics. In this study, we use a combination of rational design and first-principles density functional theory computations to tailor the properties of new hybrid organic-inorganic photovoltaic materials in order to ameliorate these issues. Starting with hybrid organic-inorganic molecules shown to self-assemble into crystalline structures, we design a nanostructured material in which inorganic charge carrier channels are separated by domains of organic absorber on the order of several nanometers thick perpendicular to the light absorption direction. By functionalizing the organic component and substituting the cations in the inorganic layer, we engineer a dipole moment to drive electrons and holes into the inorganic charge carrier channels. Furthermore, we tune the density of states of these regions via a combination of cation substitution and interactions with functional groups in the organic region in order to optimize charge carrier mobility. The combination of rational design and first-principles optimization could significantly reduce exciton recombination and increase charge carrier mobility with respect to purely organic photovoltaics.

Q1.00311 Computational Design of Photovoltaic Materials with Self Organized NanoStructures, KAZUNORI SATO, Graduate School of Engineering Science, Osaka University and PRESTO-JST, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — Chalcogenide and II-VI semiconductors, such as Cu(In,Ga)Se2, Cu2ZnSn(S, Se)4, and Cd(S, Te), are one of the most promising materials for low cost photovoltaic solar-cells. In this paper, based on first-principles calculations, we propose that self-organized nanostructures in these compounds will enhance the conversion efficiency. Our calculations are based on the KKR-CPA-LDA [1] with the self-interaction correction [2]. We also use VASP package [3] for calculating mixing energy and effective interactions of the systems by using the cluster expansion method [4]. For phase separating systems, we simulate nano-structure formation by using the Monte Carlo method. It is expected that the photo-generated electron-hole pairs are efficiently separated by the type-II interface and then effectively transferred along the quasi-one-dimensional structures. Moreover, we can expect multiplication of generated carriers due to the multi-exciton effects in nano-structures [5].

Q1.00312 Enhancing the Efficiency of Bulk Heterojunction Solar Cells via Templated SelfAssembly, CHENG PAN, HONGFEI LI, Materials Science and Engineering, Stony Brook University, BULENT AKGUN, SUSHIL SATIJIA, Center for Neutron Research, National Institute of Standards and Technology, DILIP GERSAPPE, Materials Science and Engineering, Stony Brook University, YIMEI ZHU, Center for Functional Nanomaterials, Brookhaven National Laboratory, MIRIAM RAFAILOVICH, Materials Science and Engineering, Stony Brook University — Bulk Heterojunction (BHJ) polymer solar cells are an area of intense interest due to their flexibility and relatively low cost. The mixture of polythiophene derivatives (donor) and fullerene (acceptor) is spin coated on substrate as the active layer, and are phase-separated into interconnected domains. However, due to the disordered inner structures in the active layer, donor or acceptor domains isolated from electrodes and long path conduction, the power conversion efficiency (PCE) of BHJ solar cell is low. Therefore, morphology control in bulk heterojunction (BHJ) solar cell is considered to be critical for the power conversion efficiency (PCE). Here, we present a novel approach that introduces non-photoactive polymer that organizes the poly(3-hexithiophene) (P3HT) into columnar phases decorated by [6,6]-phenyl C61-butyric acid methyl ester (PCBM) at the interface. This structure represents a realization of an idealized morphology of an organic solar cell, in which, both exiciton dissociation and the carrier transport are optimized leading to increased power conversion efficiency.

Q1.00313 Synthesis and Characterization of ZnO/polyaniline planar heterojunction solar cells, LEANDRO GUTIERREZ, CHRISTOPHER REEHL, ANNE ISAH, WILLIAM MANNERS, JIMMY BARRIENTOS, ARYA NABIZADEH, PATRICK ALBERS, MEHMET SAHINER, WEINING WANG, Seton Hall University, SAHINER COLLABORATION, WANG COLLABORATION — ZnO/polymer heterojunction has attracted much research attention because of its potential application in solar cell, LED, UV photodetection and other applications. However, there are few studies on ZnO/polymer heterojunction attempting to synthesize ZnO materials using pulsed laser deposition. Comparing with other methods, PLD has the advantage of congruent evaporation, and being able to grow high quality thin films at relatively low temperature. In our previous work in CdTe/Cds based thin films we have seen correlations between the pulsed laser deposition parameters and the electrical performance of the thin film solar cells. In this work, we report our studies on pulsed-laser-deposited (PLD) ZnO/Polyaniline (PANI) heterojunction and its potential application as solar cells. We studied how the performance of ZnO/PANI solar cells depends on the deposition condition of ZnO, such as deposition temperature, background pressure of oxygen, and ZnO film thickness. X-ray diffraction (XRD) and scanning electron microscopy were used to characterize the pulsed-laser-deposited (PLD) ZnO film. The correlation between the solar cell electrical performance and the pulsed laser deposition conditions will be discussed.

Q1.00314 Mondo Grass Berry Pigment for Visible to Near Infrared Absorption in Dye Sensitized Solar Cell1, L.A.A. DESILVA, Department of Physics, University of West Georgia, Carrollton, GA, P.K.D.D.P. PITIGALA, A.G.U. PERERA, Department of Physics and Astronomy, Georgia State University, Atlanta, GA — The development of dye sensitized solar cells (DSSC) is an exciting field in the low cost renewable energy production. Two major draw backs in the DSSCs are the narrow spectral response and the short term stability. Synthesis of artificial dyes with broad response is important in developing an efficient DSSC. Artificial dyes can add up to the cost of the device; therefore, it is important to identify natural dyes with broad absorption and required energy levels. Work presented here shows a broad spectral response with a natural dye extracted from a Mondo Grass berry (Ophiopogonjaponicus). The dye is extracted by crushing the berries and filtering to remove the pulp. A DSSC sensitized with Mondo Grass dye, and with TiO2 film screen printed on a Florien doped Tin Oxide (FTO) glass and baked for 30 minutes at 450 degree C as the working electrode and iodine/triiodide red-ox electrolyte as the hole collector was tested for its performance. An open circuit photovoltage of 495 mV and a short circuit photocurrent of 0.6 mA/cm^2 were observed under a simulated lamp equivalent to 1 sun illumination and have a broad spectral response extending from 400 nm to 750 nm.

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1 This work is supported by COSM at UWG.
Q1.00315 Pressure and PL study of dilute-N GaInNAs films for applications in photovoltaics¹, GEORGE P. LINDBERG, University at Buffalo, Department of Physics, Buffalo, NY 14260, MIWA FUKUDA, University of Oklahoma, Department of Physics and Astronomy, Norman, OK 73019, M. AL KHALIFIOU, CRHEA-CNRS, Valbonne, France, KHALID HOSSAIN, Amethyst Research Inc. Ardmore OK., IAN R. SELLERS, University of Oklahoma, Department of Physics and Astronomy, Norman, OK 73019, BERNARD A. WEINSTEIN, University at Buffalo, Department of Physics, Buffalo, NY 14260 — Multi-junction photovoltaic devices employing dilute-N GaInNAs alloys are currently of high interest for efficient solar energy conversion. The negative band-bowing produced by introducing a few percent N into GaInNAs provides a convenient way to match the 1eV component of the solar spectrum, providing recombination losses in localized states can be reduced while maintaining favorable carrier extraction. High pressure photoluminescence (PL) experiments exploring the localization of band-edge excitons in dilute-N GaInNAs films grown by plasma assisted MBE will be discussed. The effects of post-growth annealing and hydrogen incorporation on the PL spectra of the films are considered.

¹Research supported by Amethyst Research Inc. through the State of Oklahoma, ONAP program.

Q1.00316 Multilayered Nanostructured Broad Band Absorber, TIMOTHY CORRIGAN, BENJAMIN IDE, Concord University — Wasted energy in the form of heat is perhaps the largest source of lost energy making many power systems inefficient. Systems designed to convert heat into useful energy need a method of collecting the heat. We previously described a multilayer design with successive thin metallic and dielectric (non-metal and transparent) layers, where each successive metallic layer absorbs a small fraction of the radiation. However, the regular thickness of the dielectric layer causes reflection peaks, or regions where no absorption occurs. In this work we describe a similar design where we eliminated the undesirable reflection peaks using varying thicknesses of the dielectric layer.

Q1.00317 High Frequency Supercapacitors for Piezo-based Energy Harvesting, MATTHEW ERVIN, US Army Research Laboratory, CARLOS PEREIRA, Armament Research Development Engineering Center, JOHN MILLER, JME Inc., RONALD OUTLAW, The College of William and Mary, JAY RASTEGAR, RICHARD MURLAY, Omnitech Partners LLC — Energy harvesting is being investigated as an alternative to batteries for powering munition guidance and fuzing functions during flight. A piezoelectric system that generates energy from the oscillation of a mass on a spring (set in motion by the launch acceleration) is being developed. Original designs stored this energy in an electrolytic capacitor for use during flight. Here we replace the electrolytic capacitor with a smaller, lighter, and potentially more reliable electrochemical double layer capacitor (aka, supercapacitor). The potential problems with using supercapacitors in this application are that the piezoelectric output greatly exceeds the supercapacitor electrolyte breakdown voltage, and the frequency greatly exceeds the operating frequency of commercial supercapacitors. Here we have investigated the use of ultrafast vertically oriented graphene array-based supercapacitors for storing the energy in this application. We find that the electrolyte breakdown is not a serious limitation as it is either kinetically limited by the relatively high frequency of the piezoelectric output, or it is overcome by the self-healing nature of supercapacitors. We also find that these supercapacitors have sufficient dynamic response to efficiently store the generated energy.

Q1.00318 In Situ Investigations of Ion Transport at Oxide Surfaces, FARID EL GABALY, Sandia National Laboratories — Ion transport through materials driven by electric potential is essential to many processes, including electrical energy storage. Here we study in situ the behavior of oxide surfaces in the presence of applied electric fields with low-energy electron microscopy (LEEM), angle-resolved photoemission spectroscopy (ARPES), and related structural and spectroscopic measurement techniques. We measure with high spatial resolution the electric potential on the surface of yttria-stabilized zirconia (YSZ), a prototypical oxygen ion conductor, as a function of distance from a metallic electrode. The dependence of the potential distribution on temperature and oxygen gas pressure is determined. Finally we explore which types of surface sites facilitate the gas-surface reactions that create and annihilate the oxygen ions.

Q1.00319 First-principles determination of LaMnxM1-xO3 surface structures under catalytic conditions, XI RONG, ALEXIE KOLPAK, Department of Mechanical Engineering, Massachusetts Institute of Technology, KOLPAK GROUP TEAM — The design of efficient and cost-effective catalysts for the oxygen evolution reaction (OER) is crucial for the development of electrochemical conversion technologies. One of the most important factors determining the activity is the surface/interface structures of catalysts. However, little is known about the atomic and electronic structures and thermodynamic properties of realistic interface reconstructions, which are caused by different environments during fabrication, measurement, and eventual device operation. In this work, we apply first-principles density functional theory computations in combination with kinetic modeling to investigate the environment-dependent chemical and physical properties of perovskite oxide heterostructure catalysts, particularly LaMnxM1-xO3. We develop a methodology for accurate identification of constraints on the interface structure phase space and rapid computation of this identification as a function of temperature, pressure, and other chemical environments. Our work could lead to accurate and rapid prediction of surface/interface structures and properties under different environmental conditions, and contribute to the design of new high-activity OER catalysts.

Q1.00320 Self-standing paper based anodes prepared from siliconcarbonitride-MoS2 composite for Li-ion battery applications, LAMUEL DAVID, GURPREET SINGH, Kansas State University — We study synthesis of free-standing polymer derived SiCN/ MoS2 composite paper anode for Li-ion battery application. This was achieved following a two-step approach: First, polysilazane was interfaced with exfoliated MoS2 nanosheets which upon pyrolysis resulted in SiCN/MoS2 composite. Second, dispersion of SiCN/MoS2 in isopropanol was vacuum filtered resulting in formation of a self-standing composite paper. Physical and chemical characterization of the composite was carried out by use of electron microscopy. Fourier transform infrared spectroscopy (FT-IR) and Thermo-gravimetric analysis (TGA). FT-IR data indicated complete conversion of polysilazane precursor to SiCN ceramic, while electron microscopy confirmed layered structure of the paper. Thermo-gravimetric analysis showed enhanced thermodynamic stability of the composite paper up to 800 °C. Electrochemical analysis of SiCN/MoS2 composite paper anodes showed that Li-ion can reversible intercalate in the voltage range of 0-2.5 V with a first cycle discharge capacity of 770 mA h/g at a current density of 100 mA/g.

Q1.00321 Transducing Energy Loss in Water Electrolysis with a 0D Ion-Sensitive Field-Effect Transistor, NICOLAS CLEMENT, IEMN-CNRS (France), KATSUMIHIKO NISHIGUCHI, NTT Basic Research Labs (Japan), JEAN-FRANCOIS DUFRÊCHE, CEA-Marcoules (France), DAVID GUÉRIN, IEMN-CNRS (France), GILLES PATRIARCHE, LPN-CNRS (France), DAVID TROADEC, IEMN-CNRS (France), AKIRA FUJIWARA, NTT Basic Research Labs (Japan), DOMINIQUE VUILAUME, IEMN-CNRS (France) — In order to produce hydrogen as a fuel source of the future, water electrolysis is one of the most “promising” green approaches. Although electrolysis efficiency can be as high as 80%, it still means that at least 20% of the energy is lost. The use of transducers to collect the energy loss in water electrolysis is attractive. Among the various transducers, several ideas have been proposed such as an air bubble powered rotary driving apparatus or a microcantilever vibrating after impact of each bubble. However, the main source of energy lost appears at electrode interfaces with the presence of a double layer of ions acting as a resistor and capacitor. In this study, we show that using a 0D – ultra low noise - ISFET, allows getting the energy coming from the double layer fluctuation at each H2 bubble emission. Interestingly, the output signal that can be tuned with salt concentration and electrolysis current exactly corresponds to that of action potential which could be useful for bio-applications. In addition, electrical detection of bubbles emission at single bubble level also opens the door to optimization of hydrogen efficiency and further save energy for hydrogen production.
Q1.00322 Hydrogen Adsorption onto Magnesium Palladium and Magnesium Palladium Niobium Multilayer Thin Films. CHRISTIAN STEINMETZ, JEFFREY HETTINGER, TABBETHA DOBBINS, Rowan University — We report on the synthesis and characterization of magnesium palladium and magnesium niobium multilayer thin films as a possible reversible hydrogen storage material. The multilayer thin films are characterized by x-ray diffraction (XRD) and x-ray reflectivity (XRR) before and after hydrogen uptake. This study examines the optimal thickness of the magnesium film which would allow the diffusion of hydrogen to form magnesium hydride (MgH2). Thin barriers of palladium and niobium permit hydrogen to permeate while acting as a diffusion barrier to oxygen. Multilayer thin films are grown with various magnesium thicknesses via magnetron sputtering on a sapphire substrate. Thicknesses of Mg, MgH2, Pd, and Nb are reported. Likewise, interfacial roughness attributable to hydrogenation and dehydrogenation cycling measured using XRR are reported.

Q1.00323 Cryo-Milling and the Hydrogen Storage Properties of NaAlH4. KEVIN FELLER, TABBETHA DOBBINS, Rowan University — High energy ball milling of metal hydrides is a common way to both introduce catalysts (e.g. TiCl3) and to simultaneously increase the surface area. Both catalysis and increased surface area improve hydrogen storage capacity of the material. Nanostructuring of hydrides by depositing them into mesoporous templates (such as anodized alumina, MOFs, and SBA-15) has become a common way to increase surface area. However, the mesoporous template does not add hydrogen storage capacity— and thus, tends to decreased overall storage weight percent for the nanostructured hydride material. As with most materials, hydrides become brittle at low temperatures and will tend to fracture more readily. We will process Sodium Aluminium Hydride (NaAlH4) using cryogenic high energy ball milling using an in-house modified chamber SPEX Certiprep M8000 mixer/mill in order to gain a nanostructured hydride without mesoporous template material. Details of the modified mixer mill design will be presented. Ultimately, our planned future work is to study the resultant material using x-ray diffraction (Scherrer method for crystalite size), absorption/desorption temperature programmed desorption (TPD), and ultrasmall-angle x-ray scattering (USAXS) microstructural quantification to understand the role of cryomilling on enhancing the material’s ability to store (and release) hydrogen.

Q1.00324 Study of Titanium Hydride Destabilized Lithium Aluminum Hydride as a Promising Hydrogen Storage System. TROY SMITH, TABBETHA DOBBINS, Rowan University. Dept. of Physics & Astronomy — Destabilized hydrides are a class of hydrogen storage systems whereby the theoretical hydrogen desorption temperature is reduced owing to the formation of a stable product phase which is typically comprised of cations from the destabilizer and the hydride phase. This work examines the hydrogen desorption temperatures for a mixture of titanium hydride (TiH2) (as a destabilizer) and lithium aluminium hydride (LiAlH4). X-ray diffraction (XRD) and temperature programmed desorption (TPD) were used to confirm the onset of desorption at temperatures as low as 75 deg C. The thermodynamic phase diagram corresponding to the mixed system will be presented and a reaction mechanism is suggested.

Q1.00325 Monte Carlo simulation study on ammonia anchored TON zeolite for carbon dioxide capture. SOOHO LEE, Sogang university. Nano-structured computer fluids lab — 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.


Q1.00327 INSTRUMENTATION AND MEASUREMENTS —
Q1.00329 High sensitivity and label-free detection of Enterovirus 71 by nanogold modified electrochemical impedance spectroscopy , FANG-YU WANG, Department of Molecular Medicine and Bioengineering, National Chiao Tung University, Hsinchu, Taiwan, R.O.C., HSING-YUAN LI, HSING-HUA TSENG, TSAI-MU CHENG, HSIEH-LIANG CHU, Department of Biological Science and Technology, National Chiao Tung University, Hsinchu, Taiwan, R.O.C. — Enterovirus 71 (EV71), which is the most fulminant and invasive species of enterovirus, can cause children neurological complications and death within 2-3 days after fever and rash developed. Besides, EV71 has high sequence similarity with Coxackie A 16 (CA16) that makes differential diagnosis difficult in clinical and laboratory. Since conventional viral diagnostic method cannot diagnose EV71 quickly and EV71 can transmit at low viral titer, the patients might delay in treatment. A quick, high sensitive, and high specific test for EV71 detection is pivotal. Electrochemical impedance spectroscopy (EIS) has been applied for detecting bio-molecules as biosensors recently. In this study, we try to build a detection platform for EV71 detection by nanogold modified EIS probe. The result shows that our probe can detect 3.6 VP1/50 μl (one EV71 particle has 60 VP1) in 3 minutes. The test can also distinguish EV71 from CA16 and lysozyme. Diagnosis of enterovirus 71 by electrochemical impedance spectroscopy has the potential to apply in clinic.

Q1.00330 Rapid detection and quantification of free hemoglobin and haptoglobin by nanogold modified electrochemical impedance spectroscopy , YU-NING LU, HSING-YUAN LI, HSUEH-LIANG CHU, TSAI-MU CHENG, SHIN-HUA TSENG, CHIA-CHING CHANG, Department of Biological Science and Technology, National Chiao-Tung University, Taiwan, R.O.C. — Free Hemoglobin (Hb) is a metabolical substance that damage tissue and vessel. It is released from destructed red blood cell and causes infection or inflammatory of human body. In blood plasma, haptoglobin (Hp) binds free Hb with high affinity and prevents the damage which is caused by cell free Hb. Hp has three phenotypes, that are Hp1-1, Hp 2-1, and Hp 2-2. Different phenotypes of Hp has been different affinities to Hb. It is known that electrochemical impedance spectroscopy (EIS) provide more information for detecting the small amount bio-molecules, include protein and DNA. In this study, we have developed a simple, fast, reliable and sensitive platform to quantify concentration of free Hb and Hp. In this platform, detection probe has been modified with nano gold and the surface charge transfer resistance of Hb and Hp binding could be detected and quantified within 18 min. This is a whole new platform to quantify free Hb in the serum of human to our knowledge.

Q1.00331 Improved transcranial magnetic stimulation coil design with realistic head modeling, LAWRENCE CROWTHER, RAVI HADIMANI, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — We are investigating Transcranial magnetic stimulation (TMS) as a noninvasive technique based on electromagnetic induction which causes stimulation of the neurons in the brain. TMS can be used as a pain-free alternative to conventional electroconvulsive therapy (ECT) which is still widely implemented for treatment of major depression. Development of improved TMS coils capable of stimulating subcortical regions could also allow TMS to replace invasive deep brain stimulation (DBS) which requires surgical implantation of electrodes in the brain. Our new designs allow new applications of the technique to be established for a variety of diagnostic and therapeutic applications of psychiatric disorders and neurological diseases. Calculation of the fields generated inside the head is vital for the use of this method for treatment. In prior work we have implemented a realistic head model, incorporating inhomogeneous tissue structures and electrical conductivities, allowing the site of neuronal activation to be accurately calculated. We will show how we utilize this model in the development of novel TMS coil designs to improve the depth of penetration and localization of stimulation produced by stimulator coils.

Q1.00332 Near Field-Emission Scanning Electron Microscopy with Energy Analysis, DANilo ANDREA ZANIN, LORENZO GIUSEPPE DE PIETRO, HUGO CABRALE, PETER THALMANN, ANNA-LENA REDMANN, URS RASMOSER, DANilo PESCIA, MEHMET ERKBUADAK, Laboratory for Solid State Physics ETH Zurich — We report on new results about near field-emission scanning electron microscopy (NFESEM) which emphasize the potential of generating secondary electrons using a primary electron beam of low energy electrons. Based on scanning tunneling microscopy technology NFESEM uses a sharp W-tip as a cold field emitter, which scans the surface at constant distance, usually in the range of 5 to 40 nm. An applied voltage between tip and sample induces field emission at the tip. These primary electrons are then accelerated towards the target and successively scattered by its surface generating secondary electrons. The last ones, which carry information of the sample, are emitted and energy analyzed. Spatially resolved analysis of energy and polarization of secondary electrons may provide new insight into surface microscopy.

Q1.00333 Controlled manipulation of adatoms on the oxidized p(2 × 1) Cu(110) surface using NC-AFM, JOSEPH BAMIDELE, Dept. of Physics, King’s College London, U.K., ROBERT TURANSKY, Inst. of Physics, Slovak Acad. of Sciences, 84511 Bratislava, Slovakia, YASUHITO SUGAWARA, Dept. of Applied Physics, Osaka University, Japan, IVAN STICH, Inst. of Physics, Slovak Acad. of Sciences, 84511 Bratislava, Slovakia, LEV KANTOROVITCH, Dept. of Physics, King’s College London, U.K. — Experimentally, large finite regions (islands) of the p(6 × 2) reconstruction bordering (also rather substantial) regions of the p(2 × 1) reconstruction with single super-Cu atoms between some neighboring -Cu-O-Cu- rows can be created on the oxidized Cu(110) surface. We report on our combined theoretical and experimental study of the manipulation of these isolated super-Cu atoms with NC-AFM. Experiments indicate that the manipulation proceeds mostly by vertical manipulation with a small number of lateral manipulation events. Theoretical calculations were performed using the density functional theory (with particular attention paid towards including non-local correlation effects). Two Cu tip models were used terminated either with Cu or O atoms. Placing either of the two tips at various positions around the super-Cu atom on the surface, we calculated maps of the corresponding energy barriers for the transition of the super-Cu atom to the neighboring site and/or for tip adsorption and desorption. Using these comprehensive data and the virtual AFM, mimicking the actual NC AFM apparatus, we modeled the manipulation mechanism and obtained the corresponding tip response during the individual manipulation events.

Q1.00334 A 2nd Generation Interfacial X-ray Microscope, NOUAMANE LAANAIT, ZHAN ZHANG, PAUL FENTER, Argonne National Laboratory — Understanding and controlling the physical and chemical processes occurring at the interface of materials is a central theme in many of today’s scientific inquiries and technological advancements. Experimental investigations of interfaces has benefited from a large set of imaging techniques such as Probe microscopy, and Electron microscopy. Yet, numerous systems comprised of buried interfaces that are of immense significance, remain out of the reach of these methods because of their lack of depth penetration capabilities or inoperability in extreme conditions of pressure and/or temperature. Such systems can benefit from the development of complementary x-ray based imaging techniques that can operate in the above cited conditions. Combining the surface sensitivity of x-ray scattering and well-established methodology and instrumentation of transmission x-ray microscopy, a second generation interfacial x-ray microscope (IXM) is currently under development at Argonne’s advanced photon source with the aim of achieving a lateral resolution of 50 nm and collection times on the order of seconds. The IXM has been used to image surface topography of solid/gas, solid/liquid with sub-nanometer height sensitivity. These scientific results as well as the instrumentation will be presented.
Q1.00335 Development of Uncooled Micro-bolometer Arrays Based on Hole-doped Rare-Earth Manganese, E. KEVIN TANYI, GRACE YONG, CAMRON KESHAVARZ, PRAKASH SHARMA, CHRISTOPHER RUBIN, RAJESWARI KOLAGANI, Towson University, STEVEN GROSS1, Triton Services Inc. — Material properties indicate that rare earth manganites have a competitive advantage over VOx, which is a material commonly employed as bolometric sensors in state of the art uncooled imaging arrays. We will present the results of our work on developing manganite thin films for uncooled micro-bolometer arrays. By fine tuning the cation composition and stoichiometry, we have identified material compositions suitable for uncooled bolometer operation and developed thin films of these materials by Pulsed Laser Deposition (PLD) on Si. For hetero-epitaxy on Si, we employ lattice engineering schemes to circumvent problems such as chemical incompatibility and amorphization of the substrate surface due to the native oxide. We are in the process of fabricating single test bolometers and micro-bolometer arrays. We will discuss the results of materials development and device fabrication efforts and will present performance parameters and estimated figures of merit for test bolometers. We will also discuss efforts towards understanding and alleviating material problems such as the residual stresses in the thin film heterostructures which are of critical importance for the fabrication of suspended microstructures.

1We acknowledge support from the NSF grant ECCS 1128586 at Towson University.

Q1.00336 Auto-tuning system for NMR probe with LabView1, CARMEN QUEN, OLIVIA V. MATEO, OSCAR BERNAL, Department of Physics and Astronomy, California State University, Los Angeles, CA 90032 — Typical manual NMR-tuning method is not suitable for broadband spectra spanning several megahertz linewidths. Among the main problems encountered during manual tuning are pulse-power reproductibility, baselines, and transmission line reflections, to name a few. We present a design of an auto-tuning system using graphic programming language, LabVIEW, to minimize these problems. The program is designed to analyze the detected power signal of an antenna near the NMR probe and use this analysis to automatically tune the sample coil to match the impedance of the spectrometer (50 Ω). The tuning capacitors of the probe are controlled by a stepper motor through a LabVIEW/computer interface. Our program calculates the area of the power signal as an indicator to control the motor so disconnecting the coil to tune it through a network analyzer is unnecessary.

1Work supported by NSF-DMR 1105380

Q1.00337 ABSTRACT WITHDRAWN

Q1.00338 Characterization of Surface Topography by Line-Laser Light Scattering, LAWRENCE HONAKER, Liquid Crystal Institute, Kent State University, Kent, OH, HYEUNSEOK CHOI, Smart Systems Research Group, Korean Institute of Industrial Technology, Cheonan, South Korea, CHANJOONG KIM, Liquid Crystal Institute, Kent State University, Kent, OH — To characterize the topography of rough surfaces, various methods based on point-by-point analyses, such as scanning microscopy, atomic force microscopy, and profilometry, have been developed over the span of many years. However, the practical application of such methods is hampered by shortcomings such as the slow speed at which the analyses can be performed and the possibility of damaging or destroying the sample. We harness the optical properties of the reflection of plane-polarized line laser light as a non-destructive high-speed imaging method to inspect the surface. Profiles of reflected light patterns, both theoretical and experimental, have also been obtained to characterize the defects and roughness of the surface.

Q1.00339 Development and Characterization of Dynamic Light Scattering Instrumentation to Determine the Size of ZnO Nanoparticles1, CHRISTOPHER DI FATT A, JEFFERY R. SIMPSON, Department of Physics, Towson University, Z. THOMPSON, M. SCHULZE , Towson University, S. M. LEV, Urban Environmental Biogeochemistry Laboratory (UEBL) — Dynamic Light Scattering (DLS) serves as a useful tool for characterizing nanoparticles (NP) and molecules. DLS provides a high-throughput and accurate measurement of particle sizes for monodisperse (MD) spherical NPs. We are presenting the development and characterization of DLS instrumentation to measure the size of MD NPs, including ZnO. A HeNe and Argon ion laser comprise the excitation sources for the scattering experiment. We have evaluated avalanche photodiode and thermoelectrically-cooled photomultiplier tube detectors for the acquisition of the scattered light. We will determine the translational diffusion coefficient using time averaging and time-autocorrelation electronics. Considering the NPs to be MD spheres, we can determine the radius from the diffusion coefficient. ZnO NPs will be synthesized using several techniques and compared to those produced commercially. The synthesized particles are expected to range in diameter from 200 nm down to 20 nm, however, in the presence of agglomerates once suspended may extend the upper size limit for particles in suspension to 1000 nm. We will compare the DLS results on ZnO NPs with additional techniques including AFM. After size characterization, the ZnO NPs will be employed in ongoing toxicity studies in the UEBL.

1C. Di Fatta acknowledges support from the Fisher College of Science and Mathematics and Undergraduate Research Committee

Q1.00340 Inexpensive Ultrasonic Interferometer1, JOHN GROSSMANN, OLEKSII SVITELSKYI, Colgate University, Hamilton, NY 13346, ALEXEY SUSLOV, National High Magnetic Field Laboratory, Tallahassee, FL 32310 — Growing interest of small universities and colleges in research determines an increasing need in affordable laboratory equipment that would be capable of producing scientifically valuable experimental results. In this report we present the current status of our efforts to develop a simple and low-cost version of a classical experimental setup for ultrasonic pulse-echo measurements that would be easily reproducible in the electronic shop of any small educational institution. In particular, usage of a dual timer microchip LM556 allowed us to simplify the design of a probing pulse generator. Also, we propose that using modern broadband RF components in phase detection circuits will allow us to substitute the complicated and expensive superf heterodyne design of receiver with the technique of direct transformation and analysis of the echo signal right at the probe frequency. Our analysis shows that these simplifications can be achieved without compromising for sensitivity of the experiment or precision of measurements.

1This work is supported by Research Council of Colgate University

Q1.00341 FPGA for single-molecule recycling in a nanochannel, SULTAN BEHERY, BO WANG, BRIAN K. CANFIELD, LLOYD M. DAVIS, University of Tennessee Space Institute — Single-molecule (SM) trapping and detection experiments are important in studying biophysical processes on the molecular level. As an SM is too small for optical trapping, prolonged observation requires measurement of the position and active feedback to counteract diffusion. In previous work, a custom-built Field Programmable Gate Array (FPGA) circuit board was developed for SM detection and real-time electrokinetic trapping in a fused silica nanochannel. The FPGA was used as part of a feedback system to control the voltage for electrokinetic movement of solution along the nanochannel in response to the time stamps of individual photons from the excited SM. Other researchers have since shown that alternating the flow in a nanochannel can be used to recycle an SM through a stationary laser focus for repeated observations and that the times between each passage yield a measurement of the molecule’s diffusion. Improved measurements could be obtained by use of an FPGA for more precisely timed flow control. Therefore, we are now adapting the FPGA for SM trapping to use algorithms tested in a Monte Carlo simulation of SM recycling in an attempt to extend existing capabilities. This presentation discusses the custom-built FPGA board, algorithms, and ongoing nanochannel experiments.
Q1.00342 Mechanical Loss Measurements of Coated Substrates for Gravitational Wave Interferometry¹. JONATHAN NEWPORT, DAVID BELIVEA, RAYMOND ROBIE, GREGG HARR, American University. — Gravitational waves from sources such as binary star systems, supernovae explosions and stochastic background radiation have yet to be directly detected by experimental observations. Alongside international collaborators, the Laser Interferometer Gravitational-Wave Observatory (LIGO) is designed to realize direct detection of gravitational waves using interferometric techniques. The second generation of gravitational wave observatories, known as Advanced LIGO, are currently undergoing installation and commissioning at sites in Hanford, Washington and Livingston, Louisiana. The ultimate sensitivity of Advanced LIGO within select spectral bands is limited by thermal noise in the high-reflective coatings of the interferometer optics. The LIGO lab at American University is measuring the mechanical loss of coated substrates to predict thermal noise within these spectral bands. These predictions are used to ensure the ultimate design sensitivity of Advanced LIGO and to study coating and substrate materials for future gravitational wave detectors.

¹National Science Foundation

Q1.00343 Development of a Slow Positron Facility at Hebrew University of Jerusalem. AIDAN KELLEHER, Hebrew University of Jerusalem. — Positron annihilation spectroscopy provides both depth of penetration to study bulk defects in materials as well as nano-scale resolution. This measurement range is achieved by slowing positrons from a radioactive source, typically $^{22}$Na, by sending them through a moderator, typically W or solid Ne. The nearly thermal positrons are then accelerated to the desired energy by means of an electrostatic potential. The SPOT project at The Hebrew University of Jerusalem proposes to increase the luminosity of the beam by applying the best practices currently in use, as well as using a short-lived source of positrons, $^{18}$F. Simulations based on our current designs indicate this project will be able to deliver positrons in the energy range of 50-50000eV with an energy resolution of 1eV is possible. We will present the unique technical challenges of using this source of positrons, how we plan to overcome them, the results of simulations, and facility construction progress.

Q1.00344 Put forward the basic particle problems. HAN YONGQUAN, 13241357685. — The two kind of fundamental particles which constitute the material world is: superluminal particles and tachyon. First, the elementary particle velocity is a measure of quality. Second, due to the quality of superluminal particles, strong convergence for atomic, molecular attraction, such as “entity” material composed of neutron. Third, the light particles due to the quality of small, weak gravity launched into outer space, namely the Tachyon energy into light particles Fourth, The Tachyon convergence in atomic, molecular, so we can hardly observed superluminal Fifth, atom, molecule are internal Tachyon Sixth, the gravitational force between microscopic particles is greater than the static electricity. Then we can draw a conclusion: now, the quality determination is based on the superluminal mechanism determination, this conclusion is quality is relative essential reason. Author: hanyongquan TEL: 13241357685

Q1.00345 Pump-probe experiments of single-pulse femtosecond laser plasma-channel formation in fused silica. TREVOR S. BOWMAN, LLOYD M. DAVIS, University of Tennessee Space Institute. — Femtosecond laser pulses provide a means to machine structures with small heat-affected areas and with a highly non-linear mechanism that enables direct writing of nanoscale features. Fabrication at this scale can be applied to a large range of applications, including micro-optical and micro-fluidic devices. During single-shot ablation, the formation of opaque plasma in the focal region of a tightly focused beam typically limits the depth of the feature and creates a shallow crater. However, recent reports have shown the ablation of deep nanoholes with aspect ratios greater than 20. Proposed mechanisms for creating such high aspect ratio structures include nonlinear Kerr self-focusing and the reshaping of the Gaussian pulse into a Bessel profile. These mechanisms would create an elongated plasma channel beyond the focal region. We are developing a single-shot, pump-probe experiment to study the time-resolved formation and relaxation of plasma in femtosecond laser machining of fused silica. During the fabrication of high aspect ratio holes, the transmission characteristics of a frequency-doubled probe pulse with a controlled delay provide information about the plasma dynamics. We also briefly discuss time-resolved imaging of the material ejected during the ablation process.

Wednesday, March 20, 2013 2:30PM - 5:30PM
Session R0 APS: Kavli Foundation Special Session: Forefront Physics for Real World Problems: Energy, Climate, and the Environment — Hilton Baltimore Key Ballroom - Michael Turner, APS President and University of Chicago

2:30PM R0.00001 The Promise of Photovoltaics. STEVEN CHU, Secretary, U.S. Department of Energy. —

3:06PM R0.00002 Earth’s Climate History from Glaciers and Ice Cores¹, LONNIE THOMPSON, The Ohio State University. — Glaciers serve both as recorders and early indicators of climate change. Over the past 35 years our research team has recovered climatic and environmental histories from ice cores drilled in both Polar Regions and from low to mid-latitude, high-elevation ice fields. Those ice core-derived proxy records extending back 25,000 years have made it possible to compare glacial stage conditions in the Tropics with those in the Polar Regions. High-resolution records of $\delta^{18}$O (in part a temperature proxy) demonstrate that the current warming at high elevations in the mid- to lower latitudes is unprecedented for the last two millennia, although at many sites the early Holocene was warmer than today. Remarkable similarities between changes in the highland and coastal cultures of Peru and regional climate variability, especially precipitation, impy a strong connection between prehistoric human activities and regional climate. Ice cores retrieved from shrinking glaciers around the world confirm their continuous existence for periods ranging from hundreds to thousands of years, suggesting that current climatological conditions in those regions today are different from those under which these ice fields originated and have been sustained. The ongoing widespread melting of high-elevation glaciers and ice caps, particularly in low to middle latitudes, provides strong evidence that a large-scale, pervasive and, in some cases, rapid change in Earth’s climate system is underway. Observations of glacier shrinkage during the 20th and 21st century girdle the globe from the South American Andes, the Himalayas, Kilimanjaro (Tanzania, Africa) and glaciers near Puncak Jaya, Indonesia (New Guinea). The history and fate of these ice caps, told through the adventure, beauty and the scientific evidence from some of world’s most remote mountain tops, provide a global perspective for contemporary climate.

¹NSF Paleoclimate Program

3:42PM R0.00003 Physical Controls of the Earth’s Climate and Climate change, GRAEME STEPHENS, JPL, California Institute of Technology. — The Earth’s climate system and changes to it are determined by the physical processes that govern the flows of energy to and from the atmosphere and Earth’s surface. Although the energy exchanges at the top of the atmosphere are well determined from available satellite measurements, the global character of the energy flows within the climate system, and to and from the Earth’s surface in particular, are not directly measured and thus are much more uncertain. The surface energy balance is particularly important since geographical variations of its distribution drives ocean circulations, dictates the amount of water evaporated from the Earth’s surface, fuels the planetary hydrological cycle and ultimately controls how this hydrological cycle responds to forced climate change. This talk reviews our state of understanding of the physical processes that determine the energy balance, couple to the Earth’s water cycle and are responsible for the most important climate feedbacks that dictate the pace of climate change. Challenges in understanding the mechanisms responsible for feedbacks associated with clouds and precipitation, water vapor, snow cover and carbon will be highlighted. The further complexity and uncertainty that aerosols add to the cloud and precipitation feedbacks will also be reviewed. The effects of uncertainties in our understanding of the physical climate system, and feedbacks within it, will be reviewed in the context of climate change projections.
4:18PM R0.00004 Environmental Forensics: Molecular Insight into Oil Spill Weathering Helps Advance High Magnetic Field FT-ICR Mass Spectrometry\textsuperscript{1} . AMY MCKENNA, National High Magnetic Field Laboratory — The depletion of terrestrial global oil reserves has shifted oil exploration into offshore and ultra-deep water (\textgreater{} 5000 ft) oil reserves to meet global energy demands. Deep water reservoirs are currently in production in many parts of the world, including the Gulf of Mexico, but production is complicated by the water depth and thick salt caps that challenge reservoir characterization / production. The explosion aboard the Deepwater Horizon in April 2010 resulted in an estimated total release of \textasciitilde{} 5 million barrels (BP claims that they collected \textasciitilde{} 1M barrels, for a net release of 4 M) of light, sweet crude oil into the Gulf of Mexico and shifted attention toward the environmental risks associated with offshore oil production. The growing emphasis on deep water and ultra-deep water oil production poses a significant environmental threat, and increased regulations require that oil companies minimize environmental impact to prevent oil spills, and mitigate environmental damage when spills occur. Every oil spill is unique. The molecular transformations that occur to petroleum after contact with seawater depend on the physical and chemical properties of the spilled oil, environmental conditions, and deposition environment. Molecular-level knowledge of the composition, distribution, and total mass of released hydrocarbons is essential to disentangle photo- and bio-degradation, source identification, and long-term environmental impact of hydrocarbons released into the environment. Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) is unsurpassed in its ability to characterize complex mixtures at the level of elemental composition assignment. Only FT-ICR mass spectrometry can routinely achieve the required minimum resolving power necessary to elucidate molecular-level characterization of crude oil. Conversely, the spectral complexity of petroleum facilitates identification of systematic errors in the accumulation, transfer, excitation, and detection events in the FT-ICR experiment. For example, the high density of peaks at each nominal mass unit provides unprecedented insight into how excitation conditions affect ion motion during detection. Aggregated oil (i.e., tar balls, tar mats) that reached the surface exhibits a more than two-fold increase in the total number of detected species, with an increased number of oxygenated species. Principal component analysis (PCA) applied to two possible source oils (contained within the same ship) and weathered samples provide the first application of FT-ICR MS for source identification. Molecular formulae from parent and weathered oil indicate that the lightest petroleum fractions (saturated hydrocarbons) are the most readily oxidized components, and can serve as a template to determine chemical transformations that occur throughout the water column. The ability to differentiate and catalogue compositional changes that occur to oil after its release into the environment relies heavily on gains achieved in nearly all steps in the FT-ICR mass spectral experiment required to accommodate larger ion populations inherent to heavily weathered crude oil. Here, we present the requirement for FT-ICR MS for comprehensive oil spill characterization, and highlight advances made to FT-ICR MS experimental conditions developed from petroleum characterization.

\textsuperscript{1}Work supported by DMR-06-54118, NSF CHE-10-49753 (RAPID), BP/The Gulf of Mexico Research Initiative, and the State of Florida

4:54PM R0.00005 Forefront Research in Batteries for Electric Vehicles , STEPHEN HARRIS, General Motors —

Wednesday, March 20, 2013 7:30PM - 9:00PM —

Session S48 APS: Special Evening Event Hosted by the Editors of Physics Ballroom IV - Jessica Thomas, Editor, Physics

7:30PM S48.00001 Social Gathering with Pizza and Beer —

8:00PM S48.00002 Why Condensed Matter Physicists Should Pay Attention to Atomic Physics , WILLIAM D. PHILLIPS, Joint Quantum Institute / NIST — Atomic and molecular (AMO) physics has been revolutionized by the advent of ultracold atomic gases, including quantum degenerate Bose and Fermi gases. Much of the activity with cold atoms brings AMO physics into close contact with condensed matter (CM). Atoms in optical lattices (externally imposed periodic potentials) can mimic the behavior of electrons in crystals, Bose-Einstein condensed gases or Cooper-paired degenerate Fermi gases can mimic superfluid helium or superconducting materials, and atomic gases can exhibit phase transitions that are traditionally studied in solids. These and other atomic phenomena offer possibilities for measurement and control that can be quite different from those available in materials. This talk will explore some of the current intersections of AMO and CM physics and speculate about the future of this relationship.

Thursday, March 21, 2013 5:45PM - 7:15PM —

Session X1 APS: Nobel Prize Session: 2012 Nobel Prize Perspectives Ballroom I - Daniel Lidar, University of Southern California

5:45PM X1.00001 Controlling photons in a box and exploring the quantum to classical boundary , SERGE HAROCHE, Collège de France, Ecole Normale Superieure —

6:30PM X1.00002 Superposition, Entanglement, and Raising Schroedinger’s Cat , DAVID J. WINELAND, National Institute of Standards and Technology —