8:00AM A53.00001 Oil Induced Spontaneous Flow in Water- Bis(2-ethylhexyl)Sulfosuccinat (AOT) system
PARVATHALU KALAKONDA, King Abdullah University of Science and Technology — Instability and evaporation rates of oils within the layers of vesicles of a surfactant trigger the spontaneous (second flow) flow. The incorporation of oils into bis(2-ethylhexyl)sulfosuccinat (AOT) system remains incompletely characterized. We show that the second flow has a finite size that show a minimum at a particular concentration (mM) of surfactant solution. As a result, the layers are destabilized lead to explode and create the second flow. The fluorescence emission spectra and evaporation rates show that the oil diffuses into the layers of vesicles of a surfactant. We have characterized evaporation rates of oils on various concentrations (mM) of surfactant solution and observed that oil evaporation rates depend on volume and remain constant as the function of surfactant. We believe that second flow is new feature and brings a new insight into the fluid flow dynamics.

8:12AM A53.00002 Joule Heating Effects on Electrokinetic Flow Instabilities in Ferrofluids.1
CHRISTIAN BRUMME, RYAN SHAW, YILING ZHOU, RAMA PRABHAKARAN, XIANGCHUN XUAN, Clemson University — We have demonstrated in our earlier work that the application of a tangential electric field can draw fluid instabilities at the interface of a ferrofluid/water co-flow. These electrokinetic flow instabilities are produced primarily by the mismatch of electric conductivities of the two fluids. We demonstrate in this talk that the Joule heating induced fluid temperature rises and gradients can significantly suppress the electrokinetic flow instabilities. We also develop a two-dimensional depth-averaged numerical model to predict the fluid temperature, flow and concentration fields in the two-fluid system with the goal to understand the Joule heating effects on electric field-driven ferrofluid flow instabilities.

8:24AM A53.00003 Wall mode instability driven transition to turbulence in a soft microchannel1
SAGAR SRINIVAS, KUMARAN V, Indian Institute of Science — Transition to turbulence has been triggered due to structure fluid interaction at Reynolds number (Re) much lower than hard wall transition Re, in a soft walled micro channel of dimensions 40mm*1.5mm*0.16mm. Mixing index analysis indicates high degree of mixing accompanied by lower pressure drop as the channel deforms. Flow after transition velocity statistics has been extensively studied using Particle Imaging Velocimetry (PIV) along streamwise-wallnormal direction. The reduced plots of streamwise mean velocity are shown with the absence of viscous sublayer and presence of logarithmic layer with von Karman constants different from rigid wall channel. The one-point cross correlation between velocity fluctuations is non-zero at the soft surface which is in contrast to flow in hard walled channel. This indicates that the additional fluid stress exerted on the soft surface by the fluid velocity fluctuations result in net energy transfer due to shear work done at the interface. The structure flow interface acts as a source of energy for the mean turbulent kinetic energy which is typically zero at the interface for hard walled channel. We also detect the onset of wall-oscillations primarily tangential to the surface at the transition Re.

8:36AM A53.00004 The effect of viscosity variation on the stability of a buoyantly unstable miscible layer in vertical porous media1
SATYAJIT PRAMANI, TAPAN KUMAR HOTA, MANORJAN MISHRA, Indian Institute of Technology Ropar, India — We numerically show that in the absence of displacement a buoyantly unstable miscible layer with variable viscosity is less unstable than the constant viscosity layers. With the help of scaling analysis, we proved that the dynamics of variable viscosity layers with stable as well as unstable viscosity contrasts are identical in the absence of displacement. When the heavier fluid displaces the lighter one, the influence of viscosity contrast on the buoyantly unstable miscible layer is analogous to that in neutrally buoyant fluids. These findings of direct numerical simulations (DNS) in the fully nonlinear regime are consistent with the linear stability analysis (LSA). Furthermore, we perform a non-modal stability analysis of the linearized equations, which depicts the qualitative agreement with both LSA and DNS. In addition, the response of the linearized operator to external excitation has been studied through pseudospectra. The present findings are of great importance to understand the hydrodynamic mechanisms involved in geologic carbon sequestration.

8:48AM A53.00005 Untying vortex knots in fluids and superfluids.
DUSTIN KLECKNER, UC Merced, MARTIN SCHEELE, HRIDESH KEDIA, WILLIAM T. M. IRVINE, University of Chicago — Recent work has demonstrated that vortex knots appear to always untie in fluids and superfluids. Should we expect the same behavior from these two very different systems? We will discuss this unknotting behavior, both quantitatively – through helicity – and qualitatively through the geometry and topology of the vortex lines as they evolve.

9:00AM A53.00006 Relaxation of Anisotropy in Superfluid Turbulence
RENA ZIEVE, OWEN DIX, University of California - Davis — We simulate superfluid turbulence on a 3-sphere rather than using the more common periodic boundary conditions. We find that our topology naturally leads to anisotropy in a steady-state vortex tangle. A fundamental assumption in turbulence studies is that any large-scale anisotropy due to a driving velocity can be ignored at small length scales. However, there are practical concerns over how quickly the anisotropy decreases with length scale, and whether isotropic turbulence is attained above the dissipation scale. Here we examine how the anisotropy decreases upon moving from large to small length scales.

9:12AM A53.00007 Simulating transitional hydrodynamics of the cerebrospinal fluid at extreme scale.
KARTIK JAIN, Simulation Techniques and Scientific Computing, Univ., of Siegen, Germany and Center for Biomedical Computing, Simula Research Lab., Lysaker Norway, SABINE ROLLER, Simulation Techniques and Scientific Computing, University of Siegen, Germany, KENT-ANDRE MARDAL, Center for Biomedical Computing, Simula Research Lab., Lysaker Norway and Dept., of Mathematics, Univ., of Oslo, Norway — Chiari malformation type I is a disorder characterized by the herniation of cerebellar tonsils through the foramen magnum resulting in obstruction to cerebrospinal fluid (CSF) outflow. The flow of pulsating bidirectional CSF is of acutely complex nature due to the anatomy of the conduit containing it - the subarachnoid space. We report lattice Boltzmann method based direct numerical simulations on patient specific cases with spatial resolution of 24μm amounting meshes of up to 2 billion cells conducted on 50000 cores of the Hazelhen supercomputer in Stuttgart. The goal is to characterize intricate dynamics of the CSF at resolutions that are of the order of Kolmogorov microscales. Results unfold velocity fluctuations up to ∼ 10 Km/s, turbulent kinetic energy ∼ 2 times of the mean flow energy in Chiari patients whereas the flow remains laminar in a control subject. The fluctuations confine near the cranio-vertebral junction and are commensurate with the extremeness of pathology and the extent of herniation. The results advocate that the manifestation of pathological conditions like Chiari malformation may lead to transitional hydrodynamics of the CSF, and a prudent calibration of numerical approach is necessary to avoid overlook of such phenomena.
9:24AM A53.00008 Numerical Simulation of Parachutist Generated Turbulence on Parachute Inflation . XIAOLEI CHEN, XIAOLIN LI, Stony Brook University — Using the front tracking computational platform, we couple parachutists as rigid bodies with the spring-mass model for the parachute system. The rigid body generates turbulent flow which affect the parachute inflation and stability. In this talk, we will present our numerical method to solve the complex system and study the effect of the turbulence at the wake of the parachutist on the canopy opening and parachute descent. Several different turbulence models are used and compared with experiments.

9:36AM A53.00009 ABSTRACT WITHDRAWN –

9:48AM A53.00010 ABSTRACT WITHDRAWN –

10:00AM A53.00011 Tailoring boundary geometry to optimize heat transport in turbulent convection . SRIKANTH TOPPALADODDI, Yale University, University of Oxford, SAURO SUCCI, Istituto per le Applicazioni del Calcolo “Mauro Picone” (C.N.R.), JOHN WETTLAUFER, Yale University, University of Oxford, NORDITA — Turbulent Rayleigh-Bénard convection between planar horizontal boundaries is a classical example of the challenge posed by multiple interacting scales in fluid dynamics. Here, by tailoring the geometry of the upper boundary we manipulate the boundary layer — turbulent interior flow interaction, and study the turbulent transport of heat in two-dimensional Rayleigh-Bénard convection with numerical simulations using the Lattice Boltzmann method. By fixing the roughness amplitude of the upper boundary and varying the wavelength $\lambda$, we find that the exponent $\beta$ in the Nusselt-Rayleigh scaling relation, $Nu - 1 \propto Ra^\beta$, is maximized at $\Lambda \approx \lambda_{max} \approx (2 \pi)^{-1}$, but decays to the planar value in both the large ($\lambda \gg \lambda_{max}$) and small ($\lambda \ll \lambda_{max}$) wavelength limits. The changes in the exponent originate in the nature of the coupling between the boundary layer and the interior flow. We present a simple scaling argument embodying this coupling, which describes the maximal convective heat flux. Results from simulations with both top and bottom rough boundaries showing a further enhancement of heat transport will also be presented.

10:12AM A53.00012 Tracking Coherent Structures and Source Localization in Geophysical Flows 1 . ERIC FORGOSTON, Montclair State University, ANI HSIEH, Drexel University, IRA SCHWARTZ, US Naval Research Laboratory, PHILIP YECKO, Cooper Union — There has been a steady increase in the deployment of autonomous underwater and surface vehicles for applications such as ocean monitoring, tracking of marine processes, and forecasting contaminant transport. The underwater environment poses unique challenges since robots must operate in a communication and localization-limited environment where their dynamics are tightly coupled with the environmental dynamics. This work presents current efforts in understanding the impact of geophysical fluid dynamics on underwater vehicle control and autonomy. The focus of the talk is on the use of collaborative vehicles to track Lagrangian coherent structures and to localize contaminant spills.

1Research supported by the National Science Foundation and the Office of Naval Research.

10:24AM A53.00013 Neutral equivalent surface stress . CHERYL KLIPP, US Army Research Laboratory — In laboratory turbulent flows, it has been observed that the eigen axes of the Reynolds stress tensor are oriented 17 deg from the streamwise coordinate system. This has also been observed in atmospheric flows over relatively flat terrain under thermally neutral conditions. The reliability of this relationship is examined, especially for locations very near the surface. The relationship is then used as the basis for a neutral equivalent momentum transport which can be calculated in complex environments, such as urban canyons, where the influence of multiple wall normals makes more conventional measurement of momentum transport problematic.

Monday, March 14, 2016 11:15AM - 2:15PM – Session B40 GSNP DFD: Fluids and Elasticity

11:15AM B40.00001 Direct measurement of surface stress of stretched soft solids . QIN XU, ERIC DUFRESNE, Mechanical Engineering and Materials Science, Yale University — The wetting profile of liquid droplets on soft solids is determined by the competition between elasticity and solid surface stress. Near the contact point, the bulk elasticity becomes negligible such that Neumann’s classic analysis nicely captures the wetting geometry and provides an effective approach to directly measure the solid surface stress. Here, we report our experiments using confocal microscopy in studying the wetting of liquids on soft PDMS gels. While the droplets are sitting on the top, the substrates are biaxially strained. We observe that the wetting profiles and the three-phase contact angles are changing dramatically as the substrate is stretched. With Neumann’s principle, we obtain the quantitative relationship between surface stress of the PDMS and the applied strain. These results suggest a significant strain-dependence of surface energy and surface stress for our PDMS.

11:27AM B40.00002 A numerical modeling capability for the interplay between surface energy and elasticity in soft materials . DAVID HENANN, YUHAO WANG, Brown University — Surface energy is an important factor in the deformation of fluids but is typically a minimal or negligible effect in solids. However, when a solid is soft and its characteristic dimension is small, forces due to surface energy can become important and induce significant elastic deformation. The interplay between surface energy and elasticity can lead to interesting elastico-capillary phenomena. We have developed a finite-element formulation for problems involving these effects in both 2D and 3D settings and will demonstrate the simulation capability by examining two elastico-capillary problems. (1) The Rayleigh-Plateau instability in an elastic material – In a fluid, this instability causes fluid jets to break up into droplets; however, as shown in recent experiments (Mora et al., PRL, 2010), break-up is prohibited in an elastic material, resulting in a stable undulatory configuration. (2) The effect of fluid-filled droplet inclusions on a soft solid – When the matrix material is stiff, the presence of fluid-filled inclusions leads to a more compliant composite material; however, recent experiments (Style, et al., Nature Physics, 2014) have shown that when the matrix material is more compliant, the presence of droplets leads to stiffening. In this talk, we will show that our simulation capability predicts all experimentally observed phenomena and provides a straightforward route for describing nonlinear aspects of elastico-capillarity, which are difficult to address via analytics.

11:39AM B40.00003 Elastocapillary Deformations and Fracture of Soft Gels . KAREN DANIELS, NC State University, MARION GRZELKA, ENS-Cachan, JOSHUA BOSTWICK, Clemson University — When a droplet is placed on the surface of a soft gel, the surface deforms by an amount proportional to the elastocapillary length calculated from the ratio of surface tension and elastic modulus. For sufficiently large deformations, the gel can fracture due to the forces generated under the liquid-gel contact line. We observe that a starburst of channel fractures forms at the surface of the gel, driven by fluid propagating away from the central droplet. To understand the initiation of these cracks, we model the substrate as an incompressible, linear-elastic solid and quantify the elastic response. This provides quantitative agreement with experimental measurements of the number of fracture arms as a function of material properties and geometric parameters. In addition, we find that the initiation process is thermally-activated, with delay time that decreases as a function of the elastocapillary length.
11:51AM B40.00004 Surface tension and deformation in soft adhesion. KATHARINE JENSEN, Yale University — Modern contact mechanics was originally developed to account for the competition between adhesion and elasticity for relatively stiff deformable materials like rubber, but much softer materials are ubiquitous in biology, engineering, and everyday consumer products. In such soft materials, the solid surface tension can also play an important role in resisting shape change, and significantly modify the physics of contact with soft matter. We report indentation and pull-off experiments that bring small, rigid spheres into adhesive contact with compliant silicone gel substrates, varying both the surface functionalization of the spheres and the bulk elastic properties of the gels. We map the resulting deformation profiles using optical microscopy and image analysis. We examine the substrate geometry in light of capillary and elastic theories in order to explore the interplay of surface tension and bulk elasticity in governing soft adhesion.

12:27PM B40.00005 Elastocapillary Swelling: When coalesced structures curl apart. DOUGLAS HOLMES, Boston University, PIERRE-TOMAS BRUN, MIT, ANUPAM PANDEY, University of Twente, SUZIE PROTIERE, Institut Jean le Rond d’Alembert — We consider the elastocapillary rise between swellable structures using a favorable solvent. We study the elastocapillary rise and subsequent swelling-induced bending, and characterize the dynamic deformations and resulting equilibrium configurations for various beam geometries. Our analysis highlights the importance of two characteristic length scales, and uses these lengths to predict both the elastocapillary rise and the critical curvature for peeling. We predict the transition between coalesced and curled shapes to be driven by bending and bending-dominated beams using a balance of bending, stretching, and surface energies, and use a relaxed constraint on Euler’s elastica to describe the fluid ratcheting.

12:39PM B40.00006 Effects of elastocapillarity on periodic films folding and unfolding. OSAMA BILAL, ANDRE FOEHR, JINWOONG CHA, CHIARA DARAIIO, Department of Mechanical and Process Engineering, ETH-Zurich — Thin films interact with liquid surfaces through elastocapillary forces. These forces can control structural deformations of wetted thin films. Deformations arise from the interplay between the elastic strain energy in the bulk of the films, and the energy on the surface. In this work, we study the interplay between the surface tension of water and periodic patterns on different thin films. Our analysis explores the utilization of these periodically patterned films for the deployability of micro- and nano-systems. The main attention is paid to the experimental results of this phenomenon and the results are supported by numerical analysis.

12:51PM B40.00007 Wrinkles and folds in a compressed granular raft. ETIENNE JAMON-PUILLET, CHRISTOPHE JOSSENDAL, SUZIE PROTIERE, Institut Jean le Rond d’Alembert, Univ Paris 6 UPMC, CNRS UMR 7190, France — Wrinkles and folds occur in a wide variety of situations, we find them in Nature but also in man-made products. They typically appear when a thin sheet bound to a foundation is compressed. Here we demonstrate that particle laden interfaces, despite being made of discrete very hard particles, can form wrinkles and folds like a soft solid. We call granular raft a close packed monolayer of heavy, athermal particles at the interface between two fluids. We use beads of different materials with diameters ranging from 30 µm to 0.8 mm dispersed at a planar oil/water interface. Upon uniaxial compression the raft buckles out of plane like a soft elastic solid and forms a periodic wrinkling pattern, then the deformation localizes in a large unique fold/crease. This behavior is reminiscent of a compressed elastic sheet floating on water. We will highlight similarities and differences between the mechanical properties of our discrete heavy granular raft and a continuous elastic floating film. Finally we will show how elasticity and gravity contribute to rationalize the original shape of the fold we observe.

1:03PM B40.00008 Wrapping with a splash. DEEPAK KUMAR, University of Massachusetts Amherst, JOSEPH PAULSEN, Syracuse University, THOMAS RUSEL, NARAYAN MENON, University of Massachusetts Amherst — Ultrathin sheets have been used to encapsulate drops of one fluid in another. When the sheet is thin enough that bending energies are much smaller than interfacial energies, experiment and theory show that optimal wrappings are achieved without any special sheet design [1]. Here we study wrappings generated by the impact of an oil droplet onto a uniform (30-200 nm) polystyrene film floating on water. Depending on the energy of impact, a large deformation of the air-water interface is followed by formation of an oil phase wrapped around, submerged in the water. Even though the energetic cost of bending of the polymer film is very small, we find that successful wrapping requires an impact energy much larger than the energy difference between the initial and final configurations. We explore the dynamics of the fluid and the sheet in this process with a view to devising an efficient method to create optimal wrappings. [1] J.D. Paulsen, V. Dimery, C.D. Santangelo, T.P. Russell, B. Davydovitch, and N. Menon, doi:10.1038/nmat4397 (2015).

1:15PM B40.00009 Deformation of flexible micro helices under flow. MARINE DAIEFF, ANKE LINDNER, OLIVIA DU ROURE, PMMH-ESPCI, Paris, France, ALEXANDER MOROZOV, University of Edinburgh, United Kingdom, JONATHAN PHAM, ALFRED CROSBY, University of Massachusetts, Amherst, USA — The interaction of small helices with fluids is important because of its relevance to both fundamental science and technological applications, such as swimming microrobots or microflow sensors. Helically shaped flagella are also exploited by swimming microorganisms to move through their surrounding fluids. Here we study experimentally the deformation of flexible helical ribbons under flow in a microfluidic channel. The size of the helix is typically microscale for the diameter and nanoscale for the thickness. We focus on two different aspects: the overall shape of the helix and the viscous response of the helicoidal motion. We compare our measurements by thin-film theory and dimensionless parameters. The viscous flow is well described by resistive force theory. Deformation of helices by viscous flow is well-described by non-linear force extensibility. Due to the non-uniform distribution of the pitch under distributed loading, we identify both linear and non-linear behavior along the contour length of a single helix. Utilizing our system, we explore the impact of non-Newtonian fluid properties on the mechanics of helix-fluid interactions.

1:27PM B40.00010 Dynamics and propulsion of a rotating flexible helical rod near a no-slip rigid boundary. MOHAMMAD JAWED, HUSSAIN KARIMI, PEDRO REIS, Massachusetts Institute of Technology — We study the effect of a no-slip rigid boundary on the locomotion of uni-flagellar bacteria in a viscous fluid at low Reynolds number conditions, through a combination of computer simulations and experiments. In our analogue model experiments, we exploit the prominence of geometry in this class of problems to rescale the original micron-scale system at a finite distance away from a rigid boundary. The experimental results are compared against numerical simulations that combine the Discrete Elastic Rods method in conjunction with Lighthill Slender Body Theory. The no-slip boundary condition on the wall is implemented by the method of images. We first show that optimal wrappings are achieved without any special sheet design [1]. Here we study wrappings generated by the impact of an oil droplet onto a uniform (30-200 nm) polystyrene film floating on water. Depending on the energy of impact, a large deformation of the air-water interface is followed by formation of an oil phase wrapped around, submerged in the water. Even though the energetic cost of bending of the polymer film is very small, we find that successful wrapping requires an impact energy much larger than the energy difference between the initial and final configurations. We explore the dynamics of the fluid and the sheet in this process with a view to devising an efficient method to create optimal wrappings. [1] J.D. Paulsen, V. Dimery, C.D. Santangelo, T.P. Russell, B. Davydovitch, and N. Menon, doi:10.1038/nmat4397 (2015).

1:39PM B40.00011 Fluid-structure interaction of reticulated porous wings. ELIZABETH STRONG, MOHAMMAD JAWED, PEDRO REIS, MIT — Insects of the orders Neuroptera and Hymenoptera locomote via flapping flight with reticulated wings that have porous structures that confers them with remarkable lightweight characteristics. Yet these porous wings still perform as contiguous plates to provide the necessary aerodynamic lift and drag required for flight. Even though the fluid flow past the bulk of these insects may be in high Reynolds conditions, viscosity can dominate over inertia in the flow through the porous sub-features. Further considering the flexibility of these reticulated wings yields a highly nonlinear fluid-structure interaction problem. We perform a series of dynamically-scaled precision model experiments to gain physical insight into this system. Our experiments are complemented with computer simulations that combine the Discrete Elastic Rods method and a model for the fluid loading that takes into account the ‘leakiness’ through the porous structure. Our results are anticipated to find applications in micro-air vehicle aerodynamics.
1:15PM B40.00012 Switchable and Tunable Acoustic Drag on Cylinders, MARK GUTTAG, FRAN-CISCO LOJPZ JIMNEZ, MIT, PRIYANK UPADHYAYA, SHANMUGAM KUMAR, Masdar Institute, PEDRO REIS, MIT — We report results on the performance of Smart Morphable Surfaces (Smorphs) that can be mounted onto cylindrical structures to actively reduce their aerodynamic drag. Our system comprises of an elastomeric thin shell with a series of carefully designed sub-surface cavities that, once depressurized, lead to a dramatic deformation of the surface topography, on demand. Our design is inspired by the morphology of the giant cactus (Carnegia gigantea) which possesses an array of axial grooves, thought to help reduce aerodynamic drag, thereby enhancing the structural robustness of the plant under wind loading. We perform systematic wind tunnel tests on cylinders covered with our Smorphs and characterize their aerodynamic performance. The switchable and tunable nature of our system offers substantial advantages for aerodynamic performance when compared to static topographies, due to their operation over a wider range of flow conditions.

2:03PM B40.00013 Fanning the Optimal Breeze with an Abanico, GRACE GOON, JOEL MARTHELOT, PEDRO REIS, MIT, MIT EGS LAB TEAM — Flexible hand-held fans, or abanicos, are universally employed as cooling devices that are both portable and sustainable. Their to and fro axial motion allows for a vortex that increases the evaporation rate near the skin and refreshes. We study this problem in the context of fluid-structure interaction, through precision model experiments. We first characterize the elastic properties of a semi-circular thin plates with various thickness and capillary number (Ca = μU/σ) and compare their performance in a custom built apparatus. The air velocity profile that results from the flapping motion of the fan is characterized for different driving conditions. A systematic variation of the geometric and elastic parameters, along with an exploration of the parameter space of the periodic driving motion (amplitude and frequency), allows us to establish optimal design and operational conditions for maximal output of the generated airflow, while minimizing the input power.


11:15AM B53.00001 ABSTRACT WITHDRAWN

11:27AM B53.00002 Acoustical vortices on a Chip for 3D single particle manipulation and vorticity control.1, ANTOINE RIAUD, CNRS Nord pas de Calais, JEAN-LOUIS THOMAS, OLIVIER BOU MATAR, CNRS Paris, MICHAEL BAUDOIN, CNRS Nord pas de Calais — Surface acoustic waves offer most of the basic functions required for on-chip actuation of fluids at small scales: efficient flow mixing, integrated pumping, particles separation, droplet displacement, atomization, division and fusion. Nevertheless some more advanced functions such as 3D particles manipulation and vorticity control can be realized with trap individual particles in an acoustic well for single object manipulation. In this presentation, I will show how acoustics and characterize can be synthesized with a programmable electronics and an array of transducers. I will then highlight how some of their specificities can be used for acoustical tweezing and twisting.

1This work is supported by ANR Project No. ANR-12-BS09-0021-01 and ANR-12- BS09-0021-02, and Rgion Nord Pas de Calais.

11:39AM B53.00003 Coalescence-induced jumping of nanoscale droplets on super-hydrophobic surfaces, ZHI LIANG, PAWEL KEBLINSKI, Rensselaer Polytechnic Institute, NANO SCALE SCIENCE AND ENGINEERING CENTER TEAM — The coalescence-induced jumping of tens of microns size droplets on super-hydrophobic surfaces has been observed in experiments and simulations. However, whether the coalescence-induced jumping would occur for smaller, particularly nanoscale droplets, is an open question. Using molecular dynamics simulations, we demonstrate that in spite of the large internal viscous dissipation, coalescence of two nanoscale droplets on a super-hydrophobic surface can result in a jumping of the coalesced droplet from the surface with a speed of a few m/s. Similar to the coalescence-induced jumping of microscale droplets, we observe that the bridge between the coalescing nano-droplets expands and impacts the solid surface, which leads to an acceleration of the coalesced droplet by the pressure force from the solid surface. We observe that the jumping velocity decreases with the droplet size and its ratio to the inertial-capillary velocity is a constant of about 0.126, which is close to the minimum value of 0.111 predicted by continuum-level modeling of Enright et al. [R. Enright, N. Miljkovic, J. Sprittles, K. Nolan, R. Mitchell, and E. N. Wang, ACS Nano 8, 10352 (2014)].

11:51AM B53.00004 Droplet climbing on a pre-wetted conical fibre, ZHEN JIAN, ERQIANG LI, S. T. THORODDSEN, King Abdullah University of Science and Technology (KAUST) — We study the motion of a droplet on a wet conical fibre. The conical fibres are fabricated with a glass-puller, with tip diameters of several µm. With liquid is fed through the hollow fibre and travels up the outside of the cone, forming a droplet, which is initially attached near the tip. This droplet grows in size and then detaches and moves on the fibre, at velocities up to 0.25 m/s. We focus on the regime with small Bond number Bo = ρgR^2/σ and capillary number Ca = µU/σ, where the droplet motion is driven by the pressure gradient due to the continuous curvature change along the conical fibre. High-speed imaging and numerical simulations via the Gerris code are employed to investigate the dynamics of the droplet detachment and climbing. Our focus is on the interface profile near the tip, the mechanism of droplet formation and climbing, and the velocity field in the thin liquid layer on the cone.

12:03PM B53.00005 Electro-osmotic flow in bicomponent fluids1, ANDREI BAZARENKO, MARCELLO SEGA, University of Vienna — The electroosmotic flow (EOF) is a widely used technique that uses the action of external electric fields on solvated ions to move fluids around in microfluidics devices. For homogeneous fluids, the characteristics of the flow can be well approximated by simple analytical models, but in multicomponent systems such as oil-in-water droplets one has to rely to numerical simulations. The purpose of this study is to investigate physical properties of the EOF in a bicomponent fluid by solving the coupled equations of motions of explicit ions in interaction with a continuous model of the flow. To do so we couple the hydrodynamics equations as solved by a Shan-Chen Lattice-Boltzmann method to the molecular dynamics of the ions. The presence of explicit ions allows us to go beyond the simple Poisson-Boltzmann approximations, and investigate a variety of EOF regimes.

1ETN-COLLDENSE (H2020-MCSA-ITN-2014, Grant No. 642774)


12:15PM  B53.00006  Electrohydrodynamics of toroidal droplets  ,  ALEXANDROS FRAGKOPOULOS,  ERIC BERGER,  Georgia Institute of Technology,  EKAPOI PAIRAM,  King Mongkut’s Institute of Technology Ladkrabang,  ALBERTO FERNANDEZ-NIEVES,  Georgia Institute of Technology — Toroidal droplets are unstable and always transform into spherical droplets due to surface tension. This can happen via Rayleigh-Plateau instabilities, or via the shrinking of the handle. Interestingly, charging a toroidal droplet can cause expansion, rather than shrinking, of the handle. In this talk, we will discuss the use of particle image velocimetry to obtain the velocity profile inside both neutral and charged toroidal droplets as they transform into the spherical shape. In particular, we quantify the effect of surface stresses on the velocity field and, consequently, on the shape of the interface as the droplet evolves by either shrinking or expanding.

12:27PM B53.00007  Study of the (1+1)D Long Wavelength Steady States of the Bénard Problem For Ultrathin Films  ,  CHENGZHE ZHOU,  SANDRA TROIAN,  California Institute of Technology,  1200 E California Blvd.,  MC 128-95,  Pasadena, CA — We investigate the stationary states of the (1+1)D equation $h_t + [h h_{xx} + h \gamma(h)_x] = 0$ for thin films of thickness $h(x,t)$ where $x$ is the spatial variable and $t$ is time. The variable $\gamma(h)$ denotes the surface tension along the gas/liquid interface of the slender bilayer confined between two substrates enforcing thermal conduction within the gap. Equilibrium solutions include flat films, droplets, trenches/ridges and positive periodic steady states (PPSS), the latter conveniently parameterized by a generalized interfacial pressure and the global extremum in shape. We derive perturbative solutions describing PPSS shapes near the stability threshold including their minimal period, average height and free energy. Weakly nonlinear analysis confirms that flat films always undergo a supercritical unstable pitch-fork bifurcation. Globally, our numerical simulations indicate at most one non-trivial PPSS per given period and volume. The free energy of droplet states is also always lower than the relevant corresponding PPSS, suggesting that initial flat films tend to redistribute mass into droplet-like configurations. By solving the linearized eigenvalue problem, we also confirm the unstable nature of PPSS solutions far from the stability threshold.

12:39PM B53.00008  Collective oscillations and coupled modes in confined microfluidic droplet arrays1  ,  ULF D. SCHILLER,  Department of Materials Science and Engineering,  Clemson University,  JEAN-BAPTISTE FLEURY,  RALF SEEMANN,  Experimental Physics,  Saarland University,  GERHARD GOMPPE,  Institute of Complex Systems,  Forschungszentrum Jülich — Microfluidic droplets have a wide range of applications ranging from analytic assays in cellular biology to controlled mixing in chemical engineering. Ensembles of microfluidic droplets are interesting model systems for non-equilibrium many-body phenomena. When flowing in a microchannel, trains of droplets can form microfluidic crystals whose dynamics are governed by long-range hydrodynamic interactions and boundary effects. In this contribution, excitation mechanisms for collective waves in dense and confined microfluidic droplet arrays are investigated by experiments and computer simulations. We demonstrate that distinct modes can be excited by creating specific ‘defect’ patterns in flowing droplet trains. While longitudinal modes exhibit a short-lived cascade of pairs of laterally displacing droplets, transversely excited modes form propagating waves that behave like microfluidic phonons. We show that the confinement induces a coupling between longitudinal and transverse modes. We also investigate the life time of the collective oscillations and discuss possible mechanisms for the onset of instabilities. Our results on the effects of the interfacial forces, including disjoining pressure. Interestingly, a layered ordering of micelles inside the foam films (thickness < 100 nm) leads to a stepwise thinning phenomena called stratification, which results in a thickness-dependent variation in reflected light intensity, visualized as progressively darker shades of gray. Thinner, darker domains spontaneously grow within foam films. During the initial expansion, a rim forms near the contact line between the growing thinner domain and the surrounding region, which influences the dynamics of domain growth as well as stratification. Using newly developed interferometry digital imaging optical microscopy (IDIOM) technique, we capture the rim evolution dynamics. Finally, we also develop a theoretical model to describe both rim evolution and domain growth dynamics.
1:27PM B53.00012 Drop formation, pinch-off dynamics and liquid transfer of simple and complex fluids. JELENA DINIC, VIVEK SHARMA, University of Illinois at Chicago — Liquid transfer and drop formation processes underlying jetting, spraying, coating, and printing – inkjet, screen, roller-coating, gravure, nanoimprint hot embossing, 3D – often involve formation of unstable columnar necks. Capillary-driven thinning of such necks and their pinchoff dynamics are determined by a complex interplay of inertial, viscous and capillary stresses for simple, Newtonian fluids. Micro-structural changes in response to extensional flow field that arises within the thinning neck give rise to additional viscoelastic stresses in complex, non-Newtonian fluids. Using FLOW-3D, we simulate flows realized in prototypical geometries (dripping and liquid bridge stretched between two parallel plates) used for studying pinch-off dynamics and influence of microstructure and viscoelasticity. In contrast with often-used 1D or 2D models, FLOW-3D allows a robust evaluation of the magnitude of the underlying stresses and extensional flow field (both uniformity and magnitude). We find that the simulated radius evolution profiles match the pinch-off dynamics that are experimentally-observed and theoretically-predicted for model Newtonian fluids and complex fluids.

1:39PM B53.00013 Simulations of high and low viscosity micro-scale droplets splashing on a dry surface. ARNOTT BOELENS, ANDRZEJ LATKA, JUAN DE PABLO, University of Chicago — When a droplet hits a dry surface at atmospheric pressure with a high enough impact velocity, it splashes and breaks apart into many smaller droplets. However, when the ambient gas pressure is reduced, splashing is suppressed. This is contrary to intuition, which suggest a more violent splash should occur at lower gas densities due to reduced drag forces. Although splashes of high and low viscosity liquids visually look very different, they also obey the pressure effect. In this study the effect of viscosity on splashing is investigated, to get a better understanding of the pressure effect in general. Simulation results are presented comparing splashing of low viscosity ethanol with high viscosity silicone oil in air. The droplets are several hundred microns large. The simulations are 2D, and are performed using a Volume Of Fluid approach. The contact line is described using the Generalized Navier Boundary Condition. Both the gas phase and the liquid phase are assumed to be incompressible. The high viscosity silicone oil in air. The droplets are several hundred microns large. The simulations are 2D, and are performed using a Volume Of Fluid approach.

1:51PM B53.00014 Dynamics of Wetting and Wicking on Rough Surfaces. DION ANTAO, DANIEL PRESTON, SOLOMON ADERA, YANGYING ZHU, EVELYN WANG, Massachusetts Institute of Technology — Micro/nano engineering of surfaces to enhance the performance of phase-change heat transfer processes has recently gained wide interest. Interfacial phenomena at the micro/nanoscale play an important role in defining the dynamic wetting and wicking characteristics of the surfaces. Here we report experiments that characterize the dynamic wetting and wicking processes on microstructured silicon surfaces. We investigated cylindrical micropillar arrays in a square pattern with various diameter, pitch, and height to characterize key interfacial behavior over a wide range of surface roughness. The experiments were performed by dipping the microstructured sample vertically into a reservoir of de-ionized water and the spreading dynamics were captured with a high speed camera. We observed that both wetting and wicking exhibit a power law dependence on time, however they occur at different time scales. The instantaneous (~10-100 ms) wicking behavior occurs due to the interfacial tensions, and the resultant force acting at the three-phase contact line. The longer time scale (>100 ms) wicking behavior results from the balance of the capillary pressure generated within the microstructure and the viscous pressure loss from flow through the micropillar array. We develop analytical models to predict these different time scale behavior and compare them to experimental results. This work provides insight into key dynamic processes affecting micro/nanostructure enhanced phase-change heat transfer devices.

2:03PM B53.00015 ABSTRACT WITHDRAWN

Monday, March 14, 2016 2:30PM - 5:30PM — Session C43 GSNP GSOFT DFD: Sediment Transport, Geological Flows, and Avalanches

2:30PM C43.00001 Onset of erosion and sediment transport by a fluid flow over a granular bed1. ARSHAD KUDROLLI, Clark Univ — Erosion and deposition of grains by a fluid flowing past the surface of a granular bed occurs in many natural and industrial processes. While considerable number of empirical studies has been conducted, very little is in fact known in detail on conditions which lead to erosion and deposition of sediments and their transport coefficients. We discuss a series of laboratory experiments to develop the physics of erosion starting with a single particle resting on a surface in a fluid flow. Fluorescent fluid-particle index matching techniques allow us to visualize not only the particles at the surface of a granular bed but also the flow within the bed and the individual particles within the bed. We will discuss the conditions governing the onset of particle motion under simple shear and their transport as a function of bed and fluid flow properties.

3:06PM C43.00002 The cessation threshold of continuous sediment transport in Newtonian fluid1. THOMAS PHTZ, Ocean College, Zhejiang University, ORENCIO DURAN, MARUM-Center for Marine Environmental Sciences, University of Bremen — One of the classical problems in sediment transport science is to predict the threshold Shields number below which a bed of loose sediment particles sheared by a homogeneous fluid flow ceases to move continuously. Depending on the particle-fluid density ratio (s), it has been believed for many decades that this threshold is a consequence of either fluid forces being just strong enough to dislodge particles resting on the bed (small s, e.g., water) or of particle-bed impacts play an important role in sustaining sediment transport. We present a simple, unified analytical model of the cessation of continuous sediment transport, which is quantitatively consistent with measurements in water (the famous "Shields diagram") and air on Earth and Mars. This model predicts that sediment transport on Pluto (transport of nitrogen ice particles in a very thin nitrogen atmosphere) can be sustained under surface winds comparable to those on Earth and Mars. This might explain wind streaks on Pluto's surface which have puzzled the lead researchers of the New Horizons mission.

3:18PM C43.00003 Rod Climbing of Suspensions. YOJJING GUO, XIAORONG WANG, Chemical Engineering, Tongji University, Shanghai — We wish to report an unexpected effect observed for particle suspensions sucked to pass through a vertical pipe. Above a critical concentration, the suspension on the outside of the pipe may climb along the outside wall of the pipe and then display a surprising rod-climbing effect. Our study shows that the phenomenon is influenced mainly by the suspension composition, the pipe dimension and the suction speed. The effects of the pipe materials of different kinds are negligible. Increasing the suction force and the concentration increases the climbing height. Increasing the pipe diameter and wall thickness reduces the climbing effect. This behavior may be relevant to that the suspensions of the type described are all displaying markedly shear-thickening.

1Supported by the U.S. DOE Office of Science and Office of BES program under DE-FG02-13ER16401, and NSF Grant No. CBET-1359528.

1We acknowledge support from grants National Natural Science Foundation of China (Nos. 1151101041 and 41376065) and Natural Science Foundation of Zhejiang Province (No. LR16E090001).

1Supported by the U.S. DOE Office of Science and Office of BES program under DE-FG02-13ER16401, and NSF Grant No. CBET-1359528.
3:30PM C43.00004 Laboratory investigations of granular and hydrodynamic processes in tidewater glacial fjords

When a fluid flows laterally over a granular bed, grains may be transported with the flow. This process shapes much of the natural world. The boundary between states with and without grain motion has been studied for decades. However, this boundary is not well understood, since the process whereby grains are transported involves the coupling of several complex phenomena: turbulent fluid flow near a rough boundary, Darcy flow through the pore structure of the granular bed, the yield strength of granular beds comprised of frictional grains with irregular shape, and inertial effects of grains that become entrained in the flow. In order to clarify the essential physics that governs the onset of granular motion, we study this process computationally by including only the minimal features and then adding complexities one by one. We start with a simple numerical model that includes only gravity, grain-grain interactions that are repulsive and frictionless, and a purely horizontal viscous fluid flow. By varying the fluid flow rate and the effective viscosity, we find behavior that is qualitatively consistent with a large collection of experimental data known as the Shields curve. Thus, our results suggest that the main features of this curve result from a competition between grain inertia and viscous damping. We find this phase diagram to be qualitatively insensitive to secondary effects, such as friction, irregular grain shape, and restitution losses.

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3:42PM C43.00005 A phase diagram for fluid-driven sediment transport

When a fluid flows laterally over a granular bed, grains may be transported with the flow. This process shapes much of the natural world. The boundary between states with and without grain motion has been studied for decades. However, this boundary is not well understood, since the process whereby grains are transported involves the coupling of several complex phenomena: turbulent fluid flow near a rough boundary, Darcy flow through the pore structure of the granular bed, the yield strength of granular beds comprised of frictional grains with irregular shape, and inertial effects of grains that become entrained in the flow. In order to clarify the essential physics that governs the onset of granular motion, we study this process computationally by including only the minimal features and then adding complexities one by one. We start with a simple numerical model that includes only gravity, grain-grain interactions that are repulsive and frictionless, and a purely horizontal viscous fluid flow. By varying the fluid flow rate and the effective viscosity, we find behavior that is qualitatively consistent with a large collection of experimental data known as the Shields curve. Thus, our results suggest that the main features of this curve result from a competition between grain inertia and viscous damping. We find this phase diagram to be qualitatively insensitive to secondary effects, such as friction, irregular grain shape, and restitution losses.

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4:18PM C43.00006 The drag mechanics of an intruder moving in sheared granular medium

We acknowledge support from NSF DMR1206351 and the W.M. Keck Foundation.

4:30PM C43.00007 Dynamics of pull out in a granular material

We acknowledge support from NSF DMR1206351, NASA Grant No. NNX15AD38G and the W.M. Keck Foundation.

4:42PM C43.00008 How does particle shape affect the near jamming properties of granular materials?

We would like to acknowledge NSF-DMR1206351 and the W.M.Keck Foundation.

4:54PM C43.00009 The evolution of orientational order in sheared, 2D granular media of convex and concave elongated particles

Funded by U.S. Army Research Office under Grant No. W911NF-14-1-0005

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This work is supported by NSF grant DMRPD-09-1765

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We acknowledge support from NSF Grant No. DMR1206351, NASA Grant No. NNX15AD38G and the W.M. Keck Foundation.
5:06PM C43.00010 Stability and Structure of Star-Shape Granules1, YUCHEN ZHAO, JONATHAN BARES2, Duke Univ., Department of Physics, NC, KEVIN LIU, Julia R. Masterman Laboratory and Demonstration School, PA, MATTHEW ZHEN, North Carolina School of Science and Mathematics, NC, KAROLA DIERICHES, ACHIM MENGES, Institute for Computational Design, University of Stuttgart, Stuttgart, Germany, ROBERT BEHRINGER, Duke Univ., Department of Physics, NC — Columns made of convex noncohesive grains like sand collapse after being released from a confining container. While various architectures built by concave grains are stable. We explore why these structures are stable, and how stable they can be. We performed experiments by randomly pouring identical star-shape particles into hollow cylinders resting on glass or a roughened base, and then observed how stable these granular columns were after carefully lifting the cylinders. We used particles that are made of acrylics and have six 9 mm arms, which extend symmetrically in xyz directions. We investigated the probability of creating a stable column and other mechanical stability aspects. We define \( r \) as the weight fraction of particles that fall out of the column after the confining cylinder is removed. \( r \) gradually increases as the column height increases, or the column diameter decreases. We found high column stability when the inter-particle friction was greater. We also explored experiment conditions such as initial vibration of columns when they were confined and loading on the top. In order to understand the inner structure leading to stability, we obtained 3D CT reconstruction data of stable columns. We will discuss coordination number and orientation, etc.

1We acknowledge supports from W.M.Keck Foundation and Research Triangle MRSEC

2will be at CNRS

5:18PM C43.00011 Rheology of U-Shaped Granular Particles, MATTHEW HILL, SCOTT FRANKLIN, Rochester Institute of Technology — We study the response of cylindrical samples of U-shaped granular particles (staples) to extensional loads. Samples elongate in discrete bursts (events) corresponding to particles rearranging and re-entangling. Previous research on samples of constant cross-sectional area found a Weibullian weakest-link theory could explain the distribution of yield points. We now vary the cross-sectional area, and find that the maximum yield pressure (force/area) is a function of particle number density and independent of area. The probability distribution function of important event characteristics the stress increase before an event and stress released during an event both fall of inversely with magnitude, reminiscent of avalanche dynamics. Fourier transforms of the fluctuating force (or stress) scales inversely with frequency, suggesting dry friction plays a role in the rearrangements. Finally, there is some evidence that dynamics are sensitive to the stiffness of the tensile testing machine, although an explanation for this behavior is unknown.

Tuesday, March 15, 2016 11:15AM - 2:15PM – Session F12 GPC DFD GSNP: Climate Science Frontier: Cloud and Precipitation Physics 308 - Juan Restrepo, Oregon State Univ

11:15AM F12.00001 Precipitation and atmospheric moisture transport responses to increased infrared opacity, ELISABETH MOYER, University of Chicago — No abstract available.

11:51AM F12.00002 Prototypes for the dynamics underlying precipitation and temperature extremes1, J DAVID NEELIN, UCLA — Projecting changes in precipitation and temperature extreme events can be aided by a deeper understanding of the dynamics underlying such variations. For precipitation, this is closely connected to the interaction of fast, small-scale motions with variability of large-scale climate. Simple prototype models from the physics and applied math literature can point to analysis methods, connections among related quantities, and hypotheses for the dynamics, especially when the prototype models can be derived from climate-model equations. An overview will be provided including recent work with a number of collaborators. For distributions of precipitation-related variables, prototypes including Fokker-Planck solutions and first-passage problems for variations across an onset threshold yield insights into the form of present-day observed distributions and predictions for the form of the global warming changes. For example, the tails of the distribution of events and/or the tails of certain variables is likely explained in part by prototypes for tracer advection across a maintained gradient. The shape of these tails can have substantial implications for regional changes in probabilities of precipitation and temperature extremes with large-scale warming.

Supported in part by the National Science Foundation

12:27PM F12.00003 The physics of atmospheric instability, lightning, and global warming, DAVID ROMPS, University of California, Berkeley — No abstract available.

1:03PM F12.00004 Thermodynamic analysis of atmospheric convection, OLIVIER PAULUIS, Courant Institute of Mathematical Sciences — No abstract available.

1:39PM F12.00005 Aerosols, Clouds, and Precipitation as Scale Interactions in the Climate System and Controls on Climate Change, LEO DONNER, Geophysical Fluid Dynamics Laboratory/NOAA — Clouds are major regulators of atmospheric energy flows. Their character depends on atmospheric composition, dynamics, and thermodynamic state. Clouds can assume organized structures whose scales are planetary, while processes important for determining basic properties occur on the scale of microns. The range of processes, scales, and interactions among them has precluded the development of concise theories for the role of clouds in climate, and limitations in modeling clouds in complex climate models remain among the key uncertainties in understanding and projecting climate change. The distribution function of vertical velocities (updraft speeds) in clouds is an important control on climate forcing by clouds and possibly a strong correlate with climate sensitivity. (Climate forcing refers to the change in Earth’s energy balance as atmospheric composition changes, in particular, due to human activity. Climate sensitivity is defined here as the equilibrium change in globally averaged annual surface temperature as a result of doubled carbon dioxide.) Vertical velocities are central because they determine the thermodynamic environment governing phase changes of water, with both equilibrium and non-equilibrium phenomena important. The spatial and temporal spectra of relevant vertical velocities includes scales both numerically resolved by climate models and below their resolution limit. The latter implies a requirement to parameterize these smaller scale motions in models. The scale dependence of vertical velocities and emerging observational constraints on their distribution provide new opportunities for representing aerosols, clouds, and precipitation in climate models. Success in doing so could provide important breakthroughs in understanding both climate forcing and sensitivity.

Tuesday, March 15, 2016 2:30PM - 5:18PM – Session H51 GPC DFD GSNP: Climate as a Non-equilibrium and Stochastic System Hilton Baltimore Holiday Ballroom 2 - Juan Restrepo, Oregon State University
2:30PM H51.00001 Fluctuations and Response in Geophysical Fluid Dynamics. VALERO LUCARINI, University of Hamburg — The climate is a complex, chaotic, non-equilibrium system featuring a limited horizon of predictability, variability on a vast range of temporal and spatial scales, instabilities resulting into energy transformations, and mixing and dissipative processes resulting into entropy production. Despite great progress, we still do not have a complete theory of climate dynamics able to account for instabilities, equilibration processes, response to changing parameters of the system, and multiscale effects. We will outline some possible applications of the response theory developed by Ruelle for non-equilibrium statistical mechanical systems, showing how it allows for setting on firm ground and on a coherent framework concepts like climate sensitivity, climate response, and climate tipping points, and to construct parametrizations for unresolved processes. We will show results for comprehensive global climate models. The results are promising in terms of suggesting new ways for approaching the problem of climate change prediction and for using more efficiently the enormous amounts of data produced by modeling groups around the world. Ref: V. Lucarini, R. Blender, C. Herbert, F. Ragone, S. Pascale, J. Wouters, Mathematical and Physical Ideas for Climate Science, Reviews of Geophysics 52, 809-859 (2014).

3:06PM H51.00002 Balanced Dynamics in the Madden-Julian Oscillation. SHARON SESSIONS, STIPO SENTIC, New Mexico Tech, ZELJKA FUCHS, University of Split, Croatia, and New Mexico Tech, DAVID RAYMOND, New Mexico Tech — Balanced dynamics describe the response of the tropical thermodynamic environment to changes in the atmospheric vorticity patterns. Observations and numerical simulations have demonstrated that positive mid-tropospheric vorticity anomalies produce a more stable thermodynamic environment with cool anomalies at low levels and warm anomalies aloft. The increase in atmospheric stability creates more bottom-heavy convective profiles which are highly conducive for developing tropical cyclones. Balanced dynamics may also play a role in other varieties of tropical convection, including the most significant source of intraseasonal variability: the Madden-Julian Oscillation (MJO). Using data from DYNAMO—a field program aimed to investigate the dynamics of the MJO—we investigate the role of balanced dynamics in the Madden-Julian Oscillation.

3:18PM H51.00003 Stochastic dynamics of melt ponds and sea ice-albedo climate feedback. IVAN SUDAKOV, Department of Physics, University of Dayton — Evolution of melt ponds on the Arctic sea surface is a complicated stochastic process. We suggest a low-order model with ice-albedo feedback which describes stochastic dynamics of melt ponds geometrical characteristics. The model is a stochastic dynamical system model of energy balance in the climate system. We describe the equilibria in this model. We conclude the transition in fractal dimension of melt ponds affects the shape of the sea ice albedo curve.

3:30PM H51.00004 A Novel Method to Unravelling Energy Pathways in the Ocean. HUSSEIN ALUIE, University of Rochester — Large-scale currents and eddies pervade the ocean and play a prime role in the general circulation and climate. The coupling between scales ranging from $O(10^{-4})$ km down to $O(1)$ mm presents a major difficulty in understanding, modeling, and predicting oceanic circulation and mixing, where the energy budget is uncertain within a factor possibly as large as ten. Identifying the energy sources and sinks at various scales can reduce such uncertainty and yield insight into new parameterizations. To this end, we refine a novel coarse-graining framework, which accounts for the spherical geometry of the problem, to directly analyze the coupling between scales. We apply these tools to strongly eddying high-resolution simulations using LANL’s Parallel Ocean Program (POP).

4:06PM H51.00005 The impact of the diurnal insolation cycle on the tropical cyclone heat engine. MORGAN E. O’NEILL, Department of Earth and Planetary Sciences, Weizmann Institute of Science, DIAMILET PEREZ-BETANCOURT, Program in Atmospheres, Oceans and Climate, Massachusetts Institute of Technology, ALLISON A. WING, Lamont-Doherty Earth Observatory, Columbia University — A hurricane, or tropical cyclone, is understood as a heat engine that moves heat from the warm sea surface to the cold tropopause. The efficiency of this engine depends in part on the strength and duration of solar heating. Over land, peak rainfall associated with individual thunderstorms occurs in the late afternoon. Over ocean, with its markedly higher surface heat capacity, deep convection responds more to radiational cooling than daytime surface heating. However, the role of daily varying solar forcing on the dynamics of tropical cyclones is poorly understood. Recently, Dunion et al. (2014) reported significant, repeating diurnal behavior propagating outward from tropical cyclone centers, using infrared imagery from nine years of North Atlantic tropical cyclones. We study the impact of the diurnal cycle on tropical cyclones using a high resolution 3D numerical model, the System for Atmospheric Modeling (Khairoutdinov and Randall 2003). Simulations are run with and without variable sunlight. We are able to reproduce the observational finding of Dunion et al. (2014), and further identify a diurnally-varying residual circulation in the tropical cyclone at midlevels. The impact of the diurnal cycle on the equilibrium dynamics of tropical cyclones is also discussed.

4:18PM H51.00006 Towards a General Turbulence Model for Planetary Boundary Layers Based on Direct Statistical Simulation. BRAD MARSTON, BAYLOR FOX-KEMPER, JOE SKITKA, Brown University — Sub-grid turbulence models for planetary boundary layers are typically constructed additively, starting with local flow properties and including non-local (KKP) or higher order (Mellor-Yamada) parameters until a desired level of predictive capacity is achieved or a manageable threshold of complexity is surpassed. Such approaches are necessarily limited in general circumstances, like global circulation models, by their being optimized for particular flow phenomena. By using direct statistical simulation (DSS) that is based upon expansion in equal-time cumulants we offer the prospect of a turbulence model and an investigative tool that is equally applicable to all flow types and able to take advantage of the wealth of nonlocal information in any flow. We investigate the feasibility of a second-order closure (CE2) by performing simulations of the ocean boundary layer in a quasi-linear approximation for which CE2 is exact. As oceanographic examples, wind-driven Langmuir turbulence and thermal convection are studied by comparison of the statistics of quasi-linear and fully nonlinear simulations. We also characterize the computational advantages and physical uncertainties of CE2 defined on a reduced basis determined via proper orthogonal decomposition (POD) of the flow fields.

4:30PM H51.00007 Non-equilibrium Statistical Mechanics and the Sea Ice Thickness Distribution. JOHN WETTLAUFER, SRIKANTH TOPPALADODDI, Yale University — We use concepts from non-equilibrium statistical physics to transform the original evolution equation for the sea ice thickness distribution $g(h)$ due to Thomdike et al. (1975) into a Fokker-Planck like conservation law. The steady solution is $g(h) = N(q)h^{e^{-h/H}}$, where $q$ and $H$ are expressible in terms of moments over the transition probabilities between thickness categories. The solution exhibits the functional form used in observational fits and shows that for $h \ll 1$, $g(h)$ is controlled by both thermodynamics and mechanics, whereas for $h \gg 1$ only mechanics controls $g(h)$. Finally, we derive the underlying Langevin equation governing the dynamics of the ice thickness $h$, from which we predict the observed $g(h)$. This allows us to demonstrate that the ice thickness field is ergodic. The genericity of our approach provides a framework for studying the geophysical scale structure of the ice pack using methods of broad relevance in statistical mechanics.

1Supported in part by NSF DMR-1306806

2Swedish Research Council Grant No. 638-2013-9243, NASA Grant NNH13ZDA001N-CRYO and the National Science Foundation and the Office of Naval Research under OCE-1332790 for support.
Large-eddy simulation of the transient and near-equilibrium behavior of precipitating shallow convection

THIJS HEUS, Cleveland State University, AXEL SEIFERT, Deutscher Wetter Dienst, Offenbach, Germany, ROBERT PINCUS, University of Colorado, BJORN STEVENS, Max Planck Institute for Meteorology, Hamburg, Germany — Cloud-aerosol remain one of the largest uncertainties in climate modeling. Many of the postulated cloud-aerosol interactions involve precipitation to limit cloud size and life time, in particular for barely precipitating shallow cumulus clouds. If the precipitation exceeds a certain threshold, it will create feedback on the cloud field through cold pools and mesoscale organization. Such mesoscale responses have mostly been ignored so far in the discussion of aerosol indirect effects. We study the sensitivity of transient cumulus clouds to perturbations in cloud droplet number concentrations. Over time, the cloud system approaches a radiative-convective equilibrium state. The transient behavior and the properties of the near-equilibrium cloud field depend on the microphysical state and therefore on the cloud droplet number density. The primary response of the cloud field to changes in the cloud droplet number density is deepening of the cloud layer, and results in a shorter cloud life time. If the atmospheric time scales are long enough compared to the microphysical time scales, the cloud field may reach a near-equilibrium regime. In this regime, the decrease in cloud cover compensates much of the brightening of the clouds, and the overall effect on the albedo is small.

Statistical state dynamics of jet/wave coexistence in beta-plane turbulence

NAVID CONSTANTINOU, Scripps Inst. of Oceanography, Univ of California — San Diego, BRIAN FARRELL, Department of Earth and Planetary Sciences, Harvard University, PETROS IOANNOU, Physics Department, National and Kapodistrian University of Athens — Jets are commonly observed to coexist in the turbulence on time scales long compared to dissipative or advective time scales. The emergence, equilibration at finite amplitude, maintenance and stability of these structures pose fundamental theoretical problems. The emergence of jets and vortices from turbulence is not associated with an instability of the mean flow and their equilibration and stability at finite amplitude does not arise solely from the linear or nonlinear dynamics of these structures in isolation from the turbulence surrounding them. Rather the dynamics of these large-scale structures arises essentially from their cooperative interaction with the small-scale turbulence in which they are embedded. It follows that fundamental theoretical understanding of the dynamics of jets and vortices in turbulence requires adopting the perspective of the statistical state dynamics (SSD) of the entire turbulent state. In this work a theory for the jet/wave coexistence regime is developed using the SSD perspective.

A stochastic shallow cumulus ensemble model as a scale-aware parameterization of convective fluctuations

MIRJANA SAKRADZIJA, Max Planck Institute for Meteorology, AXEL SEIFERT, Deutscher Wetterdienst, THIJS HEUS, Cleveland State University, ANURAG DIPANKAR, Max Planck Institute for Meteorology — Numerical models are approaching the high-resolution limit where some aspects of deep convection and mesoscale convective systems can be explicitly modeled, while shallow cumuli are still a subgrid process that requires a parameterization. The classical assumption of a sufficiently large cloud sample within a model grid column breaks down in this regime, so it is crucial to develop scale-aware parameterizations. Therefore, we propose an approach to represent the variability of subgrid shallow cumuli about the ensemble average convective response. The shallow clouds are studied using Large Eddy Simulation (LES), where the original cloud field modeled on the grid of 25 m resolution is coarse-grained to mimic resolutions from 1 to 50 km. A canonical statistical ensemble is developed based on theoretical and LES findings and fluctuations of shallow convection are modeled by random subsampling of microstates from the convective ensemble distribution. The resulting distribution of subgrid convective states is scale-aware, and it represents stochastic fluctuations that increase with grid resolution and become substantial on the kilometre-scale grids. We find that the local cloud memory plays an important role in defining the convective ensemble statistics in a steady cumulus regime.

Effect of Microstructural Geometry for Computing Closure Models in Multiscale Modeling of Shocked Particle Laden Flow

OISHIK SEN, H.S. UDAYKUMAR, Univ of Iowa, GUSTAUF JACOBS, San Diego State University — Interaction of a shock wave with dust particles is a complex physical phenomenon. A computational model for studying this two-impact-system is the Particle-Source in Cell (PSIC) approach. In this method, the dust particles are tracked as point particles in a Lagrangian frame of reference immersed in a compressible fluid. Two-way interaction between the carrier and the dispersed phases is ensured by coupling the momentum and energy transfer between the two phases as source terms in the respective governing equations. These source terms (e.g. drag force on particles) may be computed from resolved numerical simulations by treating each macroscopic point particle as an ensemble of cylinders immersed in a compressed fluid. However the drag so computed must be independent of the geometry of the mesoscale. In this work, the effect of the stochasticity of the microstructural geometry in construction of drag laws from resolved mesoscale with planar cylinders is studied. Several different arrangements of cylinders are considered and the mean drag law as a function of the Mach Number and Volume Fraction for each arrangement is computed using the Dynamic Kriging Method. The uncertainty in the drag forces arising because of the arrangement of the cylinders for a given volume fraction is quantified as 90% credible sets and the effect of the uncertainty on PSIC computations is studied.

Wednesday, March 16, 2016 8:00AM - 11:00AM — Session K53 DFD GSOF GSNP: Granular and Multiphase Flows

8:00AM K53.00001 Ferrofluid-based Diamagnetic Particle Separation in U-shaped Microchannels

YILONG ZHOU, XIANGCHUN XUAN, Clemson University — We demonstrate in this talk a continuous-flow sheath-free separation method of diamagnetic particles in ferrofluids through U-shaped microchannels. Due to the action of a size-dependent magnetic force, diamagnetic particles are focused into a single stream in the inlet branch of the U-turn and then continuously separated into two streams in its outlet branch. We also develop a 3D numerical model to predict and understand the diamagnetic particle transport during the separation process. The numerical predictions are found to agree well with the experimental observations in a systematic study of multiple parameter effects including ferrofluid flow rate, concentration and magnet-channel distance.

8:12AM K53.00002 Smart microgels for controlling two-phase fluid structure in porous media

JING FAN, DAVID WEITZ, Harvard University — Understanding the transport of microgels in porous media directly benefits the conformance improvement technique using preformed gels in the oil industry. We develop a new type of microgels that can swell in response to specific stimuli in an aqueous environment. From a practical point of view, this enables us to deliver the microgels to the deep reservoir formation and control the permeability profile more effectively. With confocal microscopy imaging, we show that we can deliver such smart microgels to the high-permeability region in a stratified porous medium, which subsequently changes the two-phase fluid structure in the medium. From a scientific point of view, this allows for characterizing the permeability change due to homogeneous pore-clogging by soft particles instead of surface clogging; using the typical microgels this can hardly be done because we cannot place gel particles with comparable size to the pore uniformly into a porous medium. This study may shed light on understanding many other processes involving the transport of soft particles in porous structures.

8:24AM K53.00003 Effect of Microstructural Geometry for Computing Closure Models in Multiscale Modeling of Shocked Particle Laden Flow

OISHIK SEN, H.S. UDARQUMAR, Univ of Iowa, GUSTAUF JACOBS, San Diego State University — Interaction of a shock wave with dust particles is a complex physical phenomenon. A computational model for studying this two-impact-system is the Particle-Source in Cell (PSIC) approach. In this method, the dust particles are tracked as point particles in a Lagrangian frame of reference immersed in a compressible fluid. Two-way interaction between the carrier and the dispersed phases is ensured by coupling the momentum and energy transfer between the two phases as source terms in the respective governing equations. These source terms (e.g. drag force on particles) may be computed from resolved numerical simulations by treating each macroscopic point particle as an ensemble of cylinders immersed in a compressed fluid. However the drag so computed must be independent of the geometry of the mesoscale. In this work, the effect of the stochasticity of the microstructural geometry in construction of drag laws from resolved mesoscale with planar cylinders is studied. Several different arrangements of cylinders are considered and the mean drag law as a function of the Mach Number and Volume Fraction for each arrangement is computed using the Dynamic Kriging Method. The uncertainty in the drag forces arising because of the arrangement of the cylinders for a given volume fraction is quantified as 90% credible sets and the effect of the uncertainty on PSIC computations is studied.
8:36 AM K53.00004 Time dependent behavior of impact angle in turbulent pipe flows experiment erence erosion.1, AMADOR GUZMAN, Pontificia Universidad Catolica de Chile, DIEGO OYARZUN2, Universidad de Santiago de Chile, MAGDALENA WALCZAK3, JAVIERA AGUIRRE1, Pontificia Universidad Catolica de Chile — Erosion-corrosion in pipe systems transporting slurry turbulent flows is of a great importance in industrial and mining applications, where large volumes of suspended solids are sent up to hundreds of kilometers, to be further processed. The slurry is typically sent over large diameter steel pipes, which not always have an anti-abrasion coating. During the transport, the thickness of the pipe diminishes and eventually leaks and breaks, due to the combined effects of wear and corrosion. The processes of pipe degradation are further enhanced by the content of the slurry electrolytes that might switch from neutral to aggressive. The understanding of these processes in terms of operational parameters is critical for anticipating and mitigating a catastrophic outcome. This paper describes turbulent flow numerical simulations in a slurry transporting steel pipe with an emphasis on the correlation between the time dependent impact angle in the vicinity of the steel pipe and the rate of material loss. Full numerical simulations in a 3D long domain by using an Eulerian –Eulerian two phase flow approach coupled to a r–e Tolman turbulent model are performed for different solid particle concentration and flow velocity and compared to existing experimental and numerical results for validation with and without gravity. Time dependent axisymmetric turbulent flow simulations are performed for determining both the time dependent behavior of the axial and radial velocities near the pipe wall and the impact angle.1

1Financial support from Conicyt through the Fondecyt proposal 1141107 is acknowledged
2Assistant Professor of Mechanical Engineering
3Associate Professor of Mechanical Engineering
4Doctoral student and research assistant

8:48 AM K53.0005 Caustics and the growth of droplets1, RAMA GOVINARAJAN, S RAVICHANDRAN, TIFR Centre for Interdisciplinary Sciences, Hyderabad, India, SAMRIDDHI RAY, International Centre for Theoretical Sciences, TIFR, Bangalore, P DEEPU, TIFR Centre for Interdisciplinary Sciences, Hyderabad, India — Caustics are formed when inertial particles of very different velocities collide in a flow, and are a consequence of the dissipative nature of particle motion in a suspension. Using a model vortex-dominated flow with heavy droplets in a saturated environment, we suggest that the caustic characteristics form only within a neighborhood around a vortex, the square of whose radius is proportional to the product of circulation and particle inertia. Droplets starting close to this critical radius congregate very close together, resulting in large spikes in (Lagrangian) number density. Allowing for merger when droplets collide, we show that droplets starting out close to the critical radius display a much more rapid growth in size than those starting elsewhere, and a large fraction of the large droplets are those that originate within the caustics-forming region. We test these predictions in a two-dimensional simulation of turbulent flow. We hope that our study will be of interest in long-standing problems of physical interest such as the mechanism of broadening of droplet spectra in a turbulent flow.

1Support from the Ministry of Earth Sciences, Government of India for the project Coupled physical processes in the Bay of Bengal and monsoon air-sea interaction under OMM is gratefully acknowledged

9:00 AM K53.0006 Soft Sphere Suspensions: Flow and Relaxation, MARCEL WORKAMP, JOSHUA A. DIJKSMAN, Physical Chemistry and Soft Matter, Wageningen University — We experimentally study the role of particle elasticity on the rheology of soft sphere suspensions. Experiments allow us to probe the role of elastic timescales, relaxation and anisotropy in a custom 3D printed shear cell. We find robust rheological features, such as a flow instability, that are not well captured by existing models for suspension flows. In addition, we find relaxation effects after shear even in the absence of shear or thermal fluctuations. We aim to integrate these findings in the emerging unified framework for structured fluids.

9:12 AM K53.0007 Impact cratering on granular beds: From the impact of raindrops to the strike of hailstones1, LEONARDO GORDILLO, JUNPING WANG, FRED JAPARDI, WARREN TEDDY, MING GAO, XIANG CHENG, CEMS - University of Minnesota — Impact craters generated by the impact of liquid drops onto a granular bed strongly depend on the material properties of impactors. As an example, impact cratering by liquid drops and by solid spheres exhibits qualitatively different power-law scalings for the size of resulting impact craters. While the basic energy conservation and dimensional analysis provide simple guiding rules, the detailed dynamics governing the relation between these power-law scalings is still far from clear. To analyze the transition between liquid-drop and solid-sphere impact cratering, we investigate impact cratering by liquid drops for a wide range of viscosities over 7 decades. Using high-speed photography and laser profilometry, we delineate the liquid-to-solid transition and show the emergence of the two asymptotic behaviors and their respective power laws. We find that granular avalanches triggered by impacts are crucial in understanding the energy partition between impacted surfaces and impactors, which directly determines the observed scaling relations. A simple model is constructed for the initial stage of the impact that explains the energy partition during crater formation.

1We acknowledge the support of NSF CAREER DMR-1452180. LG acknowledges fundings from CONICYT/BECAS CHILE 74160007.

9:24 AM K53.0008 Scaling of liquid-drop impact craters in granular media1, RUNCHEN ZHAO, QIANYUN ZHANG, HENDRO TJUGITO, MING GAO, XIANG CHENG, University of Minnesota — Granular impact cratering by liquid drops is a ubiquitous phenomenon, directly relevant to many important natural and industrial processes such as soil erosion, drip irrigation, and dispersion of micro-organisms in soil. Here, by combining the high-speed photography with high precision laser profilometry, we investigate the liquid-drop impact dynamics on granular surfaces and monitor the morphology of resulting craters. Our experiments reveal novel scaling relations between the size of granular impact craters and important control parameters including the impact energy, the size of impinging drops and the degree of liquid saturation in a granular bed. Interestingly, we find that the scaling for liquid-drop impact cratering in dry granular media can be quantitatively described by the Schmidt-Holsapple scaling originally proposed for asteroid impact cratering. On the other hand, the scaling for impact craters in wet granular media can be understood by balancing the inertia of impinging drops and the strength of impacted surface. Our study sheds light on the mechanism governing liquid-drop impacts on dry/wet granular surfaces and reveals a remarkable analogy between familiar phenomena of raining and catastrophic asteroid strikes.

1Scaling of liquid-drop impact craters in granular media

9:36 AM K53.0009 Scaling of granular convective velocity and timescale of asteroidal resurfacing, TOMOYA YAMADA, KOUSUKE ANDO, TOMOKATSU MOROTA, HIROAKI KATSURAGI, Department of Earth and Environmental Sciences, Nagoya University — Granular convection is one of the well-known phenomena observed in a vertically vibrated granular bed. Recently, the possible relation between granular convection and asteroidal surface processes has been discussed. The granular convection on the surface of small asteroids might be induced by seismic vibration resulting from meteorite impacts. To quantitatively evaluate the timescale of asteroidal resurfacing by granular convection, the granular convective velocity under various conditions must be revealed. As a first step to approach this problem, we experimentally study the velocity scaling of granular convection using a vertically vibrated glass-beads layer. By systematic experiments, a scaling form of granular convective velocity has been obtained. The obtained scaling form implies that the granular convective velocity can be written by a power-law product of two characteristic velocity components: vibrational and gravitational velocities. In addition, the system size dependence is also scaled. According to the scaling form, the granular convective velocity is almost proportional to gravitational acceleration. Using this scaling form, we have estimated the resurfacing timescale on small asteroid surface.
The high-viscosity oil suspension bounces. Increasing solvent viscosity increases the rebound energy. To gain insight into the underlying mechanism, we model the suspension as densely packed elastic spheres experiencing viscous lubrication drag between neighbors. The model reproduces the observed trends. Plots of elastic compression and drag experienced by the particles show that rebounds are made possible by (1) a fraction of the impact energy being stored during initial contact via elastic compression, (2) a rapid broadening of local lubrication drag interactions at the initial impact site into a spatially uniform upward force throughout the drop. Including finite wall drag to the presence of ambient air into the numerical model diminishes and eventually cuts off the rebound.

10:00AM K53.00011 Percolation velocity dependence on local concentration in bidisperse granular flows, RYAN P. JONES, HONGYI XIAO, ZHEKAI DENG, PAUL B. UMBANHOWAR, RICHARD M. LUEPTOW, Northwestern University — The percolation velocity, \( u_p \), of granular material in size or density bidisperse mixtures depends on the local concentration, particle size ratio, particle density ratio, and shear rate, \( \dot{\gamma} \). Discrete element method computational results were obtained for bounded heap flows with size ratios between 1 and 3 and for density ratios between 1 and 4. The results indicate that small particles percolate downward faster when surrounded by large particles than large particles percolate upward when surrounded by small particles, as was recently observed in shear-box experiments. Likewise, heavy particles percolate downward faster when surrounded by light particles than light particles percolate upward when surrounded by heavy particles. The dependence of \( u_p/\dot{\gamma} \) on local concentration results in larger percolation flux magnitudes at low concentrations of large (or light) particles compared to high concentrations of small (or heavy) particles, while local volumetric flux is conserved. The dependence of \( u_p/\dot{\gamma} \) on local concentration can be incorporated into a continuum model, but the impact on global segregation patterns is usually minimal.

1Partially funded by Dow Chemical Company and NSF Grant No. CBET-1511450

10:12AM K53.00012 Impact of Overburden on Segregation in Sheared Granular Flow, ALEXANDER M. FRY, PAUL B. UMBANHOWAR, RICHARD M. LUEPTOW, Northwestern University — Dense granular materials tend to segregate into size or density graded regions when subjected to shear. Previous experiments demonstrated that overburden – normal confining pressure on a granular system – can slow the rate of size segregation in an annular shear cell. Here, we explore the effects of overburden on sheared granular material through Discrete Element Method (DEM) simulations in a planar shear cell geometry where shear is applied by a moving bottom wall, while a massive upper wall provides the overburden. Segregation decreases with increasing overburden, but the picture is complicated by concurrent changes in the streamwise velocity profile. To decouple these effects, we also test an idealized system in which a desired streamwise velocity profile – and therefore shear rate – is imposed by applying additional horizontal forces to each particle. Based on this approach, we link the effect of overburden on segregation to the grain-scale behavior of the system. Partially funded by Procter & Gamble.

10:24AM K53.00013 Impact of a hydrophobic granular stream in water, BRIAN UTTER, Bucknell University, HARRY MANDELES, JACOB PARKHOUSE, James Madison University — We experimentally investigate the flow of a stream of hydrophobic granular particles impacting a water surface from above. The granular sample is composed of a mixture of hydrophobic and hydrophilic grains and the concentration, stream diameter, and drop height are independently controlled. While granular flows are common in nature and industry, effects of surface chemistry on flow behavior have received relatively little attention. The present experiment complements rheological measurements performed in parallel and aims to elucidate prior experiments on hydrophobic samples in a rotating drum. The present experimental geometry allows us to compare the behavior of granular streams to prior work on impacts of solids and fluid streams. Sequential images of the granular stream in water are taken and analyzed. We present data on the size, length, and shape of the aggregate streams with variations in concentration, entering stream diameter, and drop height. We find that increased hydrophobic grain concentration leads to increased aggregation due to an effectively cohesive interaction mediated by entrained air. At lower concentrations, the stream exhibits a lateral instability. Finally, we will make connections to rheology and rotating drum results.

1This work was supported by NSF CBET award 1067598.

10:36AM K53.00014 Numerical Simulation and Performance Optimization of a Magnetophoretic Bio-separation chip, MATIN GOLOZAR, JEFF DARABI, MAJID MOLKI, Southern Illinois University Edwardsville — Separation of micro/nanoparticles is important in biomedicine and biotechnology. This research presents the modeling and optimization of a magnetophoretic bio-separation chip for the isolation of biomaterials, such as circulating tumor cells (CTCs) from the peripheral blood. The chip consists of a continuous flow through microfluidic channels that contains locally engineered magnetic field gradients. The high gradient magnetic field produced by the magnets is spatially non-uniform and gives rise to an attractive force on magnetic particles that move through the flow channel. The computational model takes into account the magnetic and fluidic forces as well as the effect of the volume fraction of particles on the continuous phase. The model is used to investigate the effect of two-way particle-fluid coupling on both the capture efficiency and the flow pattern in the separation chip. The results show that the microfluidic device has the capability of separating CTCs from their native environment. Additionally, a parametric study is performed to investigate the effects of the channel height, substrate thickness, magnetic bead size, bioparticle size, and the number of beads per cell on the cell separation performance.

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10:48AM K53.00015 A Statistical investigation of sloshing parameter impact on offshore separators, MD MAHMUD, Lamar University, RAFIQUIL KHAN, Cameron Corporation, QIANG XU, Louisiana State University — Offshore separators has been the subject of intense investigations for last several decades both by experiment and by simulation. Although various engineering solutions have been proposed to minimize sloshing impacts/intensity and some others have developed new methods to describe these movements, the ability of the mathematical models are developed to characterize sloshing phenomenon. However, a comprehensive statistical study of the impact of sloshing on offshore separators is not yet studied. In this study, statistical approach will be considered to determine the significant parameters. Principal component analysis techniques are considered to identify the significant parameters for liquid sloshing. Computation Fluid Dynamics (CFD) technique using ANSYS Fluent software. The input parameters considered are acceleration, wave frequencies, amplitudes in various sea state conditions. The measured variables include height, volume, kinetic energy, height of the free surface, vorticity. Mathematical correlations may be developed from the data collected.
11:15AM L53.00001 Non-equilibrium Stokes-Einstein relation via active microrheology of hydrodynamically interacting suspensions. HENRY CHU, ROSEANNA ZIA, Cornell University — In our recently developed non-equilibrium Stokes-Einstein relation, we showed that, in the absence of hydrodynamic interactions, the stress in a suspension is given by a balance between fluctuation and dissipation. Here, we generalize our theory for systems of hydrodynamically interacting colloids, via active microrheology, where motion of a Brownian probe through the medium reveals rheological properties. The strength of probe forcing compared to the entropic restoring force defines a Péclet number, Pe. In the absence of hydrodynamics, the first normal stress difference and the osmotic pressure scale as $Pe^4$ and $Pe^2$ respectively when probe forcing is weak, and as $Pe$ for strong probe forcing. As hydrodynamics become important, interparticle forces give way to lubrication interactions. Hydrodynamic coupling leads to a new low-$Pe$ scaling of the first normal stress difference and the osmotic pressure as $Pe^4$, and high-$Pe$ scaling as $Pe^2$, where $0.799 < \delta < 1$ as hydrodynamics vary from strong to weak. For the entire range of the strength of hydrodynamic interactions and probe forcing, the new phenomenological theory is shown to agree with standard micromechanical definitions of the stress. We further draw a connection between the stress and the energy storage in a suspension, and the entropic nature of such storage is identified.

11:27AM L53.00002 Distinctive viscoelastic and viscoplastic nanomechanics of ionically cross-linked polyelectrolyte complexes under intermittent relaxation and creep. BIAO HAN, TIANZHU MA, Drexel University School of Biomedical Eng., Sci., and Health Systems, DAEYEEON LEE, VIVEK SHENOY, University of Pennsylvania, School of Engineering and Applied Science, LIN HAN, Drexel University School of Biomedical Eng., Sci. and Health Systems — This study aims to reveal unique nanoscale viscoelastic and viscoplastic properties of ionically cross-linked polyelectrolyte networks. Layer-by-layer PAH/PAA complexes were tested by four continuous loading cycles in aqueous solutions. In each cycle, AFM-nanoindentation via a microspherical tip ($R=5\mu m$) was applied up to $1\mu N$ force, followed by a 30-60 sec hold at either a constant indentation depth to measure relaxation, or a constant force to measure creep. At a highly cross-linked, neat neutral state ($0.01M$, pH 5.5), instantaneous modulus increased by 2.7-fold from first to last cycle, while the degree of relaxation (>$95\%$) remain consistent. These results indicate repeated loading increases local cross-link density, while relaxation is consistently dominated by cross-link breaking and re-formation. In contrast, under creep, modulus increased by a similar 3.5-fold, and degree of creep is significantly attenuated from $\approx 50\%$ to $45\%$ from first to last cycle. Results from creep suggest constant viscous flow of polymer chains in the absence of permanent anchorage. As a result, an irreversible deformation ($\approx$370nm) was observed after multiple creep cycles, suggesting the presence of viscoplasticity.

11:39AM L53.00003 Non-equilibrium Stokes-Einstein relation via active microrheology of hydrodynamically interacting suspensions. HENRY CHU, ROSEANNA ZIA, Cornell University — In our recently developed non-equilibrium Stokes-Einstein relation, we showed that, in the absence of hydrodynamic interactions, the stress in a suspension is given by a balance between fluctuation and dissipation. Here, we generalize our theory for systems of hydrodynamically interacting colloids, via active microrheology, where motion of a Brownian probe through the medium reveals rheological properties. The strength of probe forcing compared to the entropic restoring force defines a Péclet number, $Pe$. In the absence of hydrodynamics, the first normal stress difference and the osmotic pressure scale as $Pe^4$ and $Pe^2$ respectively when probe forcing is weak, and as $Pe$ for strong probe forcing. As hydrodynamics become important, interparticle forces give way to lubrication interactions. Hydrodynamic coupling leads to a new low-$Pe$ scaling of the first normal stress difference and the osmotic pressure as $Pe^4$, and high-$Pe$ scaling as $Pe^2$, where $0.799 < \delta < 1$ as hydrodynamics vary from strong to weak. For the entire range of the strength of hydrodynamic interactions and probe forcing, the new phenomenological theory is shown to agree with standard micromechanical definitions of the stress. We further draw a connection between the stress and the energy storage in a suspension, and the entropic nature of such storage is identified.

11:51AM L53.00004 Sticky-probe active microrheology. DEREK HUANG, ROSEANNA ZIA, Cornell University — We study the strongly nonlinear flow behavior of a sticky colloidal dispersion via active microrheology, where the motion of a Brownian probe driven by external forces through the suspension is tracked to infer material properties. Most prior work focused on repulsive hard spheres and the influence of Brownian and hydrodynamic forces on rheological behavior, but in many biological suspensions, particles exert attractive forces on one another. Previous attempts to model the effects of particle attractions on sheared suspensions yield that interparticle attractions increase suspension stress and viscosity, but these results are limited to weak shearing flows in macroscopic systems. In our microrheological model, probe motion through the suspension distorts the configuration of particles; the Péclet number, probe forcing compared to thermal forces, gives the extent of this distortion. The equilibrium microstructure and its distortion under probe forcing are also influenced by the strength of interparticle attractions relative to thermal forces. We determine the equilibrium and non-equilibrium microstructure and examine the forcing and attraction contributions to particle motion and suspension stress.

12:03PM L53.00005 Stress diffusion in models for shear banding. ELIYAN MASNADA, PETER OLMSTED, Georgetown Univ — Understanding shear banding is of utmost importance from both theoretical and experimental point of view and consequently it has been studied for several decades [1]. Despite this study numerous aspects of shear banding remains poorly understood. Because of the intrinsic inhomogeneity in the shear banded state, applicable constitutive models must be include spatial inhomogeneities, leading to a so-called ‘diffusive’ term in the equation of motion for the slow variables that carry stress [2,3]. Such terms are also vital in describing the interaction of bulk shear banding flows with walls and incorporation of wall slip. In this work, we consider different sources of ‘diffusion’ in polymer models in which concentration degrees of freedom are negligible. The simplest models used are consistent with diffusive terms whose origin is intrinsically dissipative, such as due to hydrodynamic interactions. By contrast, models in which elastic effects such as finite chain stiffness contribute to stress diffusion are inconsistent with simple diffusive models, and we propose alternative consistent models. [1] P. D. Olmsted, Rheol. Acta, 47, 293-300 (2008). [2] C.-Y. D. Lu et al, Phys. Rev. Lett., 84, 642 (2000). [3] A. W. El-Kareh and L. G. Leal, J. Non-Newton. Fluid Mech., 33, 257 (1989).

12:15PM L53.00006 Strength of self-pinning in coffee drops. ANDRZEJ LATKA, KIMBERLY KAWCZINSKI, SIDNEY NAGEL. James Franck Institute, University of Chicago — The equilibrium contact angle $\theta_c$ of a liquid drop placed on a solid surface is uniquely determined by a balance of surface tension forces according to Young’s Equation, yet is rarely observed in real systems. Due to contact angle hysteresis, liquids can make contact with a surface at any angle before the receding and advancing contact angle: $\theta_R < \theta_c < \theta_A$. A particularly striking example of this phenomenon is the familiar coffee stain. For coffee $\theta_R = 0$, thus as the drop evaporates the contact line remains pinned at its initial location. This results in the majority of the coffee being deposited in a characteristic ring at the drop’s original boundary. We investigate how solid particles suspended in a liquid could so strongly influence contact angle hysteresis, by measuring the receding contact angle of a droplet at various times during the evaporation process. For low solute concentrations, $\theta_R$ slowly decreases as the drop evaporates, but remains positive. Surprisingly, we find that increasing the solute concentration results in $\theta_R = 0$ and a fully pinned contact line almost immediately after the drop is deposited.
12:27PM L53.00007 Microfluidics of soft granular gels, RYAN NIXON, Univ of Florida – Gainesville, TAPOMOY BHATTACHARJEE, W. GREGORY SAWYER, THOMAS E. ANGELINI, University of Florida — Microfluidic methods for encapsulating cells and particles typically involve drop making with two immiscible fluids. The main materials constraint in this approach is surface tension, creating inherent instability between the two fluids. We can eliminate this instability by using miscible inner and outer phases. This is achieved by using granular micro gels which are chemically miscible but physically do not mix. These microgels are yield stress materials, so they flow as solid plugs far from shear gradients, and fluidize where gradients are generated — near an injection nozzle for example. We have found that tuning the yield stress of the material by varying polymer concentration, device performance can be controlled. The solid like behavior of the gel allows us to produce infinitely stable jets that maintain their integrity and configuration over long distances and times. These properties can be combined and manipulated to produce discrete particulate bunches of an inner phase, flowing inside of an outer phase, well enough even to print a Morse code message suspended within flow chambers about a millimeter in diameter moving at millimeters a second.

12:39PM L53.00008 Lift-enhanced Electrical Pinched Flow Fractionation for Particle and Cell Separation.1, Cory G. Thomas, Andrew Todd, Xinyu Lu, Xiangchun Xu, Clemson University — Pinched flow fractionation (PFF) is a microfluidic technique that utilizes the laminar flow profile in microchannels to continuously separate particles or cells by size. The flow can be either pressure-driven or electric-field-driven. We demonstrate in this work that the wall-induced electrical lift force can be exploited to significantly increase the particle or cell displacement in electrical PFF due to its strong size dependence. This enhanced particle and cell separation is implemented by a simple elongation of the pinched segment in electrical PFF. It is demonstrated through both a binary and a ternary separation of polymer particles and biological cells based on surface charge and/or size. We also develop a numerical model to predict and understand this lift-enhanced electrical PFF.

1This work was supported by the Honors and Creative Inquiry programs at Clemson University.

12:51PM L53.00009 Particle Size Effect on Wetting Kinetics of a Nanosuspension Drop: MD Simulations, BAIOU SHI, EDMUND WEBB, Lehigh University — The behavior of nano-fluids, or fluid suspensions containing nanoparticles, has garnered tremendous attention recently for applications in advanced manufacturing. In our previous results from MD simulations, for a wetting system with different advancing contact angles, cases where self-pinning was observed were compared to cases where it was not and relevant forces on particles at the contact line were computed. To advance this work, the roles of particle size and particle loading are examined. Results presented illustrate how particle size affects spreading kinetics and how this connects to dynamic droplet morphology and relevant forces that exist nearby the contact line region. Furthermore, increased particle size in simulations permits a more detailed investigation of particle/substrate interfacial contributions to behavior observed at the advancing contact line. Based on changes in spreading kinetics with particle size, forces between the particle and liquid front are predicted and compared to those computed from simulations. At high loading, particle/particle interactions become relevant and forces computed between particles entrained to an advancing contact line will be presented.

1:03PM L53.00010 Numerical Computation of Mass Transport in Low Reynolds Number Flows and the Concentration Boundary Layer, Nicholas A. Licata, Nathaniel J. Fuller, University of Michigan-Dearborn — Understanding the physical mechanisms by which an individual cell interacts with its environment often requires detailed information about the fluid in which the cell is immersed. Mass transport between the interior of the cell and the external environment is influenced by the flow of the extracellular fluid and the molecular diffusivity. Analytical calculations of the flow field are challenging in simple geometries, and not generally available in more realistic cases with irregular domain boundaries. Motivated by these problems, we discuss the numerical solution of Stokes equation by implementing a Gauss-Seidel algorithm on a staggered computational grid. The computed velocity profile is used as input to numerically solve the advection-diffusion equation for mass transport. Special attention is paid to the case of two-dimensional flows at large Péclet number. The numerical results are compared with a perturbative analytical treatment of the concentration boundary layer.

1:15PM L53.00011 Cell mechanics through analysis of cell trajectories in microfluidic channel, Samuel Bowie, Alexander Alexeev, Todd Sulchek, Georgia Institute of Technology — The understanding of dynamic cell behavior can aid in research ranging from the mechanistic causes of diseases to the development of microfluidic devices for cancer detection. Through analysis of trajectories captured from video of the cells moving in a specially designed microfluidic device, insight into the dynamic viscoelastic nature of cells can be found. The microfluidic device distinguishes cells viscoelastic properties through the use of angled ridges causing a series of compressions, resulting in differences in trajectories based on cell stiffness. Trajectories of cell passing through the device are collected using image processing methods and data mining techniques are used to relate the trajectories to cell properties obtained from experiments. Furthermore, numerical simulation of the cell and microfluidic device are used to match the experimental results from the trajectory analysis. Combination of the modeling and experimental data help to uncover how changes in cellular structures result in changes in mechanical properties.

1:27PM L53.00012 New analysis method for passive microrheology, Kengo Nishi, Christoph Schmidt, Univ Göttingen, Fred Mackintosh, Vrije Universiteit — Passive microrheology is an experimental technique used to measure the mechanical response of materials from the fluctuations of micron-sized beads embedded in the medium. Microrheology is well suited to study rheological properties of materials that are difficult to obtain in larger amounts and also of materials inside of single cells. In one common approach, one uses the fluctuation-dissipation theorem to obtain the imaginary part of the material response function from the power spectral density of bead displacement fluctuations, while the real part of the response function is calculated using a Kramers-Kronig integral. The high-frequency cut-off of this integral strongly affects the real part of the response function in the high frequency region. Here, we discuss how to obtain more accurate values of the real part of the response function by an alternative method using autocorrelation functions.

1:39PM L53.00013 Effect of droplet shape on ring stains from dried liquid, Melvin Santiago, Department of Physics, Case Western Reserve University, Cleveland, OH 44106-7079, Katherine Brown, Department of Physics, Hamilton College, Clinton NY 13323, Harsh Mathur, Department of Physics, Case Western Reserve University, Cleveland, OH 44106-7079 — A landmark experimental paper on coffee stains by Deegan et al included a simple theoretical analysis of circular droplets [1]. The analysis was based on a model informally called the Maxwell House equations. It describes the evolving height profile of the droplet, the evaporation of the solvent and the outflow of solute to the rim of the droplet. Since typical droplets are not circles, here we extend the analysis to more general shapes. We find that for thin droplets the height profile may be determined by solving Poisson’s equation in a domain corresponding to the footprint of the droplet. Evaporation is treated in a simple approximation via an electrostatic analogy and is dominated by the sharp edges of the droplet. Assuming zero vorticity allows us to analyze the solute flow in droplets of arbitrary shape. We compare circular droplets to other shapes including long linear droplets, ring shaped droplets and droplets with an elliptical footprint. [1] R.D. Deegan et al, Nature 389, 827 (1997).
1:51PM L53.00014 Lie Algebraic Analysis of Thin Film Marangoni Flows: Multiplicity of Self-Similar Solutions, ZACHARY NICOLAOU, SANDRA TROJAN, California Institute of Technology, 1200 E. California Blvd., MC 128-95, Pasadena, CA — The rapid advance of an insoluble surfactant monolayer on a thin liquid film of higher surface tension is controlled by distinct flow regimes characterized by the relative strength of viscous, Marangoni and capillary forces. Such flows play a critical role in human pulmonary and ocular systems. During the past quarter century, researchers have focused exclusively on self-similar solutions to the governing pair of nonlinear PDEs for the film thickness, \( H(r/t^a) \), and surface concentration, \( f(r/t^b)/t^b \), in the limit where the Marangoni or capillary terms vanish, where \( r \) denotes the spatial variable, \( t \) is time, and \( a \) and \( b \) are fractional exponents. Using Lie algebraic techniques, we demonstrate for the first time the existence of several embedded symmetries in this system of equations which yield multiple self-similar solutions describing more complex scaling behavior, even when all three forces are incorporated. A special and previously unrecognized subset of these solutions reveals the dynamical behavior of film thinning and surfactant distribution near the origin, which ultimately controls the downstream flow. Finite element simulations confirm the suite of scaling exponents obtained analytically.

2:03PM L53.00015 Convective flows generated by evaporation: experiments, linear stability analysis and numerical simulations, JOCELYN DUNSTAN, Postdoc, KYOUNG JIN LEE, Professor, SIMON PARK, Senior Lecturer, RAYMOND E. GOLDSTEIN, Professor — A novel form of convection was observed in a suspension of non-motile Photobacterium phosphoreum bacteria. The pattern resembles classical bioconvection, however this strain has limited if any motility, which excludes this possible explanation. After performing a series of control experiments we found that the convection was actually driven by the evaporation of the salty bacterial medium, and the same kind of plumes were observed using polystyrene beads suspended in water with salt added. A mathematical model was formulated for the process and studied using a linear stability analysis and finite element method simulations, reproducing most of the observed experimental features. From the linear stability analysis, a threshold in salt concentration to observe convective motion was obtained, as well as the wavelength of the pattern at the onset of the instability. This was complemented by finite element simulations, which produced plume dynamics remarkably similar to the experimental observations. Evaporation-driven convection on the millimeter scale has not been studied extensively, and its effect may have been underestimated in other experiments.

11:30AM - 11:30AM — Exhibit Hall EF —

M1.00001 POLYMER PHYSICS —

M1.00002 Morphology Evolution and Dynamic Viscoelastic Behavior of Ternary Elastomer Blends under Shear, JIA DONG, XIANGGULI LIU, CHARLES C HAN, DUJIN WANG, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry CAS — The influence of nanoparticle geometry, such as size and shape, on the phase morphology of partially miscible binary polymer blends under and after shear has been examined by rheological and rheo-optical techniques. The phase morphologies of the solution-polymerized styrene-butadiene rubber and low vinyl content polyisoprene (SBR/LPI) blend systems were affected by the dispersion status of fillers which were determined by filler shapes and shear strength. Under weak shear flow, the domain morphology of the OMMT filled blend was much thinner than that of the SiO\(_2\) filled blend. Under strong shear flow, the string-like phase interface of the OMMT filled blend was much blurred compared with that of the SiO\(_2\) filled blend. After shear cessation, the orientation status of OMMT sheets determined the orientation of newborn domains. Combined morphology observation and rheological analysis showed that the anisotropic structure and the unfavorable bending energy of OMMT sheets played important roles on phase morphology and its evolution process during or after shear.

M1.00003 Selective crystallization of regioregularity controlled polythiophene for enhancing mechanical stability and electronic performance, HYEONG JUN KIM, KAISST, HOJEONG YU, POESTECH, JAEHAN KIM, JINSUNG KIM, TAEK SOO KIM, KAIST, — Considering the many potential applications of organic electronics in portable electronic devices, it is of great importance to develop an electro-active material that possesses mechanical stability and high electronic performance. Coexistence of both properties, however, is very difficult to achieve because good electronic performance is associated with long conjugation length, and high crystallinity often results in stiffness and brittleness. Herein, we utilize P3HT with two different regioregularities: high RR (98) P3HT has high electronic properties but poor mechanical resilience, and low RR P3HT (68) exhibits high elasticity and ductility but poor electronic performance. Selective crystallization of high RR P3HT induced by solution assembly allows construction of percolated networks of high RR P3HT nanowires (NWs) embedded in low RR P3HT matrix. Only 5 wt high RR P3HT is required to reach a hole mobility comparable to that of high RR P3HT, and high RR NWs embedded in film exhibits 20 times higher elongation at break. Selective self-assembly allows us to overcome the fragile nature of highly crystalline conjugated polymers without losing their electronic properties.

M1.00004 Development of flash nanoprecipitation as a scalable platform for production of hybrid polymer-inorganic Janus particles, VICTORIA E. LEE, ROBERT K. PRUD'HOMME, RODNEY D. PRIESTLEY, Princeton University — Polymer Janus particles, containing two or more distinct domains, can act as supports for inorganic nanoparticles, stabilizing them against aggregation and templating anisotropic functionalization of the microparticles. This anisotropy can be advantageous for applications such as biofuel upgrading, biomonosensors, and responsive materials. Here, we introduce flash nanoprecipitation (FNP) as a scalable, fast process to create hybrid polymer-inorganic Janus particles with control of particle size and anisotropy. During FNP, polymer Janus particles form by rapid intermixing of a polymer solution with a poor solvent, inducing polymer precipitation and phase separation. Inorganic nanoparticles are then adsorbed selectively onto one domain of the polymer support by exploiting electrostatic interactions between the charged particles. By tuning polymer concentration and ratio in the feed stream, the particle size and anisotropy can be controlled. We further demonstrate that these hybrid particles can simultaneously stabilize emulsions and selectively catalyze the degradation of dye in one phase.

1The authors thank the financial support from National Natural Science Foundation of China (No.51173195).

2With support from the Princeton Imaging Analysis Center.
M1.00005 Control of dynamical self-assembly of strongly Brownian nanoparticles through convective forces induced by ultrafast laser. SERIM ILDAY, GURSOY B. AKGUC, ONUR TOKEL, CHAITH MAKEY, OZGUN YAVUZ, KORAY YAVUZ, IHOR PAVLOV, F. OMER ILDAY, OCUZ GULSEREN, Bilkent Univ — We report a new dynamical self-assembly mechanism, where judicious use of convective and strong Brownian forces enables effective patterning of colloidal nanoparticles that are almost two orders of magnitude smaller than the laser beam. Optical trapping or tweezing effects are not involved, but the laser is used to create steep thermal gradients through multi-photon absorption, and thereby guide the colloids through convective forces. Convective forces can be thought as a positive feedback mechanism that helps to form and reinforce pattern, while Brownian motion act as a competing negative feedback mechanism to limit the growth of the pattern, as well as to increase the possibilities of bifurcation into different patterns, analogous to the competition observed in reaction-diffusion systems. By steering stochastic processes through these forces, we are able to gain control over the emergent pattern such as to form-deform-reform of a pattern, to change its shape and transport it spatially within seconds. This enables us to dynamically initiate and control large patterns comprised of hundreds of colloids. Further, by not relying on any specific chemical, optical or magnetic interaction, this new method is, in principle, completely independent of the material type being assembled.

M1.00006 Amphiphilic Soft Janus Particles as Interfacial Stabilizers, WENDA WANG, SUNNY NIU, CHRIS SSO, ROBERT PRUDHOMME, RODNEY PRIESTLEY, Princeton Univ, PRIESTLEY POLYMER GROUP TEAM, PRUD'HOMME RESEARCH GROUP Team — Janus particles, which incorporate two or more “faces” with different chemical functionality, have attracted great attention in scientific research. Amphiphilic Janus particles have two faces with distinctly different hydrophobicity. This can be thought of as colloidal surfactants. Theoretical studies on the stabilization of emulsions using Janus particles have confirmed higher efficiency. Herein we synthesize the narrow distributed amphiphilic Janus particles via Precipitation-Induced Self-Assembly (PISA). The efficiency of the amphiphilic Janus particles are tested on different oil/water systems. Biocompatible polymers can also be used on this strategy and may potentially have wide application for food emulsion, cosmetics and personal products.

M1.00007 Time-resolved SANS studies on block copolymer micelles with varying core-solvent interactions, TYLER COOKSEY, AVANTIKA SINGH, MARIA MARQUEZ, MEGAN ROBERTSON, University of Houston — The self-assembly of block copolymer micelles occurs through a relaxation process dominated by the exchange of individual polymer chains. The objective of this work is to probe the single chain exchange of block copolymer micelles with varying core-solvent interactions, utilizing time-resolved neutron scattering (TR-SANS). The interactions between the core-forming polymer and the solvent has many implications for the micelle structure, including the aggregation number, micelle size, and interfacial tension. However, few studies have investigated the effect of the core polymer-solvent interactions on the dynamics of micelle formation. We will focus our study on poly(epsilon-caprolactone-block-ethylene oxide) block copolymers forming micelle structures in mixtures of water and tetrahydrofuran (THF). It was observed that changing the THF concentration, which varies the degree of repulsion between the core and solvent, greatly influences the single chain exchange rate in this system.

M1.00008 Spectroscopic Analysis of 10MAG/LDAO Reverse Micelles to Determine Characteristic Properties and Behavioral Extrema, JOSHUA BERG, CARA MAWSON, ZACH NORM, NATHANIEL NUCCI, Rowan University — Reverse micelles are spontaneously organizing complexes of surfactant that encapsulate a nanoscale pool of water in a bulk non-polar solvent. Reverse micelle (RM) mixtures have a wide range of applications, including biophysical investigation of protein systems. A new RM mixture composed of decyl-1-monooleylcer (10MAG) and lauryldimethylammonium-N-oxide (LDAO) was recently described. This mixture has the potential to prove more widely applicable for use of RMs in applications that involve encapsulation of macromolecules, yet little is known about the phase behavior or size of reverse micelles created by this mixture. Data describing such behaviors for this mixture are presented here. We have used dynamic light scattering (DLS) and fluorescence spectroscopy to investigate the size and partitioning behavior of RMs in varying mixtures of 10MAG, LDAO, water, pentane, and hexanol. These data demonstrate that the 10MAG/LDAO RM mixture exhibits markedly different phase and RM size behavior than that of commonly used RM surfactant mixtures. The implications of these findings for use of the 10MAG/LDAO mix for RM applications will also be addressed.

M1.00009 Photolithography and Fluorescence Correlation Spectroscopy used to examine the rates of exchange in reverse micelle systems, ZACH NORM, CARA MAWSON, KYRON JOHNSON, SARAH KESSLER, ANNE REBECCA, NATHAN WOLF, MICHAEL LIM, NATHANIEL NUCCI, Rowan University — Reverse micelles are molecular complexes that encapsulate a nanoscale pool of water in a surfactant shell dissolved in non-polar solvent. These complexes have a wide range of applications, and in all cases, the degree to which reverse micelles (RM) exchange their contents is relevant for their use. Despite its importance, this aspect of RM behavior is poorly understood. Photolithography is employed here to create micro and nano scale fluidic systems in which mixing rates can be precisely measured using fluorescence correlation spectroscopy (FCS). Micro-channel patterns are etched using reactive ion etching process into a layer of silicon dioxide on crystalline silicon substrates. Solutions containing mixtures of reverse micelles, proteins, and fluorophores are placed into reservoirs in the patterns, while diffusion and exchange between RMs is monitored using a FCS system built from a modified confocal Raman spectrometer. Using this approach, the diffusion and exchange rates for RM systems are measured as a function of the components of the RM mixture.

M1.00010 Self-assembly of mixed lipids into bicelles and vesicles: molecular dynamics simulations, HARI SHARMA, ZILU WANG, ELENA DORMIDONTOVA, Department of Physics and Institute of Materials Science, University of Connecticut, Storrs, CT — Formation of complex supramolecular nanostructures, such as micelles, bicelles, vesicles (liposomes) etc. via self-assembly of simple molecules has provided a new pathway for the design and development of effective drug carriers. Solid nanoparticles or functional biopolymers, such as RNA, DNA, peptides can be encapsulated into these carriers for controlled delivery or selective targeting. We performed coarse grained molecular dynamics simulation using the MARTINI force field to study the self-assembly of a binary surfactant mixture composed of long and short phospholipids, DPPC and DHPC, in the ratio 3:1. We found that at low temperature lipids self-assemble into a bicelle (nanodisc) with the longer lipid mainly forming the interior and short lipid the rim of the bicelle. At higher temperature the nanodisc transforms into a vesicle with homogeneously distributed lipids. The structural changes of these nanodiscs and vesicles imposed by gold nanoparticle encapsulation and pegylation will be addressed.

M1.00011 Directed Assembly of Gold Nanoparticles via Polymer Single Crystals, SHAN MEI, HAO QI, TIAN ZHOU, CHRISTOPHER LI, None, SOFTWARE LAB TEAM — Gold nanoparticles (AuNPs) have attracted great attention due to their unique properties and potential applications. In recent years, more efforts have been made to the assembly of AuNPs into various ordered structures such as AuNP wires and sheets in order to transfer their properties from nanoscale to macroscale, as well as exploring new properties. In this work we report a method to assemble AuNPs into well defined, free standing frame structure using poly(ethylene oxide) (PEO) lamellar single crystal as the template. By controlling the single crystal size and functioning pattern, we are able to tune the width and size of the AuNP frame. We consider this approach to be an efficient and precise way to assemble AuNP and this methodology could be applied to other metal or semiconductor NPs.
M1.00012 Synthesis of Poly(N-isopropylacrylamide) Microcapsules for Drug Delivery Applications via UV Aerosol Photopolymerization. NICOLE ROBERSON, DANIEL DENMARK, SARATH WITANACHCHI, University of South Florida — Hybrid drug delivery systems composed of thermo-responsive polymers and magnetic nanoparticles have been developed using chemical methods to deliver controlled amounts of a biotherapeutic to target tissue. These methods can be expensive, time intensive, and produce impure composites due to the use of surfactants during polymer synthesis. In this study, UV aerosol photopolymerization is used to synthesize N-isopropylacrylamide (NIPAM) monomers, N,N-methylenebisacrylamide (MBA) crosslinker, and irgacure 2959 photoinitiator into the transporting microcapsule for drug delivery. The method of UV aerosol photopolymerization allows for the continuous, cost effective, and time efficient synthesis of a high concentration of pure polymers in a short amount of time; toxic surfactants are not necessary. Optimal NIPAM monomer, MBA crosslinker, and irgacure 2959 photoinitiator concentrations were tested and analyzed to synthesize a microcapsule with optimal conditions for controlled drug delivery. Scanning Electron Microscope (SEM) imaging reveals that synthesis of polymer microcapsules of about 30 micrometers in size is effective through UV aerosol photopolymerization. Findings will contribute greatly to the field of emergency medicine.

M1.00013 Tertiary phase diagram of cellulose, ionic liquid and organic solvent. XIN ZHANG, DOUG HENDERSON, Department of Materials Science and Engineering, University of Maryland, MADHUSUDAN TYAGI, YIMIN MAO, NCNR, NIST, Gaithersburg, MD, ROBERT M. BRIBER, HOWARD WANG, Department of Materials Science and Engineering, University of Maryland — Cellulose is the most abundant natural polymer on earth, and widely used in products from clothing to paper. Fundamental understanding of molecular solutions of cellulose is the key to realize advanced technologies beyond cellulose fibers. It has been reported that certain ionic liquid/organic solvent mixtures dissolve cellulose. In this study, the tertiary phase diagram of microcrystalline cellulose, 1-Ethyl-3-methylimidazolium acetate (EMIMAc), and dimethylformamide (DMF) mixtures has been determined using optical cloud point method and small angle neutron scattering (SANS). Data indicate that a molar ratio of EMIMAc to cellulose repeating unit equal or greater than 3 is necessary but not sufficient in forming one-phase homogeneous solutions. A miscibility gap exists in the dilute regime, where a minimum of 5 mol% of EMIMAc in DMF is needed to form homogenous solutions. SANS show that cellulose chains adopt Gaussian-like conformation in homogenous solutions. The solution exhibits the characteristics of upper critical solution temperature. Clustering of cellulose chains occurs at low EMIMAc/DMF or EMIMAc/cellulose ratio, or at low temperatures. The mechanism of cellulose dissolution in tertiary mixture is discussed.

M1.00014 Thin blend films of cellulose and polyacrylonitrile. RUI LU, XIN ZHANG, Department of Materials Science and Engineering, University of Maryland, College Park, MD, YIMIN MAO, NCNR, NIST, Gaithersburg, MD, ROBERT BRIBER, HOWARD WANG, Department of Materials Science and Engineering, University of Maryland, College Park, MD — Cellulose is the most abundant renewable, biocompatible and biodegradable natural polymer. Cellulose exhibits excellent chemical and mechanical stability, which makes it useful for applications such as construction, filtration, bio-allowing and packaging. To further expand the potential applications of cellulose materials, their alloying with synthetic polymers has been investigated. This study focused on films comprising cotton linter cellulose (CLC) and polyacrylonitrile (PAN) blends with various compositions spanning the entire range from neat CLC to neat PAN were spun cast on silicon wafers from common solvents in dimethyl sulfoxide / ionic liquid mixtures. The morphologies of thin films were characterized using optical microscopy, atomic force microscopy, scanning electron microscopy and X-ray reflectivity. Morphologies of as-cast films are highly sensitive to the film preparation conditions; they vary from featureless smooth films to self-organized ordered nano-patterns to hierarchical structures spanning over multiple length scales from nanometers to tens of microns. By selectively removing the PAN-rich phase, the structures of blend films were studied to gain insights in their very high stability in hot water, acid and salt solutions.

M1.00015 Process Dependence of Cellulose Nanofiber Fabrication. DOUG HENDERSON, XIN ZHANG, Department of Materials Science and Engineering, University of Maryland, College Park, MD, YIMIN MAO, NCNR, NIST, Gaithersburg, MD, SOO-HWAN JANG, LIANGBING HU, ROBERT BRIBER, HOWARD WANG, Department of Materials Science and Engineering, University of Maryland, College Park, MD — Cellulose nanofibers (CNF) are the most abundant natural nanomaterial on earth with potential applications in renewable energy, polymer nanocomposites and biodegradable natural polymer. Cellulose exhibits excellent chemical and mechanical stability, which makes it useful for applications such as construction, filtration, bio-allowing and packaging. To further expand the potential applications of cellulose materials, their alloying with synthetic polymers has been investigated. This study focused on films comprising cotton linter cellulose (CLC) and polyacrylonitrile (PAN) blends with various compositions spanning the entire range from neat CLC to neat PAN were spun cast on silicon wafers from common solvents in dimethyl sulfoxide / ionic liquid mixtures. The morphologies of thin films were characterized using optical microscopy, atomic force microscopy, scanning electron microscopy and X-ray reflectivity. Morphologies of as-cast films are highly sensitive to the film preparation conditions; they vary from featureless smooth films to self-organized ordered nano-patterns to hierarchical structures spanning over multiple length scales from nanometers to tens of microns. By selectively removing the PAN-rich phase, the structures of blend films were studied to gain insights in their very high stability in hot water, acid and salt solutions.

M1.00016 Multi-scale Characterization of Cellulose TEMPO-Nanofiber Suspension. YIMIN MAO, KAI LIU, BENJAMIN HSIAO, Chemistry Department, Stony Brook University — Cellulose nanofiber (CNF) suspensions were characterized at multiple length scales. CNF suspension was prepared by applying 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) oxidation method to dry wood pulp. TEMPO method was able to produce fine fibers with a cross section dimension being in the order of magnitude of several nanometers, and length being several hundred nanometers. The surface was negatively charged. Charge density was characterized by Zeta-potential measurement. Both small-angle X-ray (SAXS) and small-angle neutron scattering (SANS) methods were employed to examine fiber dimensions in solution. Data fitting indicated that newly-developed ribbon model was able to capture the essence of CNF's geometry, which is also computationally economic. The rectangular-shaped cross section was consistent to cellulose's crystal structure, and was able to provide insights into how cellulose crystals were biologically synthesized and packed in nature. Multi-angle dynamic light scattering (DLS) was used to gain insights in their very high stability in hot water, acid and salt solutions.

M1.00017 Controlling the structure and rheology of TEMPO-oxidized cellulose in zinc chloride aqueous suspensions for fabricating advanced nanopaper. SHA WANG, XIN ZHANG, LIANGBING HU, ROBERT BRIBER, HOWARD WANG, Dept. Materials Science and Engineering, University of Maryland, College Park, LINXIN ZHONG, State Key Laboratory of Pulp and Paper Engineering, South China University of Technology — Due to its abundance, low-cost, biocompatibility and renewability, cellulose has become an attractive base material for a number of applications. A strong scattering-angle dependence of autocorrelation function was observed. The characterization is useful to gain insights into how cellulose crystals were biologically synthesized and packed in nature. Multi-angle dynamic light scattering (DLS) was used to characterize TEMPO-oxidized cellulose in zinc chloride aqueous suspensions for fabricating advanced nanopaper. Scanning Electron Microscope (SEM) imaging reveals that cellulose nanofiber suspension can be rapidly obtained by dissolving TOC in 65 wt. % zinc chloride aqueous solutions at room temperature, whereas a transparent suspension quality of CNF, and can provide guideline for follow-up research aimed for a variety of applications.
M1.00018 All-or-none folding of a polymer in confinement\textsuperscript{1}, MARK TAYLOR, Hiram College — A flexible homopolymer chain with sufficiently short-range interactions undergoes a discontinuous transition from an expanded coil to a compact crystallite analogous to the all-or-none folding transition exhibited by fast-folding proteins. One anticipates that geometric confinement will reduce the entropy of the unfolded chain, thereby stabilizing the folded state and shifting the transition to a higher temperature. In this work we study a flexible square-well N-mer chain (monomer diameter \( d \)) located between two hard walls forming a slit-like pore (width \( W \)) with the chain end-tethered to one wall. We carry out Monte simulations with Wang-Landau sampling to construct the single-chain density of states and use both microcanonical and canonical analyses to characterize phase transitions. When the slit width is similar to the size of the folded chain we observe a modest stabilization effect. Further reduction of the slit width geometrically prohibits the chain from folding into the free-chain ground state. However, a discontinuous all-or-none folding transition still occurs to a flattened crystallite that spans the pore. All-or-none folding persists even to the limit of a very narrow pore (\( W \approx d \)) where the ground-state structure is a quasi-two-dimensional crystal.

\textsuperscript{1}Funding: NSF DMR-1204747

M1.00019 Exploring the existence of two Tg's in thin, supported polymer films\textsuperscript{1}, ERIC CHEN, ETHAN GLOR, GABRIEL ANGRAND, ZAHRA FAKHRAAI, Univ of Pennsylvania, FAKHRAAI GROUP TEAM — Ellipsometry has commonly been used to characterize the glass transition temperature (Tg) and other properties of nanoscale thin films. In some ultra-thin films the glass transition broadens and even becomes two distinct transitions, as previously observed in free-standing polystyrene, thin films. However, for most polymers, the second, lower Tg is located below the compensation temperature and is secondary to the primary Tg. We present ellipsometry measurements of a supported polymer film, Epon 828 cured with diethanolamine, designed in a manner to avoid most of the complications associated with the primary Tg. We have designed a vacuum stage with a base pressure of \(<10^{-4} \text{ torr}, \text{ equipped with a Linkam temperature stage with a temperature range of 153 K-873 K to study the properties of thin polymer films, supported on a substrate at a wide temperature range and explore the existence of two Tgs in these systems. The stage was machined from aluminum and used inrasil quartz windows to allow the transmission of polarized light without distortion. The vacuum allows for accurate ellipsometry measurements of the properties of thin polymer films, such as expansion coefficient and Tg, at temperatures well below room temperature, without artifacts due to water condensation.

\textsuperscript{1}MRSEC (NSF-DMR-11-20901)

M1.00020 Limits of single-molecule super-resolution microscopy in thin polymer films, MUZHOU WANG, MARCELO DAVANCO, JAMES M. MARR, J. ALEXANDER LIDDLE, JEFFREY W. GILMAN, National Institute of Standards and Technology — Structural characterization by super-resolution microscopy has become increasingly widespread, particularly in the biological community. The technique is powerful because it can produce real-space images with resolutions of tens of nanometers, while sample preparation is relatively non-invasive. Previous studies have applied these techniques to important scientific problems in the life sciences, but relatively little work has explored the attainable limit of resolution using samples of known structure. In this work, we apply photo-activated localization microscopy (PALM) to polymer films that have been nanopatterned using electron-beam lithography. Trace amounts of a rhodamine spiroamide dye are dispersed into nanostructured poly(methyl methacrylate), and UV-induced switching of the fluorophores enables nanoscale localization of single molecules to generate a final composite super-resolution image. Features as small as 50 nm are clearly resolvable. To determine the ultimate resolution limit, we investigate sources of error in the system, particularly from systematic mislocalizations due to the effect of fluorophore orientation on the single-molecule point-spread function.

M1.00021 Phase separated microstructure and dynamics of polyurethane elastomers under strain, CIPRIAN IACOB, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802 USA, AJAY PAUL, ALI CAGAEL, Electronic Systems Division, St. Jude Medical, Rogers, MN, USA, JAMES RUNT, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802 USA — The molecular mobility of polyurethane elastomers is of the utmost importance in establishing physical properties for ranges from automotive tires and shoe soles to more sophisticated aerospace and biomedical applications. In many of these applications, chain dynamics as well as mechanical properties under external stresses/strains are critical for determining ultimate performance. In order to develop a complete understanding of their mechanical response, we explored the effect of uniaxial strain on the phase separated microstructure and molecular dynamics of the elastomers. We utilize X-ray scattering to investigate soft segment and hard domain orientation, and broadband dielectric spectroscopy for interrogation of the dynamics. Uniaxial deformation is found to significantly perturb the phase-separated microstructure and chain orientation, and results in a considerable slowing down of the dynamics of the elastomers. Attenuated total reflectance Fourier transform infrared spectroscopy measurements of the polyurethanes under uniaxial deformation are also employed and the results are quantitatively correlated with mechanical tensile tests and the degree of phase separation from small-angle X-ray scattering measurements.

M1.00022 Phase behavior of the thermoresponsive polymer Poly(N-isopropyl acrylamide) at variable pressure, ALFONS SCHULTE, Department of Physics and College of Optics and Photonics, University of Central Florida, Orlando, FL 32817-2385, KORA-LEE CLAUDE, SIMON PINZEK, PETER MILLER-BUSCHBAUM, CHRISTINE PAPADAKIS, TU Mnchen, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — Stimuli-responsive such as Poly(N-isopropyl acrylamide) (PNIPAM) exhibit lower critical solution temperature (LCST) behaviour. At ambient pressure it is associated with the release of water and coil to globule transition of the polymer chains, leading to phase separation. Using turbidimetry we measure the P-T phase diagram over an extended range of pressure (0.1 – 400 MPa) and temperature (-10 to 40 oC). The phase boundary shows an elliptic profile, i.e. the cloud point temperature first increases and then decreases with pressure. This is reflected in the change in Gibbs free energy, isothermal compressibility, and isobaric heat capacity. The role of solvent-solvent interaction and addition of co-solvents is discussed.

M1.00023 Complex Curve Kinetics of the Hydroxyl-Epoxy Reaction in DGEBA Epoxy Hardened with Diethanolamine, WINDY ANCIPINK, JOHN MCCOY, New Mexico Institute of Mining and Technology, JAMIE KROPKA, MATHIAS CELINA, Sandia National Laboratories — The curing of a diglycidyl ether of bisphenol-A Epoxy (Epon 828) with diethanolamine (DEA) involves a fast amine-epoxide reaction followed by a slower hydroxyl-epoxide reaction. At curing temperatures below 100\(^\circ\)C, the time scales of these two reactions are well separated, and the hydroxyl addition can be studied as an isolated reaction. The hydroxyl-epoxide reaction is of great interest due to the complex kinetics involved, which are brought about by competing reactions. The reaction kinetics are believed to be tertiary amine catalyzed and are well fit to a modified form of the Kamal-type equation. Here we study the complex long term reaction kinetics at various temperatures, by using isothermal modulated differential scanning calorimetry, micro calorimetry, and infrared spectroscopy. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

M1.00024 Relaxation Characteristics of 828 DGEBA Epoxy Over Long Time Periods, JASMINE HOO, RILEY C. REPGRÖPPE, BRIAN WISLER, GABRIEL K. ARECHEDERRA, JOHN D. MCCOY, New Mexico Institute of Mining and Technology, JAMIE M. KROPKA, KEVIN N. LONG, Sandia National Laboratories — The mechanical relaxation response in uniaxial compression of a diglycidyl ether of bisphenol-A epoxy was studied over long time periods. The epoxy, 828DEA, was Epon 828 cured with diethanolamine (DEA). A sample was compressed at constant strain rate and held at various strain levels for days to allow the sample to relax. The sample was then compressed further and held once more. The relaxation curves were fit with a stretched exponential function. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
M1.00025 Effect of Structure on Charge Mobility in Partially Ordered Polymeric Systems. WAYLON LUO, KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, University of Akron — The performance of thin film organic semiconductor devices depends on the mobility of the charge carriers, which is strongly affected by the structure of the material. 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 present Monte Carlo simulations of a coarse-grained lattice model for dense polymeric systems with a semiflexible component that undergoes a transition to (partially) ordered states at low temperatures. To investigate charge transport, the lattice polymer configurations become part of a model device, which consists of a layer of the material between two electrodes at different potentials. We determine the mobility from Monte Carlo simulations of charge carriers. To model the effect of polymer chain connectivity on charge transport we include an energetic barrier to hopping between sites on different chains; energetic disorder is taken into account by averaging over many polymer configurations. We find that ordering in the material leads to strong mobility anisotropies with increased mobility for transport parallel to the ordered domains and reduced mobility for perpendicular transport.

M1.00026 Improved electrosplintering processing of PU/PEDOT:PSS for electronic textile applications1, ERIN EVKE2, Materials Engineering, AARON CLIPPINGER3, Biomedical Engineering, CLAYSON SPACKMAN, JOHNSON SAMUEL, Mechanical, Aerospace and Nuclear Engineering, RAHMI OZISIK, Materials Engineering; Rensselaer Polytechnic Institute — Poly(3,4-ethylenedioxythiophene)/poly(4-styrenesulfonate), PEDOT:PSS, is an electrically conductive polymer used in electronic textile (e-textile) applications, such as e-textiles, stretch sensors, and resistive heaters. In the current study, PEDOT:PSS is blended with varying concentrations of polyurethane (PU) to investigate the flexibility of PU/PEDOT:PSS fibers that are produced via a modified electrosplintering process where the jet is collected close to the tip of the needle, thereby, enabling the collection of straight fibers by a rotating spool. The electrical conductivity and mechanical properties of PU/PEDOT:PSS fibers are characterized to understand the effect of PU concentration and the processing parameters.

M1.00027 Monte-Carlo simulations of a coarse-grained model for α-oligothiophenes. AMANI AL-MUTAIRI, JUTTA LUETTMER-STRATHMANN, Department of Physics, University of Akron — The interfacial layer of an organic semiconductor in contact with a metal electrode has important effects on the performance of thin-film devices. However, the structure of this layer is not easy to model. Oligothiophenes are small, π-conjugated molecules with applications in organic electronics that also serve as small-molecule models for polythiophenes. α-heptithiophene (6T) is a six-ring molecule, whose adsorption on noble metal surfaces has been studied extensively (see, e.g., Ref. [1]). In this work, we develop a coarse-grained model for α-oligothiophenes. We describe the molecules as linear chains of bonded, discotic particles with Gay-Berne potential interactions between non-bonded ellipsoids. We perform Monte Carlo simulations to study the structure of isolated and adsorbed molecules. [1] M. Kiel et al. Phys. Rev. B 75, 195439 (2007).

M1.00028 Conductance Thin Film Model of Flexible Organic Thin Film Device using COMSOL Multiphysics. CAROLYN CARRADERO-SANTIAGO, JOSEE VEDRINE-PAULUS, University of Puerto Rico at Humacao — We developed a virtual model to analyze the electrical conductivity of multilayered thin films placed above a graphene conducting and flexible polyethylene terephthalate (PET) substrate. The organic layers of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) as a hole conducting layer, poly(3-ethylthiophene-2,5-diyli) (P3HT), as a p-type, phenyl-C61-butyric acid methyl ester (PCBM) and as n-type, with aluminum as a top conductor. COMSOL Multiphysics was the software we used to develop the virtual model, and simulate and model the propagation of physical phenomena represented by differential equations such as heat transfer, fluid flow, electromagnetism, and structural mechanics. In this work, we used the AC/DC, electric currents module we defined the geometry of the model and properties for each of the six layers: PET/graphene/PEDOT:PSS/P3HT/PCBM/aluminum. We analyzed the model with varying thicknesses of graphene and active layers (P3HT/PCBM). This simulation allowed us to analyze the electrical conductivity, and visualize the model with varying voltage potential, or bias across the plates, useful for applications in solar cell devices.

M1.00029 Photopatterned surface relief gratings in azobenzene-amorphous polycarbonate thin films1, MORTEN VOLLMANN, Technical University Berlin, PETER GETEK, University of Applied Sciences Berlin, KELLIE OLEAR, CODY COMBS, BENJAMIN CAMPOS, EDMUND WITKOWSKI, The College of New Jersey, ERIN CAIN, Temple University, DAVID MCGEE, The College of New Jersey — Photoinduced orientation of azobenzene chromophores in polymeric host materials has been broadly explored for optical processing applications. Illumination of the chromophore with polarized light rotates the trans isomer perpendicular to the polarization, resulting in spatially modulated birefringence. The photoinduced anisotropy may also drive mass transport, with surface relief patterns being observed in a wide variety of systems. Here we report photoinduced birefringence in a guest-host system of Disperse Red 1- amorphous polycarbonate (DR1-APC). Birefringence was induced with a 490 nm laser and probed at 633 nm, with typical values of Δn = 0.01 in 2 micron thick films. Illumination of DR1-APC with intensity and/or polarization gratings also resulted in sinusoidal surface relief patterns with periodicity 1-3 micron as controlled by the interbeam crossing angle of the 490 nm writing beams; the surface modulation was measured as atomic force microscopy. Photopatterned DR1-APC is useful for applications given the ease of thin-film fabrication and the high glass transition temperature of APC, resulting in robust optically-induced surface gratings.

M1.00030 Morphology of conjugated polymer/insulating polymer blends from inkjet printing and its correlation to the function of field-effect transistors. HUIPENG CHEN, GUOCHEN ZHENG, LIQIN HU, HUIHUANG YANG, TAILIANG GUO, Fuzhou University — Printed electronics is a rapidly developing field of research which covers any electronic devices or circuits that can be processed using direct printing techniques. Among those printing techniques, inkjet printing is a technique of increasing interest for organic field-effect transistors (FETs) due to its fully data driven and direct patterning. In this work, the morphology of conjugated polymer/insulating polymer blends from inkjet printing and their FET properties has been investigated. The crystallinity and packing of conjugated polymer has been examined by synchrotron x-ray diffraction. The detailed information about the interface and domains of polymer blends were investigated by small angle neutron scattering. It is found that the domains and polymer interface were crucial to the FET properties. Finally, the relationship between morphology and function has been established for polymer blends FET from inkjet printing.
M1.00031 Solvent-vapor concentration impacts selectivity during polymeric transformation in molecular-semiconductor thin films, GEOFFREY PURDUM, Dept. of Chemical and Biological Engineering, Princeton University, THOMAS GESSNER, R. THOMAS WEITZ, BASF SE, GMV 67056, Germany, YUEH-LIN LOO, Dept. of Chemical and Biological Engineering, Princeton University. Post-deposition processing allows precise control over the structural development of molecular-semiconductor thin films. In particular, solvent-vapor annealing converts thin films of a core-chlorinated naphthalene diimide from its triclinic polymorph to its monoclinic polymorph. By tuning the concentration of solvent vapor, we can simultaneously impact the morphology of the resulting monoclinic thin film. At low solvent-vapor concentrations, transformation in-plane is isotropic; we observe comparable transformation rates along the b- and c-axes, resulting in plate-like domains. At high solvent-vapor concentrations, transformation along the c-axis is instead favored, resulting in the formation of needle-like domains. Extended solvent-vapor annealing at these conditions can lead to isolated needles in the active channels of field-effect transistors; these devices exhibit electron mobilities exceeding 1 cm²/Vs.

M1.00032 Charge conduction in partially fluorinated discotic liquid crystals, MITCHELL POWERS, ZHE LI, ROBERT TWIEG, BRETT ELLMAN, Kent State University. Motivated by the role of electrostatic interactions on stacking of partially fluorinated conjugated compounds, we present mobility measurements of, e.g., 1,4-difluoro-2,3,6,7,10,11-hexakisphenantraoxiphenylene (2F-HAT5) in discotic mesophases across a wide range of temperature and applied electric field. Charge conduction in this case is well described by a disorder driven hopping model. 2F-HAT5 exhibits a mobility of approximately 2x10⁻³ cm²/Vs, similar to the parent triphenylene, and has a weak temperature dependence throughout its discotic mesophase, which extends below room temperature. We compare results on this and related compounds to various theoretical models.

M1.00033 Gated Seebeck Using Polymerized Ionic Liquid Gate Dielectrics, ELAYNE THOMAS, BHOOSHAN POPERE, HAIYU FANG, MICHAEL CHABINYC, RACHEL SEGALMAN, Univ of California - Santa Barbara. Thermoelectric materials have the ability to convert a temperature gradient into usable electrical power via the Seebeck effect. This phenomenon is directly related to the material’s Seebeck coefficient and electrical conductivity, which are in turn linked to its electron (or hole) mobility and carrier concentration. Organic semiconductors show promise for thermoelectric applications due to their flexibility and low-temperature manufacturing techniques; however, the role of ionized dopants on charge transport in these materials remains poorly understood. In this work, we use polymerized ionic liquids (PILs) as a gate dielectric in organic field-effect transistors to directly control the concentration of charges in the conducting channel. We report a method to tune the carrier concentration in the transistor channel via electrostatic gate modulation. We observe carrier concentration levels that are comparable to traditional doping methods with the added ability to precisely tune the concentration of charges induced. With this process, we aim to gather new information on the effect of ions on the performance of organic semiconductors in hopes of better understanding charge transport in conducting polymers on a molecular level.

M1.00034 Electrospun Composite Nanofibers of Semiconductive Polymers for Coaxial PN Junctions, WILLIAM SERRANO, SYLVIA THOMAS, University of South Florida at Tampa. The objective of this research is to investigate the conditions under P3HT and Activink, semiconducting polymers, form 1 dimension (1D) coaxial p-n junctions and to characterize their behavior in the presence of UV radiation and organic gases. For the first time, fabrication and characterization of semiconductor polymer single fiber coaxial arrangements will be studied. Electrospinning, a low cost, fast and reliable method, with a coaxial syringe arrangement will be used to fabricate these fibers. With the formation of fiber coaxial arrangements, there will be investigations of dimensionality crossovers e.g., from one-dimensional (1D) to two-dimensional (2D). Coaxial core/shell fibers have been realized as seen in a recent publication on an electrospun nanofiber p-n heterojunction of oxides (BiFeO₃ and TiO₂, respectively) using the electrosprining technique with hydrothermal method. In regards to organic semiconducting coaxial p-n junction nanofibers, no reported studies have been conducted, making this study fundamental and essential for organic semiconducting nano devices for flexible electronics and multi-dimensional integrated circuits.

M1.00035 A novel Graphene Oxide film: Synthesis and Dielectric properties, BETUL CANIMKURBEY, SAIT EREN SAN, Gebze Technical University, MUHAMMAD YASIN, National University of Science and Technology, MUHAMMET ERKAN KSE, Gebze Technical University. In this work, we used Hummers method to synthesize Graphene Oxide (GO) and its parallel plate impedance spectroscopic technique to investigate dielectric properties. Graphene Oxide films were coated using drop casting method on ITO substrate. To analyze film morphology, atomic force microscopy was used. Dielectric measurements of the samples were performed using impedance analyzer (HP-4194) in frequency range (100 Hz to 10MHz) at different temperatures. It was observed that the films' AC conductivity σac varied with angular frequency, ω as ωⁿ, with S<1. The electrical properties of GO showed changes depending on both frequency and temperature. We observed GO film contains direct current (DC) and Correlated Barrier Hopping (CBH) conductivity mechanisms at low and high frequency ranges, respectively. Using solution processed Graphene Oxide will provide potential for organic electronic applications through its photon absorption and transmittance capability in the visible range and excellent electrical parameters.

M1.00036 Synthesis and Characterization of Plant based Polythiophene Copolymers for Light Harvesting Applications, UDARI KODITHUWAKKU, PRASHANTHA MALAVI ARACHCHI, DILRU RATNAWEEERA, University of Sri Jayewardenepura,Sri Lanka. Polythiophenes became more attractive in diverse applications due to some of their inherent properties including thermal and environmental stability as well as optical and electronic conductive properties. Commonly thiophene monomers are obtained by byproducts of crude oils. The current study discusses for the first time the synthesis and characterization of light harvesting polythiophenes copolymers from thiophene derivatives extracted from Tagetes species. There were mainly two thiophene derivatives, 5-(3-butien-1-ynyl)-2, 2-bithienyl and 2, 2’, 5, 2”-terthiophenyl (terthiophene), in the roots of the plant. Chemical oxidative radical polymerization was followed during the synthesis of copolymers with various block compositions of plant based terthiophenes and 3-hexyl terthiophenes. Structural characterization of the synthetic products was done using FTIR, NMR, UV-vis, XRD and DSC techniques. Polythiophene homopolymers obtained from plant based terthiophenes have limited processability of solar cells due to poor solubility in common organic solvents. A significant solubility improvement was observed with copolymers having minor contributions of 3-hexylthiophenyl.

1Research Grants, University of Sri Jayewardenepura, Sri Lanka
M1.00037 Synthesis and Photoelectrochemistry Characterization of Polymer based on 4,7-Di(thiophen-2-yl)-benzo[c][1,2,5]thiadiazole, (DTBT).  LUC MARIA LAZO JIMENEZ, Instituto de Ciencias Nucleares, UNAM, MEXICO. BERNARDO ANTONIO FRONTANA-URIBE, Centro Conjunto de Investigación en Química Sustentable, CCIQS-UNAM-UAEM. — Poly[4,7-di(thiophen-2-yl)-benzo[c][1,2,5]thiadiazole], P(DTBT), is used in polymer:PCMB blends as active layer on organic photovoltaic devices, (OPV); DTBT-based polymers show well-reversible oxidation and reduction electrochemical processes. These processes indicate their high electrochemical stability suitable for n- and p-doping. This is a typical feature benzothiadiazole containing molecules. In the present study the synthesis conditions of the monomer, 4,7-di-(thiophen-2-yl)-benzo[c][1,2,5]-thiadiazole based on Stille coupling reactions has been investigated and its respective polymer P(DTBT) was prepared by repetitive potential-sweep anodic oxidation of the corresponding monomer DTBT onto Pt disk or indium tin oxide (ITO) electrodes. Electrochemical cyclic voltammetry (CV) was performed to determine the HOMO and the LUMO energy levels of the conjugated DTBT and P(DTBT), both exhibit amphoteric redox properties, n- and p- doping process. The optical gap estimated from electrochemical measurements of the polymer P(DTBT) was found to be 1.77 eV, which is close to the reported band gap (1.1-1.2eV) determined by optical absorption technique. Photoelectrochemical characterization of P(DTBT) was realized from UV-Vis-NIR spectra recorded at different applied potentials. These result are correlated with the charge-transfer phenomena in the polymers applied as active layer on OPV's.

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M1.00038 Electrospinning Nanofiber Based Organic Solar Cell, ZHENHUA YANG, YING LIU, STONY BROOK UNIVERSITY, MARIA MOFFA, CNR-Istituto Nanoscienze, CHANG-YONG NAM, Brookhaven National lab, DARIO PISIGNANO, CNR-Istituto Nanoscienze, MIRIAM RAFAILOVICH, STONY BROOK UNIVERSITY — Bulk heterojunction (BJH) polymer solar cells are an area of intense interest due to their potential to result in printable, inexpensive solar cells which can be processed onto flexible substrates. The active layer is typically spin coated from the solution of polythiophene derivatives (donor) and fullerenes (acceptor) and interconnected domains are formed because of phase separation. However, the power conversion efficiency (PCE) of BJH solar cell is restricted by the presence of unfavorable morphological features, including dead ends or isolated domains. Here we MEH-PPV:PV:PCBM electrospin nanofiber into BHJ solar cell for the active layer morphology optimization. Larger interfacial area between donor and acceptor is attained with electrospinning method and the high aspect ratio of the MEH-PPV:PV:PCBM nanofibers allow them to easily form a continuous pathway. The surface morphology is investigated with atomic force microscopy (AFM) and scanning electron microscopy (SEM). Electrospin nanofibers are discussed as a favorable structure for application in bulk-heterojunction organic solar cells.

M1.00039 Asymmetric Zinc Phthalocyanines as Dye-Sensitized Solar Cells, GULENAY TUNC, YUNUS YAVUZ, AYESGUL GUREK, BETUL CANIKMURBEY, ARIF KOSEMEN, SAIT EREN SAN, VEFA AHSEN, Gebze Technical University — Dye-sensitized solar cells (DSSCs) have received increasing attention due to their high incident to photon efficiency, easy fabrication and low production cost. Tremendous research efforts have been devoted to the development of new and efficient sensitizers suitable for practical use. In TiO2-based DSSCs, efficiencies of up to 11.4% under simulated sunlight have been obtained with rutheniumpolypyrrolid complexes. However, the main drawback of ruthenium complexes is the lack of absorption in the red region of the visible light and the high cost. For this reason, dyes with large and stable π-conjugated systems such as porphyrins and phthalocyanines are important classes of potential sensitizers for highly efficient DSSCs. Phthalocyanines (Pcs) have been widely used as sensitizers because of their improved light-harvesting properties in the far-red and near-IR spectral regions and their extraordinary robustness [1]. In this work, a series of asymmetric Zn(II) Pcs bearing a carboxylic acid group and six helixy groups either at the peripheral or non-peripheral positions have been designed and synthesized to investigate the influence of the COOH group and the positions of helixy groups on the dye-sensitized solar cell (DSSC) performance.

M1.00040 Highly conductive polymer electrolyte membranes modified with polyethylene glycolbis-carbamate, GUOPENG FU, Univ of Akron, JANELL DEMPSEY, John Carroll University, THEIN KUY, Univ of Akron — By virtue of its non-flammability and chemical stability, polyethylene glycol (PEG) networks have shown potential application in all solid-state polymer electrolyte membranes (PEM). However, room temperature ionic conductivity of these PEG based PEMs is inherently low. Plasticization of these PEMs is needed to improve the ionic conductivity. Several groups have employed this strategy to increase the ionic conductivity of the membranes. However, it is desirable to achieve plasticization without sacrificing the mechanical properties of the membrane. One way to achieve this is to incorporate low molecular weight, polyethylene glycol bis-carbamate (PEGBC) plasticizer. Here we report on plasticization of PEMs using a high molecular weight polyethylene glycol diamine and ethylene carbonate (EC). The PEGBC modified PEMs has higher ionic conductivity and a better moisture stability relative to the unmodified PEM. Moreover, PEGBC modified PEMs has a better stability relative to ethylene carbonate based liquid electrolyte with enhanced ionic conductivity.

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M1.00041 Neutron Vibrational Spectroscopy and modeling of polymer/dopant interactions, ADAM MOULE, THOMAS HARRELSON, University of California, Davis, YONGQIANG CHENG, ANIBAL RAMIREZ-CUESTA, Oak Ridge National Lab, ROLAND FALLER, University of California, Davis, DAVID HUANG, University of Adelaide, Australia — Neutron vibrational spectroscopy (VISION and ORNL) is a powerful technique to determine the configurations of organic species in amorphous samples. We apply this technique to samples of the semiconducting polymer poly(3-hexylthiophene) (P3HT) with chlorine-vaporized donor dopants. The formation of donorn-acceptor and acceptor-n-acceptor configurations outside of the crystalline domains have never been investigated. Application of density functional theory modeling using crystal field theory and for the single molecule approach yield a variety of configurations of the polymer backbone and side chains. These results demonstrate that only 1% of the volume corresponds to the assumed crystal structure solved using x-ray diffraction. In addition we report on the n- and p-doping processes of the polymer P(DTBT) and the polymer P3HT.

1 M1.00042 Single- and Multilayered Nanostructures via Laser-Induced Block Copolymer Self-Assembly, PAWEL MAJEWSKI, KEVIN YAGER, ATIKUR RAHAMAN, CHARLES BLACK, Brookhaven Natl Lab — We present a novel method of accelerated self-assembly of block copolymer thin films utilizing laser light, called Laser Zone Annealing (LZA). In our approach, steep temperature transients are induced in block copolymer films by rastering narrowly focused laser line over the light-absorbing substrate. Extremely steep temperature gradients accelerate the process of self-assembly by several orders-of-magnitude compared to conventional oven annealing, and, when coupled to photo-thermal shearing, lead to global alignment of block copolymer domains assessed by GISXAS diffraction studies and real-space SEM imaging. We demonstrate monolithic alignment of various block-copolymer thin films including PS-b-PMMA, PS-b-PEO, PS-b-P2VP, PS-b-PI and observe different responsiveness to the shearing rate depending on the characteristic relaxation timescale of the particular material. Subsequently, we use the aligned polymeric films as templates for synthesis of single- and multi-layered arrays of inorganic, metallic or semiconducting nanowires and nanomeshes and investigate their anisotropic electro-optical properties.

Research carried out in part at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.
M1.00043 Temperature dependent structural, elastic, and polar properties of ferroelectric polyvinylidene fluoride (PVDF) and trifluoroethylene (TrFE) copolymers, FU-CHANG SUN, AVINASH DONAGARE, ALEXANDRU ASARIEL, University of Connecticut, PAMIR ALPAY, University of Connecticut, SERGE NAKHMANSON, University of Connecticut, UNIVERSITY OF CONNECTICUT TEAM — We use molecular dynamics to calculate the structural, elastic, and polar properties of crystalline ferroelectric β-poly(vinylidene fluoride), PVDF (CH₂CF₂), with randomized trifluoroethylene TrFE (CH₂CF₂), as a function of TrFE content (0-50%) in the temperature range of 0-400 K. There is a very good agreement between the experimentally obtained and the computed values of the lattice parameters, thermal expansion coefficients, elastic constants, polarization, and pyroelectric coefficients. A continuous decrease in Young’s modulus with increasing TrFE content was observed and attributed to the increased intramolecular and intermolecular repulsive interactions between fluorine atoms. The computed polarization decreased slightly with temperature, but there was no significant change in the transition temperatures. Our results show that molecular dynamics can be used as a practical tool to predict the mechanical and polarization-related behavior of ferroelectric poly(vinylidene fluoride). Such an atomic model can thus serve as a guide for practical applications of this important multifunctional polymer.

M1.00044 Understanding Nonlinear Dielectric Properties in a Biaxially Oriented Poly(vinylidene fluoride) Film at Both Low and High Electric Fields, YUE LI, College of Polymer Science and Engineering, Sichuan University, LEI ZHU, Department of Macromolecular Science and Engineering, Case Western Reserve University, CASE WESTERN RESERVE UNIVERSITY TEAM, SICHUAN UNIVERSITY TEAM — Understanding nonlinear dielectric behavior in polar polymers is crucial to their potential application as next generation high energy density and low loss dielectrics. In this work, we studied nonlinear dielectric properties of a biaxially oriented poly(vinylidene fluoride) (BOPVDF) film under both low and high electric fields. It was observed that the low-field dielectric nonlinearity for the BOPVDF disappeared above 10 Hz at room temperature, suggesting that the low-field dielectric nonlinearity originated from ionic migration of impurity ions rather than dipolar relaxation of the amorphous segments. Above the coercive field (EC ~70 MV/m), bipolar dielectric displacement-electric field (D-E) loop tests were used to extract the nonlinear behavior for pure PVDF crystals, which had a clear origin of ferroelectric switching of polar crystalline dipoles and domains and nonpolar-to-polar (α → δ → β) phase transformations. Using HVBDS, it was observed that the ferroelectric switching of polar crystalline dipoles and domains in BOPVDF above the EC always took place between 20 and 500 Hz, regardless of a broad range of temperature from -30 to 100 °C. This behavior was drastically different from the amorphous PVDF dipoles, which had a strong dependence on frequency over orders of magnitude.

M1.00045 Correlating Thin-Film Radical Density with Charge Transport in Open-Shell Conducting Macromolecules, MARTHA HAY, ELIZABETH JERGENS, BRYAN BOUDOURIS, Purdue University — Within the class of radical polymers, stable open-shell species serve as the medium for charge transport by undergoing oxidation-reduction (redox) reactions. The kinetics of these reactions is rapid enough that they are not considered rate-limiting in the electronic interactions of these materials. Rather, the proximity of these radical sites is paramount as a synthetic handle. Unfortunately, controlling the density of radicals has proven challenging in radical polymer systems. Often radical functionality is imparted to a polymer, rather than polymerizing a radical-containing monomer unit. This can prove troublesome as longer reaction times, in the interest of higher functionality, can lead to the elimination of radicals. Thus, the consequential altering of the radical electronic interactions is not well understood. We have synthesized a series of polymer monomers with controlled radical densities such that the radical density was preserved from monomer to polymer synthesis. As such, we attribute any change in the macroscopic transport properties to a change in the spacing between radical sites. These results elucidate the role of radical site distribution on the electronic performance of nitroxide-based radical polymers.

M1.00046 Polyvinylidene fluoride molecules in nanofibers, imaged at atomic scale by aberration corrected electron microscopy, DARRELL RENEKER, JOSEPH GORSE, DINESH LOLLA, The University of Akron, CHRISTIAN KISIELOWSKI, Lawrence Berkeley National Laboratory, JIAYUAN MIAO, PHILIP TAYLOR, Case Western Reserve University, GEORGE CHASE, The University of Akron — Atomic scale features of polyvinylidene fluoride molecules (PVDF) were observed. Electron micrographs of thin, self-supporting PVDF nanofibers showed conformations and relative locations of atoms in segments of polymer molecules. Rows of CF₂ atomic groups, at 0.25 nm intervals, marked the paths of segments of the PVDF molecules. The fact that an electron microscope image of a segment of a PVDF molecule depended upon the particular azimuthal direction, along which the segment was viewed, enabled observation of twist around the molecular axis. The 0.2 nm side-by-side distance between the two fluorine atoms attached to the same carbon atom was clearly resolved. Morphological and chemical changes produced by energetic electrons, ranging from no change to fiber scission, over many orders of magnitude of electrons per unit area, provide quantitative new insights into radiation chemistry. Relative movements of segments of molecules were observed. Synergism between high resolution electron micrographs and images created by molecular dynamic modeling was demonstrated. This paper is at the threshold of growing usefulness of electron microscopy to the science and engineering of polymer and other molecules.

M1.00047 Design of Free-Standing Microstructured Conducting Polymer Films for Enhanced Particle Removal from Non-uniform Surfaces, JENNIFER LASTER, NICHOLAS DEOM, BRYAN BOUDOURIS, STEPHEN BEAUDOIN, Purdue University — Particle removal from surfaces is important for a wide range of industrial applications (e.g., microelectronics fabrication). One of the main forces of particle adhesion to a surface is the van der Waals attraction force, which will be the focus of this effort. The surface features of interacting bodies can play a controlling role in the adhesion of particles by increasing or decreasing the amount of mass within the range of strong van der Waals forces. In order to control these interactions, specific geometries can be designed in order to manipulate the micro- and nanostructure of a material, which can conform to the features of a corresponding substrate increasing the overall contact area between the two surfaces. In this work, microstructured films of the conducting polymer polypyrrole (PPy) were synthesized through template-assisted electropolymerization techniques. The removal of fluorescently-labeled polystyrene beads from aluminum surfaces of varying roughness was measured and compared for microstructured and flat PPy films. The microstructured films were found to have an overall increase in the amount of particles removed from the aluminum surfaces; this demonstrates the ability to manipulate particle adhesion through advanced nanostructured polymer templating.

M1.00048 Out-of-plane Block Copolymer Microdomains in High Aspect-Ratio Templates, KARIM GADELRAB, WUBIN BAI, ALFREDO ALEXANDER-KATZ, CAROLINE ROSS, Massachusetts Inst of Tech-MIT — Directed self-assembly DSA of block copolymers BCP proved to be a power approach for nanoscale fabrication. In addition, BCP with highly incompatible blocks (high Flory-Huggins interaction parameter χ) offer improvement in resolution of the BCP patterns. Unfortunately, high-χ BCPs usually exhibit large differences in surface affinity between the two blocks, forming a surface layer of the lower surface energy block and favoring in-plane orientation of lamellae or cylindrical microdomains. Here, we explore the conditions under which a high χ BCP creates an out-of-plane lamellar structure using high aspect ratio trenches with preferential walls. We employ self-consistent field theory SCFT and single mode expansion of Ginzburg-Landau free energy expression in the weak segregation limit to analytically construct a phase diagram and attribute to the out-of-plane lamellar microdomain structure. It is found that the transition from the in-plane lamellar structure necessitates a coupling between aspect ratio and surface functionality. In particular, strong side wall attraction results in out-of-plane lamellae when the trench aspect ratio is greater than unity. The results are validated for a polystyrene-block-polydimethylsiloxane (PS-b-PDMS) system within trenches made using interference lithography.

1 This work is supported by NSF(DMR-1402733)

2 Support from Coalescence Filtration Nanofiber Consortium and from the Office of Basic Energy Sciences Contract No. DE-AC02-05CH11231

3 This work is supported by NSF(DMR-1402733)
M1.00049 Vertically Aligned Nanoplate Particles Directed by Block Copolymer Domains for Anisotropic Properties, NADIA KROOK, University of Pennsylvania, JEFFREY METH, DuPont, CHRISTOPHER MURRAY, ROBERT RIGGLEMAN, RUSSELL COMPOSTO, University of Pennsylvania — During common processing methods, anisotropic fillers in polymer nanocomposites align in the direction of flow, parallel to the surfaces, thus enhancing properties in the plane of the substrate. This research aims to create thin film nanocomposites with perpendicularly aligned anisotropic particles to improve properties in the out-of-plane direction. The demonstrated work explores vertical orientation of rare-earth fluoride nanofibres in lamellar-forming polystyrene (PS) to establish a platform that controls the alignment of any planar particle. Currently, gadolinium fluoride (GdF3) rhombus nanoparticles with the longest and shortest diagonal dimensions of ~30 nm and ~25 nm, respectively, have been specially synthesized with the potential to intercalate the block copolymer (BCP) domains. By employing a ternary brush blend to neutralize silicon substrates to both BCP domains, vertical nanofibre orientation has been enabled with an optimum film thickness of ~110 nm. The GdF3 surfaces are chemically modified to drive the plates to a specific BCP domain. After surface modification, the dispersion of GdF3 in homopolymer will first be shown followed by morphology results from integrating GdF3 into the BCP using scanning and transmission electron microscopy.

M1.00050 The role of ultra-fast solvent vapor annealing on the directed self-assembly of block polymer thin films, CHLOE DRAPES, G. NELSON, M. GRANT, J. WONG, A. BARUTH, Creighton University — The directed self-assembly of nano-structures in block polymer thin films via solvent vapor annealing is complicated by several factors, including evaporation rate. Solvent vapor annealing exposes a disordered film to solvent(s) in the vapor phase, increasing mobility and tuning surface energy, with the intention of producing an ordered structure. Recent theoretical predictions reveal the solvent evaporation affects the resultant nano-structuring. In a competition between phase separation and kinetic trapping during drying, faster solvent removal can enhance the propagation of a given morphology into the bulk of the thin film down to the substrate. Recent construction of a purpose-built, computer controlled solvent vapor annealing chamber provides control over forced solvent evaporation down to 15 ms. This is accomplished using a pneumatically actuated nitrogen flow into and out of the chamber. Furthermore, in situ spectral reflectance, with 10 ms temporal resolution, monitors the swelling and evaporation. Presently, cylinder-forming polystyrene-block-polylactide thin films were swollen with 40% (by volume) tetrahydrofuran, followed by immediate evaporation under a variety of designed conditions. This includes various evaporation times, ranging from 15 ms to several seconds, and four unique rate trajectories, including linear, exponential, and combinations. Atomic force microscopy reveals specific surface, free and substrate, morphologies of the resultant films, dependent on specific evaporation conditions. Funded by the Clare Boothe Luce Foundation and Nebraska EPSCoR.

M1.00051 Towards ultra-fast solvent vapor annealing, the development of a computer controlled solvent vapor annealing chamber, GUNNAR NELSON, J. WONG, C. DRAPES, M. GRANT, A. BARUTH, Creighton Univ, Omaha, NE — Despite the promise of fast and cheap nanoscale ordering of block polymer thin films via solvent vapor annealing, a standardized, scalable production scheme remains elusive. Solvent vapor annealing exposes a nano-thin film to the vapors of one or more solvents with the goal of forming a swollen and mobile state to direct the self-assembly process by tuning surface energies and mediating unfavorable chain interactions. We have shown that optimized annealing conditions, where kinetic and thermal properties for crystal growth are extremely fast (<1s), exist at solvent concentrations just below the order-disorder transition of the film. However, when investigating the propagation of a given morphology into the bulk of a film during drying, the role of solvent evaporation comes under great scrutiny. During this process, the film undergoes a competition between two fronts; phase separation and kinetic trapping. Recent results in both theory and experiment point toward this critical element in controlling the resultant morphologies; however, no current method includes a controllable solvent evaporation rate at ultra-fast time scales. We report on a computer-controlled, pneumatically actuated chamber that provides control over solvent evaporation down to 15 ms. Furthermore, in situ spectral reflectance monitors solvent concentration with 10 ms temporal resolution and reveals several possible evaporation trajectories, ranging from linear to exponential to logarithmic. Funded by Dr. Randolph Ferlic Summer Research Scholarship and NASA Nebraska Space Grant.

M1.00052 Directed Self-Assembly of Block Copolymers in Thin Films on Polymer Nano-Stripes, DONG-EUN LEE, HO-JONG KANG, DONG HYUN LEE, Dankook University, NANO FUNCTIONAL MATERIALS LAB. TEAM — In this study, we report directed self-assembly (DSA) of block copolymers in thin films on nano-stripes of polymers. Unique nano-stripes of poly(tetrafluoro ethylene) (PTFE) having ~20 nm of amplitude and ~200 nm of pitch were simply generated by physically rubbing a PTFE bar on various substrates like Si wafers, glass, and polyimide due to its low friction coefficient and high wear rate. The resulting nano-stripes were extremely oriented along the rubbing direction. Then, various asymmetric polystyrene-block-poly(2-vinylpyridine) copolymers (PS-b-P2VP) were directly self-assembled on the nano-stripes of PTFE by solvent-annealing in vapor of tetrahydrofuran (THF). As a result, PS-b-P2VP exhibited extremely ordered P2VP cylinders oriented normal to the surface in large area on the underlying nano-stripes of PTFE. In addition, as utilizing the BCPs as templates, hexagonal arrays of metal nanoparticles were generated in large area for further application. BCP thin films and arrays of metal nanoparticles were characterized by atomic force microscopy (AFM) and scanning electron microscopy (SEM).

M1.00053 Perpendicular Orientation of Nanodomains on Versatile Substrates through Self-Neutralization Induced by Star-Shaped Block Copolymers, MOOSEONG KIM, SANGSHIN JANG, KYU SEONG LEE, HONG CHUL MOON, JONGHEON KWAK, JICHEOL PARK, GUMHYE JON, JIN KON KIM, POSTECH — A novel self-neutralization concept is introduced by designing molecular architecture of a block copolymer. Star-shaped 18 arm poly(methyl methacrylate)-block-polystyrene copolymers ((PMMA-b-PS)18) exhibiting lamellar and PMMA cylindrical nanodomains are synthesized. When a thin film of (PMMA-b-PS)18 is spin-coated on a substrate, vertically aligned lamellar and cylindrical nanodomains are obtained without any pre- or post-treatment, although thermal annealing for a short time (less than 30 min) is required to improve the spatial array of vertically aligned nanodomains. This result is attributed to the star-shaped molecular architecture that overcomes the difference in the surface affinity between PS and PMMA chains. Moreover, vertical orientations are observed on versatile substrates, for instance, semiconductor (Si, SiOx), metal (Au), PS or PMMA-brushed substrate, and a flexible polymer sheet of polyethylene naphthalate.

M1.00054 The morphology of A2B miktoarm polymer in thin film, HYEYOUNG KIM, Univ of Mass - Amherst, BEOM-GOO KANG, University of Tennessee, ZHIWEI SUN, JAEWON CHOI, THOMAS RUSSELL, Univ of Mass - Amherst — The morphologies of A2B mikto-arm polymer consisted of poly(2-vinyl pyridine) and polystyrene ((P2VP)2PS) in thin film were examined. Solvent vapor annealing produces films with lamellae perpendicular to the substrate within a very short time. The change in the morphology for different periods of time, corresponding to different swelling ratios was observed by grazing incidence small angle x-ray scattering and scanning force microscopy. This morphology showed the smaller height difference between PS and P2VP microdomains, when compared to the corresponding diblock copolymer. We also observed the long-range ordering formed on the saw-tooth pattern. Thermal annealing, on the other hand, resulted in the lamellae being oriented parallel to the substrate, where unusual behavior was depending on the film thickness and surface energy of substrate.
M1.00055 Simple, generalizable route to highly aligned block copolymer thin films. ZHE QIANG, KEVIN CAVICCHI, BRYAN VOGT, University of Akron, UNIVERSITY OF AKRON TEAM — Macroscopic alignment of block copolymer domains in thin films is desired for many applications, such as cell responsive surfaces or optical polarizers. Alignment generally requires specialized tools that apply external fields, shear force gradient, or produce topological patterned substrates. This requirement limits the broad academic application of aligned BCPS. Here, we describe a simple modification of commonly used solvent vapor annealing (SVA) process for macroscopic alignment of BCPS. Adhering a flat, crosslinked elastomer pad to the BCP film leads to differential swelling between the elastomer pad and BCP to produce a shear force that aligns the ordered BCP domains. The role of elastomer properties, solvent quality, drying rate and degree of segregation of the block copolymer will be discussed to provide generalized rules for alignment with this technique. Cylindrical nanostructures formed in polystyrene-block-polydimethylsiloxane can be transformed into arrays of silica lines and increasing the thickness from a monolayer to bilayer can effectively halt the spacing of the lines. These results illustrate a generalized method for BCP alignment and potential route for the generation of complex hierarchical assembled structures.

M1.00056 Sulfation effect on levan polysaccharide chains structure with molecular dynamics simulations. BINNAZ COSKUNKAN, Yeditepe University, DENIZ TURGUT, DENIZ RENDE, Rensselaer Polytechnic Institute, SEYDA MALTA, Yeditepe University, NIHAT BAYSAL, RAHMI OZISIK, Rensselaer Polytechnic Institute, EBRU TOKSOY-ONER, Marmara University — Diversity in conformations and structural heterogeneity may make polysaccharides the most challenging biopolymer type for experimental and theoretical characterization studies. Levan is a biopolymer chain that consists of fructose rings with β-(2-6) linkages. It is a glycan that has great potential as a functional biopolymer in foods, feeds, cosmetics, pharmaceutical and chemical industries. Sulfated polysaccharides are group of macromolecules with sulfated groups in their hydroxyl parts with a range of important biological properties. Sulfate groups and their positions have a major effect on anticoagulant activity. It is expected that sulfate modified levan has anticoagulant activity such as heparin. In the current study, the effect of sulfation on the structure and dynamics of unmodified and sulfate modified levan are investigated via fully atomistic Molecular Dynamics simulations in aqueous media and varying salt concentrations at 310 K.

M1.00057 The Effects of pH and Temperature on the Nanostructure of Chitosan Films. RAMONA LUNA, AHMED TOUHAMI, University of Texas Rio Grande Valley — Developing a method that can mimic tissue-like environment for cell cultures and molecular studies can help reduce the loss of some cell functions that occur when investigations are performed in vitro. Of particular interest is chitosan (CS): abundant and renewable biopolymer that is also biodegradable and non-toxic. The present study focuses on synthesizing CS films under various conditions and for multiple applications. We are using several techniques to characterize the physicochemical properties of the synthesized films. The contact angle technique is used to determine the hydrophobicity, hydrophilicity, and the surface free energy. The atomic force microscopy is used to determine the nanostructure, and nanomechanical properties. Here we specifically investigated the effect of the pH and the temperature on the nanostructure of the CS films. AFM images showed remarkable changes in the surface nanostructures that increase the roughness of the films when the pH of the solution increases. However, the surface free energy of these films has not shown any significant changes with the pH. By investigating the properties of these films, the needed biomaterial platform for a specific biological system can be designed and manipulated to increase its performance and lifetime.

M1.00058 Characterization of Nanoparticle Aggregation in Biologically Relevant Fluids. KATHLEEN MCENNIS, JOERC LAHANN, University of Michigan — Nanoparticles (NPs) are often studied as drug delivery vehicles, but little is known about their behavior in blood once injected into animal models. If the NPs aggregate in blood, they will be shunted to the liver or spleen instead of reaching the intended target. The use of animals for these experiments is costly and raises ethical questions. Typically dynamic light scattering (DLS) is used to analyze aggregation behavior, but DLS cannot be used because the components of blood also scatter light. As an alternative, a method of analyzing NPs in biologically relevant fluids such as blood plasma has been developed using nanoparticle tracking analysis (NTA) with fluorescent filters. In this work, NTA was used to analyze the aggregation behavior of fluorescent polystyrene NPs with different surface modifications in blood plasma. It was expected that different surface chemistries on the particles will change the aggregation behavior. The effect of the surface modifications was investigated by quantifying the percentage of NPs in aggregates with this technique. Cylindrical nanostructures formed in polystyrene-block-polydimethylsiloxane can be transformed into arrays of silica lines and increasing the thickness from a monolayer to bilayer can effectively halt the spacing of the lines. These results illustrate a generalized method for BCP alignment and potential route for the generation of complex hierarchical assembled structures.

M1.00059 Ring Structure of Center of Spacetime, DNA, and Extraterrestrial Being. DAYONG CAO, AEAA — There is a balance of the flat universe between the stellar matter and the dark massenergy (include dark matter and dark energy) which make of dark hole which has the center of the spacetime. The Einstein’s equation has the other formula of the structure of the center of spacetime. There are also balance system between the solar system and its companion dark hole, and between the Milky-Way galaxy and its center of the huge dark hole. The model of stellar matter can explain of the structure of molecule by electromagnetic interaction (of the spacetime effect). The ring structure both the nucleic acid and protein is like the structure of the center of the spacetime. It produced by an interaction of double helix between dark massenergy and stellar matter when the companion dark hole of sun seasonal impacted near solar system, and took dark comets and dark massenergy on the earth, and made extinction while they were producing new DNA of lives, broke the old one to the petroleum, natural gas, and coal. DNA of extraterrestrial being who live on system of the companion dark hole with the double helix. A new big extinction is coming for human being and extraterrestrial being.

M1.00060 Coacervate Core Micelles for the Dispersion and Stabilization of Organophosphate Hydrolyase in Organic Solvents. CAROLYN MILLS, ALLIE OBERMEYER, XUEHUI DONG, BRADLEY D. OLSEN, Massachusetts Institute of Technology — Bulk organophosphate (OP) nerve agents are difficult to decontaminate on site and dangerous to transport. The organophosphate hydrolyase (OPH) enzyme is a efficient catalyst for hydrolyzing, and thus decontaminating, these compounds, but suffers from poor stability in the hydrophobic bulk OP environment. Here, we exploit the complex coacervation phase separation phenomenon to form complex coacervate core micelles (C3Ms) that can protect this OPH enzyme under these conditions. Stable C3Ms form when mixing a charged-neutral block copolymer methyl-quinaternized poly(4-vinylpyridine)-block-poly(oligo(ethylene glycol) methacrylate) (Q4vp-b-POEGMA), a homopolymer poly(acrylic acid) (PAA), and OPH under a certain conditions. The C3Ms are then transferred into two organic solvents, ethanol and dimethyl methylphosphonate (DMMP), which is a good simulant for the physical properties of the OP compounds. The C3Ms retain their nanostructures in the organic solvents. The activity test of OPH indicates that the C3Ms successfully protect OPH activity in organic solvents.

1A generalized method for block copolymer thin film alignment: solvent vapor annealing with shear.

1Supported by: NSF and MBRS RISE Program.

1This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730.
M1.00061 Fluorescence Recovery after Photobleaching in Confined Polymer Thin Films , LAURA A. G. GRAY, CLIFFORD P. BRANGWYNNE, RODNEY D. PRIESTLEY, Princeton Univ, Dept. of Chemical and Biological Engineering — Over the past twenty years many studies have shown a reduction in the glass transition temperature (Tg) of thin polymer films confined on the nanoscale when supported on non-adsorbative substrates or free-standing. The depth dependence of Tg has been measured using thin layers of fluorescently tagged polymer to localize the dye within a larger polymer film stack, revealing a decrease in local Tg tens of nanometers into the film. These results have been explained by the propagation of enhanced mobility from the free-surface into the film. Atomic force microscopy measurements of molecular mobility have been made in confined polymer systems. Here, we present the results of fluorescence recovery after photobleaching (FRAP) experiments investigating the mobility of fluorescently doped and labeled methacrylate-based polymers confined in thin film geometries. Bleaching and recovery was monitored using a laser-scanning confocal microscope that enabled us to bleach arbitrary micron-sized shapes to monitor diffusion in polymer melts.

M1.00062 Using Atomic Molecular Dynamics Simulations to Guide Development of Coarse-Grained Models of Polyethylene glycol (PEG), Elastic-like peptides (ELP) and Collagen-like peptides (CMP) For Biomaterial Design . FRANCESCA STANZIONE, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716, ARTHI JAYARAMAN, Department of Chemical and Biomolecular Engineering, Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716. — Molecular dynamics (MD) is a well established technique to study the structure and dynamics of biomolecular systems. While atomistic simulations maintain chemical details, they are computationally intensive, thus limiting the accessible time, the length scales and the sampling. To overcome these limitations, coarse-grained (CG) models have proven to be successful in reproducing experimentally relevant length and time scales with reasonable computational expense. CG models can be developed to be phenomenological by effectively reproducing experimental results or can be developed by mapping rigorously to structural information provided by atomistic MD simulations. The latter method is recommended for biomolecules and biomaterials since atomistic simulations capture the detailed effect of the medium on interactions that affect the structure, dynamics and functional properties of the biomolecules, and that can be programmed into the CG models. In this poster we highlight three different cases where atomistic MD simulations provide such essential information to guide CG models: Polyethylene glycol, Elastic-like peptides and Collagen-like peptides based biomaterials.

M1.00063 The influence of ionic strength on DNA diffusion in gel networks , YUANXI FU, AH-YOUNG JEE, HYEONG-JU KIM, STEVE GRANICK, Institute for Basic Science — Cations are known to reduce the rigidity of the DNA molecules by screening the negative charge along the sugar phosphate backbone. This was established by optical tweezer pulling experiment of immobilized DNA strands. However, little is known regarding the effect of cations on the motion of ions in DNA. We have studied in real time the Brownian diffusion of fluorescent labeled lambda-DNA in an agarose gel network in the presence of salt with monovalent or multivalent cations. Each movie was analyzed using home-written program to yield a trajectory of center of the mass and the accompanying history of the shape fluctuations. Some preliminary findings is that ionic strength has a profound influence on the slope of the trace of mean square displacement (MSD) versus time.

M1.00064 Active microrheology of entangled blends of DNA and Actin link polymer flexibility to induced molecular deformations and stress propagation , ROBERT FITZPATRICK, RAE ROBERTSON-ANDERSON, University of San Diego, ANDERSON RESEARCH TEAM — Actin is a ubiquitous structural protein in the cytoskeleton that gives cells shape and rigidity, and plays important roles in mechanical processes such as cell motility and division. Actins diverse roles stem from its ability to polymerize into semiflexible filaments that are less than one persistence length (17 m) in length, and form entangled networks that display unique viscoelastic properties. We previously found that entangled actin networks propagate microscale forces over several persistence lengths (£60 m) and takes minutes to relax. DNA, oppositely, has thousands of persistence lengths (50 nm) per chain, exhibits minimal force propagation, and takes only seconds to re-equilibrate. To directly determine the role of flexibility in mechanical response and force propagation of entangled networks, we use optical tweezers and fluorescence microscopy to investigate blends of actin and DNA. We use optically driven microspheres to perturb the network far from equilibrium and measure the force the network creates in response to the induced force. We simultaneously track partially labeled actin filaments during the perturbation and subsequent relaxation period. We characterize filament deformation and show explicitly how induced microscale forces propagate through the network.

M1.00065 Deep image analysis of entangled ring-shaped DNA . HYEONG-JU KIM, AH-YOUNG JEE, STEVE GRANICK, Institute for Basic Science — Ring-shaped DNA entangled in aqueous actin networks and observed by super-resolution microscopy (STED; stimulated emission depletion) offers rich data for comparison with unresolved questions of polymer physics. Using home-written software, we calculated not only the center of mass (CoM) and CoM trajectories of hundreds of molecules, but also analyzed conformation dynamics with statistical analysis including wavelet transformation and a correlation matrix approach. The analysis reveals some surprising aspects unanticipated by classical theories.

M1.00066 Quantifying the effects of cyclic defects on the mechanical properties of polymer gels , RUI WANG, MINGJIANG ZHONG, KEN KAWAMOTO, JEREMIAH JOHNSON, BRADLEY OLSEN, Massachusetts Institute of Technology — Understanding the correlation between the topology and properties of polymer gels is an outstanding challenge in polymer science. Classical theories of gel elasticity assume acyclic tree-like network topology; however, all polymer gels inevitably possess cyclic defects: loops that have profound, yet previously unpredictable, effect on gel properties. Here, we develop a modified phantom network theory that describes the effects of loops on the modulus of polymer gels. We demonstrate that small loops (primary and secondary loops) have vital effect on the modulus; whereas this negative impact decreases rapidly as the loop order increases, especially for networks with higher junction functionalities. Loop effect is non-local, which can propagate to its neighborhood strands. We show that adjacent loops weaken the network cooperatively, resulting in the nonlinear decrease of the dimensionless modulus (G/kT, where v is the total density of polymer strands) with the loop fraction. The theory is in good agreement with the experimental data without any fitting parameters.

M1.00067 Degrafting of polymer brushes from substrates enables insight about the brush structure and facilitates surface patterning . ROHAN PATIL, North Carolina State Univ, SALOMON TURGMAN-COHEN, Kettering University, JIRI SROGL, North Carolina State Univ, DOUGLAS KISEROW, US Army Research Office, JAN GENZER, North Carolina State Univ — Polymers end-grafted to surfaces or interfaces, commonly referred to as polymer brushes, enable tailoring physico-chemical properties of material surfaces. Many applications of polymer brushes require information about the molecular weight (MW) and grafting density (GD) of polymer brushes. For brushes synthesized by surface initiated polymerization (SIP) determining these attributes was always a challenge. We have developed a simple method of measuring MW and GD of these systems by degrading SIP from silica-based surfaces by using tetrabutyl ammonium fluoride (TBAF), which attacks selectively Si-O bonds and enables complete degrading of polymer (methyl methacrylate) (PMMA) brushes from silica based substrates without damaging the backbone. The rate of PMMA degrading decreases with reaction time and depends on the concentration of TBAF, temperature, and the initial GD of the system. The molecular weight distribution of the degraded PMMA was measured using size exclusion chromatography. The GD was calculated from known MW and dry thickness of the PMMA brush. Spatial patterns of degraded regions on the substrate can be prepared by either localizing the TBAF to certain regions or by gradually immersing homogeneous samples into TBAF solution.
M1.00068 Driving Organic Molecule Crystallization with Surface Reconstructions

JESSICA BICKEI, GIANFRANCO TROVATO, Cleveland State University — This work examines how surface reconstructions can drive crystallization of organic molecules via self-assembly. Organic electronic molecules have low conductivities compared to inorganic materials, but crystallizing these polymers increases their conductivity. This project uses surface reconstructions with periodically repeating topographies to drive the crystallization process. The samples are grown by placing a drop of a dilute PEDOT solution on the clean Si(001)-(2x1) or Si(111)-(7x7) surface reconstruction and heating the surface up to both evaporate the solvent and promote diffusion of the polymer to the thermodynamically defined lowest energy position. The resulting samples are characterized by scanning tunneling microscopy (STM) with respect to their crystallinity and electronic properties. Of particular interest is whether there is a preferential location for the PEDOT molecule to adsorb and whether there are any conformational changes upon adsorption that modify the HOMO-LUMO gap. This work is being done in a new pan-style RHK-STM enclosed in a glovebox at Cleveland State University. The glovebox has O2 and H2O levels of less than 1ppm. This allows for sample preparation and imaging in a controlled environment that is free from contamination.

M1.00069 The Study of Interpenetration Length between dPS Films and PS-grafted Layers

HOYEON LEE, SEONGJUN JO, Yonsei University, TOYOAKI HIRATA, Kyushu University, NORIFUMI L. YAMADA, J-PARC, KEIJI TANAKA, Kyushu University, DU YEOL RYU1, Yonsei University — In polymer thin film system, the type of interfacial interaction is a critical parameter to determining the thermal and physical properties of polymer films. Interestingly, the interfacial energy of grafted substrates with polymer chains is remarkably altered by simply controlling grafting density, which has been referred to as autophobicity. In this study, we investigated the interpenetrating interfaces between deuterated polysyrene (dPS) and grafted substrates with the same chemical identity. PS-grafted substrates were prepared using a grafting-to approach with hydroxyl end-functionalized polystyrene (PSOH) in a dry brush regime, where the brush thickness and grafting density were determined based on the chain length (or molecular weight, Mw) of PSOHs. The interpenetration lengths (ξ) at interfaces between dPS and PS-grafted layers were characterized using neutron reflectivity (NR) measurements (performed at the SOFIA beam-line at J-PARC, Japan).

M1.00070 Glass transition dynamics and charge carrier mobility in conjugated polyfluorene thin films

HUI QIN, DAN LIU, TAO WANG, Wuhan University of Technology — Conjugated polymers are commonly used in organic optoelectronic devices, e.g. organic photovoltaics (OPVs), light-emitting diodes (LEDs) and field effect transistors (FETs). In these devices, the conjugated polymers are prepared as thin films with thicknesses in the range of tens to hundreds of nanometers, and are interfaced with different function layers made from organic or inorganic materials. We have studied the glass transition temperature (Tg) of poly(9, 9-dioctylfluorene)-co-N-(1, 4-butylphenyl)diphenylamine) (TFB) thin films supported on different substrates, as well as their SCLC charge carrier mobility in photodiodes. Both Monotonotic and non-monotonotic Tg deviations are observed in TFB thin films supported on Si/SiOx and PEDOT-PSS, respectively. With low to moderate thermal crosslinking, the thickness dependent Tg deviation still exists, which diminishes in TFB films with a high crosslinking degree. The vertical charge carrier mobility of TFB thin films extracted from the SCLC measurements is found increase with film thickness, a value increases from 1 to 50 x 10-6 cm2 V-1 s-1 in the thickness range from 15 to 180 nm. Crosslinking was found to reduce the carrier mobility, while the mobility increase with the film thickness. The Tg deviations are also discussed using the classic layered models in the literature. Our results provide a precise guide for the fabrication and design of high performance optoelectronic devices.

M1.00071 Bending and Fracture in Thin Polymer Films during Capillary Origami Assembly

TIMOTHY TWOHIG, ANDREW CROLL, North Dakota State Univ — Capillary origami uses liquid tension to bend thin films into useful shapes and structures. The ability to scale this process to the microscopic range has led to growing interest in capillary origami and many potential applications. Clearly, the creation of three dimensional structures from flat sheets depends deeply on a combination of properties: fluid tensions, film thickness, film modulus and importantly the films fracture properties. In fractions and film modulus and importantly the films fracture properties. Fractures in a film are a critical component of macroscopic origami but macroscopic methods for creating these fractures are not possible at the microscopic scale. We present an experimental investigation of the interplay of capillary forces and material properties in the creation of controlled fractures in thin polymer films. Specifically, we use capillary forces to lift and bend a thin polymer film to the point of fracture using a variety of film thicknesses and material properties and attempt to model the basic underlying physics. We observe the creation of delaminations and fractures at pre-determined sites that can be tailored to specific shapes to be utilized in capillary origami.

M1.00072 Confinement Effect on the Effective Viscosity of Plasticized Polymer Films1

FEI CHEN, D. PENG, Boston University Physics Department, Y. OGATA, K. TANAKA, Kyushu University Department of Applied Chemistry, Z. YANG, Soochow University Department of Polymer Science and Engineering, Y. FUJII, National Institute for Materials Science (Japan), C. H. LAM, Hong Kong Polytechnic University Department of Applied Physics, OPHELIA K. C. TSUI, Boston University Physics Department — We have measured the effective viscosity of polystyrene films with a small (4 wt%) added amount of dioctyl phthalate (DOP) deposited on silica. A broad range of molecular weights, Mw, from 13.7 to 2,100 kg/mol was investigated. Our result shows that the thin films with Mw <100 kg/mol, the addition of DOP causes the effective viscosity to decrease by a factor of 4, independent of Mw. But for the higher Mw films, the effective viscosity of the DOP added films creeps towards that of the neat films with increasing Mw. A model assuming the effective viscosity to be dominated by enhanced surface mobility for the lower Mw films, but surface-promoted interfacial slippage for the higher Mw films is able to account for the experimental observations.

1 We are grateful to the support of National Science Foundation through the project DMR-1310536.

M1.00073 Adhesion and Wetting in Soft Polymeric Systems

ANDREY DOBRYNIN, ZHEN CAO, Univ of Akron, MARK STEVENS, Sandia National Laboratories — We have developed a generalized model of particle/surface interactions describing adhesion and wetting phenomena. We show that for an elastic nanoparticle with radius Rp and shear modulus Gp interacting with an elastic substrate having shear modulus Gs the crossover between adhesion and wetting-like behavior is determined by a dimensionless parameter β = Gp/Rp−2/3Γ−1/3. In the limit of small values of the parameter β <1, our model reproduces JKR model for particle adhesion on elastic substrates (adhesion regime). However, in the opposite limit, β>1, the capillary forces play a dominant role and determine particle/substrate interactions (wetting regime). We extended our approach to describe the detachment of rigid nanoparticles from elastic surfaces. Simulation results confirm that the detachment force, f∗, depends on a dimensionless parameter δ = Gs/Rp−2/3, which corresponds to the ratio of the surface energy of the neck and the substrate elastic energy. In the case when δ <1, the critical detachment force approaches a critical value calculated in the framework of the JKR model, f∗ = 1.5πWp/Rp (JKR regime). However, in the opposite limit, the critical detachment force scales as f∗ Ω Gp/3<1/3 Gs 1/2, which corresponds to the necking regime. All simulation data can be described by a crossover function

f∗ Ω Gp/3<1/3 Gs 1/2, with a critical exponent

1 NSF DMR-1409710
M1.00074 Novel adhesion properties of irreversibly adsorbed polymer chains. ZHIZHAO CHEN, MANI SEN, JUSTIN CHEUNG, DEBORAH BARKLEY, NAISHENG JIANG, WENDUO ZENG, MAYA K. ENDÖH, TADANORI KOGA, Stony Brook University — The stability of thin polymer films on solids is of vital interest in traditional technologies and in new emerging nanotechnologies. We recently found that nanoscale structures of polymer chains adsorbed onto a silicon (Si) substrate (“adsorbed nanolayers”) play a crucial role in the thermal stability of the film. To understand the adhesion mechanism at the adsorbed polymer-free polymer interface, we mimicked the interface by preparing bilayers where a 200 nm-thick polymer film and an adsorbed nanolayer, both prepared on Si, were pressed together at high temperature. The bilayers were then subjected to an adhesion test by measuring the critical normal force required to separate the two films. Polystyrene was used as a model. The results are intriguing as they show an absence of adhesion between the “flattened” adsorbed chains, which lie flat on the solid, and the chemically identical free chains. On the other hand, the “loosely adsorbed” polymer chains, which are formed as a result of limited adsorption space on the solid surface, do display a degree of adhesion with the bulk polymer. We postulate that the loosely adsorbed chains act as “connectors” which promote adhesion effectively across the solid-polymer interface.

³We acknowledge the financial support from NSF Grant No. CMMI-1332499.

M1.00075 Entropic Segregation of Short Polymers to the Surface of a Polydisperse Blend. PENDAR MAHMOUDI, MARK MATSEN, University of Waterloo — Surface effects become particularly important for micro-sized and even more so for nano-sized objects. Naturally, enthalpic preferences will cause certain components of a multi-component material to segregate to a surface, but in polymeric materials this can also happen as a result of purely entropic reasons. To demonstrate this, we consider the effect of a surface on a binary blend of chemically identical long and short polymers, using self-consistent field theory. Despite the absence of any enthalpic preference, the short polymers are found to segregate to the surface. We investigate how the amount of the surface excess and its decay length depends on the polymeric model, the molecular weights of the two polymers and the blend composition.

³This work was supported by NSERC of Canada.

M1.00077 Capillary wrinkling of thin bilayer polymeric sheets. YERGOU TATEK, SOLOMON NEGASH, Addis Ababa University, MESFIN TSIGE, The Univesity of Akron — Detailed atomistic Molecular Dynamics simulations are performed to explore the effect of tacticity on the glass transition temperature as well as other pertinent structural properties of films of polystyrene (PS) chains adsorbed onto two distinct types of solid substrates. The investigated systems consist of thin films made of isotactic, syndiotactic and atactic PS chains adsorbed on graphite and hydroxylated silica surfaces. The structure of the films is investigated in terms of film density profiles and side chains and backbone orientations. Simulations results reveal a marked dependence of the film structure on substrate type while the absence of a strong correlation between structure and tacticity is observed. Moreover, it is found that the glass transition temperature is also substrate dependent and takes larger values for films adsorbed on graphite surface, irrespective of chain tacticity.

M1.00078 Role of monomer sequence and backbone structure in polypeptoid and polypeptide polymers for anti-fouling applications. ANASTASIA PATTERSON, GEORGIOS RIZIS, UC Santa Barbara, BRANDON WENNING, Cornell University, JOHN FINLAY, Newcastle University, CHRISTOPHER OBER, Cornell University, RACHEL SEGALMAN, UC Santa Barbara — Polymeric coatings rely on a fine balance of surface properties to achieve biofouling resistance. Bioinspired polymers and oligomers provide a modular strategy for the inclusion of multiple functionalities with controlled architecture, sequence and surface properties. In this work, polypeptoid and polypeptide functionalized coatings based on PEO and PDMS block copolymers were compared with respect to surface presentation and fouling by Ulva linza. While polypeptoids and polypeptides are simple isomers of each other, the lack of backbone chirality and hydrogen bonding in polypeptoids leads to surprisingly different surface behavior. Specifically, the polypeptoids surface segregate much more strongly than analogous polypeptide functionalized polymers, which in turn affects the performance of the coating. Indeed, polypeptoid functionalized surfaces were significantly better both in terms of anti-fouling and fouling release than the corresponding polypeptide-bearing polymers. The role of specific monomer sequence and backbone chemistry will be further discussed in this poster.

M1.00079 Conformation and hydration of surface grafted and free polyethylene oxide chains in solutions. UDAYA DAHAL, Department Dept. of Physics and Institute of Materials Science, Univ. of Connecticut, ZILU WANG, Dept. of Physics and Institute of Materials Science, Univ. of Connecticut, ELENA DORMIDONTOVA, DDept. of Physics and Institute of Materials Science, Univ. of Connecticut — Due to the wide application of polyethylene oxide (PEO), ranging from biomedicine to fuel cells, it is one of the most studied polymers in the scientific world. In order to elucidate detailed molecular-level insights on the impact of surface grafting on PEO conformation, we performed atomistic molecular dynamics simulations of PEO chains in solution and in flat gold surface in different solvents. We examined the hydration as well as conformation of the free chain compared to the grafted polymer in pure water and mixed solvents. We find that grafted chains are stiffer and have a stronger tendency to form helical structures in isotactic acid or mixture of isotactic acid and water solution than the free chains in corresponding solutions. For grafted chains exposed to pure water the random coil conformation is retained at low grafting density, but becomes stretched and more dehydrated as the grafting density or temperature increases.

³This research is supported by NSF (DMR-1410928).
M1.00080 Charge transport and structural dynamics in ultra-thin films of polymerized ionic liquids1, MAXIMILIAN HERES, TYLER COSBY, Univ of Tennessee, Knoxville, STEFAN BERDZINSKI, VERONICA STREHME, Department of Chemistry and Institute for coatings and surface chemistry, Hochschule Niederrein University of Applied Sciences, ROBERTO BENSON, JOSHUA SANGORO, Univ of Tennessee, Knoxville — Ion conduction and structural dynamics in a series of ultra-thin films of imidazolium based polymerized ionic liquids are investigated using broadband dielectric spectroscopy, atomic force microscopy, and ellipsometry. No alteration in the characteristic charge transport rate is observed between bulk sample and films as thin as 12nm. These results are discussed within the recent approaches proposed to explain the confinement effects on structural dynamics in polymers and low molecular weight ionic liquids.

1 NSF DRM Polymers Program

M1.00081 Molecular dynamics simulations and morphology analysis of TEM imaged PVDF nanofibers1, JIAYUAN MIAO, Case Western Reserve University, DARrell RENEKER, MESFIN TSIGE, University of Akron, PHILIP TAYLOR, Case Western Reserve University — With the goal of elucidating the structure of polyvinylidene fluoride (PVDF) nanofibers, all-atom molecular dynamics simulations were performed, and the results compared with structures observed in high resolution transmission electron microscopy (TEM) at the molecular level. Simulation shows that the stability of the 13-phase PVDF nanofiber is influenced by its thickness and processing history. When exposed to irradiation, as in a TEM observation, the structure is then further modified by the effects of chain scission. The transformation from the 13 phase into a paraelectric phase can explain the spindle formation and serpentine motion of molecular segments observed by Zhong et al. (Polymer, 54, 2013, 3745-3756) in irradiated PVDF nanofibers. From a comparison between simulated and experimental TEM images it was possible to identify numerous features that are useful in unveiling the inherent structure of PVDF nanofibers. The experimental TEM images appear to match well with those predicted by a model based on 1a-phase PVDF, while also being consistent with an alternative model (Nanoscale 2015, DOI: 10.1039/c5nr01619c).

M1.00082 Processing and characterization of natural fiber reinforced thermoplastic composites using micro-braiding technique1, SATOSHI KOBAYASHI, Tokyo Metropolitan Univ, SHINJI OGIHARA, Tokyo University of Science — In the present study, we investigate fatigue properties of green composites. A hemp fiber yarn reinforced poly(lactic acid) composite was selected as a green composite. Unidirectional (UD) and textile (Textile) composites were fabricated using micro-braiding technique. Fatigue tests results indicated that fatigue damages in UD composites was splitting which occurred just before the final fracture, while matrix crack and debonding between matrix and fiber yarn occurred and accumulated stably in Textile composites. These results were consistent with modulus reduction and acoustic emission measurement during fatigue tests.

M1.00083 Deformation Behavior during Processing in Carbon Fiber Reinforced Plastics, SHINJI OGIHARA, Tokyo University of Science, SATOSHI KOBAYASHI, Tokyo Metropolitan University — In this study, we manufacture the device for measuring the friction between the prepreg curing process and subjected to pull-out tests with it The prepreg used in this study is a unidirectional carbon/epoxy, produced by TORAY designation of T700SC/2592. When creating specimens 4-ply prepregs are prepared and laminated. The 2-ply prepregs in the middle are shifted 50mm. In order to measure the friction between the prepreg during the cure process, we simulate the environment in the autoclave in the device, and we experiment in pull-out test. Test environment simulating temperature and pressure. The speed of displacement should be calculated by coefficient of thermal expansions (CTE). By calculation, 0.05mm/min gives the order of magnitude of displacement speed. In this study, 3 pull-out speeds are used: 0.01, 0.05 and 0.1mm/min. The specimen was heated by a couple of heaters, and we controlled the heaters with a temperature controller along the curing conditions of the prepreg. We put pressure using 4 bolts. Two strain gages were put on the bolt. We can understand the load applied to the specimen from the strain of the bolt. Pressure was adjusted the tightness of the bolt according to curing conditions. By using such a device, the pull-out test performed by tensile testing machine while adding temperature and pressure. During the 5 hours, we perform experiments while recording the load and stroke. The shear stress determined from the load and the stroke, and evaluated.

M1.00084 Localized Memory Effect of Elastomers Filled with Nanoparticles1, SHOBO LI, XIAORONG WANG, Chemical Engineering, Tongji University, Shanghai — When a filler-reinforced elastomer compound is oscillatory sheared or pressed at a small fixed strain (e.g., 2%) for a period of time, it can produce a localized memory perturbation in its dynamic spectrum. Typically, a localized memory appears near the apparent strain at which maximum loss modulus and holding the system at two strains can produce one or two holes depending on the deformation history. While this discovery of localized memory effect seems to be significant and compelling, its generality in vulcanized elastomers containing various fillers has not yet been tested extensively. In this work, we intend to expand on our previous work of a colloidal silica-filled model system to carbon black-filled real rubbers. We also examine the effect of filler volume fraction in rubber compounds on the spectral memory phenomenon.

M1.00085 Mechanical Properties of Cellulose Microfiber Reinforced Polyolefin, SATOSHI KOBAYASHI, HIROYUKI YAMADA, Tokyo Metropolitan Univ — Cellulose microfiber (CeF) has been expected as a reinforcement of polymer because of its high modulus and strength and lower cost. In the present study, mechanical properties of CeF/polyolefin were investigated. Tensile modulus increased with increasing CeF content. On the other hand, tensile strength decreased. Fatigue properties were also investigated with acoustic emission measurement. Softness of the composites gradually decreased with loading. Drastic decrease in stiffness was observed just before the final fracture. Based on the Mori-Tanaka’s theory, the method to calculate modulus of CeF were proposed to evaluate dispersion of CeF.

M1.00086 Soft composites with the twisted plywood microstructure, a lesson from nature.1, YONGJIN KIM, ALFRED CROSBY, Univ of Mass - Amherst, CROSBY RESEARCH GROUP TEAM — The twisted plywood microstructure, consisting of rigid structural units within a continuous matrix, is known to be prevalent in many natural materials, including exoskeletons of crustacean, scales of fish, and even bones of mammals. Although it is yet to be resolved whether this structure is a product of evolution or an inevitable consequence of chirality of building blocks, nature utilizes the structure extensively to create various components. Previous studies have focused on fabricating and characterizing synthetic composites with similar structures; however, these composites have been based on a rigid matrix, e.g. an epoxy resin, and hard fibers, e.g. carbon fibers. For this combination of materials, it has been difficult to deconvolute the specific roles of each component. For a better understanding of the advantage of the structure, we have developed flexible composites, comprising a soft matrix and hard fiber bundles at two different size scales. Macroscopic engineered samples were created by combining elastomer and hard fibers, while sub-micron composites are fabricated from self-assembled nanoparticle ribbons and hydrogel matrices. The advantageous mechanical response of these flexible plywood composites is characterized and presented.

1 This material is based upon work supported by, or in part by, the U. S. Army Research Laboratory and the U. S. Army Research Office under contract/grant number W911NF-15-1-0358
M1.00087 Modeling heterogeneous polymer-grafted nanoparticle networks having biomimetic core-shell structure  BADEL L. MBANGLA, VICTOR V. YASHIN, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA 15261, USA, NIELS HOLLEN-ANDERSEN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA 15261, USA — Inspired by the remarkable mechanical properties of such biological structures as mussel adhesive fibers, we use 3D computational modeling to study the behavior of heterogeneous polymer-grafted nanoparticle (PNG) networks under tensile deformation. The building block of a PNG network is a nanoparticle with grafted polymer chains whose free ends' reactive groups can form both permanent and labile bonds with the end chains on the nearby particles. The tunable behavior of cross-linked PNG networks in tension is an excellent candidate for designing novel materials with enhanced mechanical properties. Here, we consider the PNG networks having the core-shell structures, in which the type and strength of the inter-particle bonds in the outer shell differ from those in the core. Using the computer simulations, we obtain and compare the ultimate tensile properties (strength, toughness, ductility) and the strain recovery properties for the uniform samples and various core-shell structures. We demonstrate that the core-shell structures could be designed to obtain highly resilient self-healing materials.

M1.00088 Effects of Dimensionality and Flexibility of Conductive Fillers in Nanocomposites on Percolating Network Formation and Electrical Conductivity  SEULKI KWON, HYUN WOO CHO, BONG JUNE SUNG, Department of Chemistry, Sogang University, Seoul 121-742, Republic of Korea — We conduct extensive langevin dynamics(LD) simulation to explore how the dimensionality and flexibility of conductive fillers in polymer nanocomposites influence their percolation network formation and electrical conductivity. The percolation network formation of nanoparticles in polymer matrices is critical to obtaining desired properties of polymer nanocomposites. Some nanofillers such as carbon nanotubes(CNTs) and graphene nanosheets, are so flexible that they become either wavy or crumpled. Such a variability in nanofiller conformation brings a change to the percolation network, but has been often ignored in the theoretical and computational investigation. We consider three kinds of nanofillers of different dimensionality: zero-dimensional(0D) nanospheres, one-dimensional(1D) nanorods, and two-dimensional(2D) nanoplates. We estimate the percolation network concentration(\(\phi_\text{p}^c\)) and electrical conductivity with careful finite-size scaling. When the sizes of nanofillers are comparable, the dimensionality of nanofillers influences on \(\phi_\text{p}^c\) and electrical conductivity of nanocomposites significantly. The effect of flexibility of nanofillers is less significant than that of dimensionality.

M1.00089 Structure, Nanomechanics and Dynamics of Dispersed Surfactant-Free Clay Nanocomposite Films  XIAO ZHANG, JING ZHAO, University of Akron, CHAD. SNYDER, National Institute of Standards and Technology, ALAMGIR KARIM, University of Akron, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY COLLABORATION — Natural Montmorillonite particles were dispersed as tactoids in thin films of polycaprolactone (PCL) through a flow coating technique assisted by ultra-sonication. Wide angle X-ray scattering (WAXS), Grazing-incidence wide angle X-ray scattering (GI-WAXS), and transmission electron microscopy (TEM) were used to confirm the dispersion of these tactoids. The characterization techniques are in conjunction with its nanomechanical properties via strain-induced buckling instability for modulus measurements (SIEBIMM), a high throughput technique to characterize thin film mechanical properties. The linear strengthening trend of the elastic modulus enhancements was fitted with Halpin-Tsai (HT) model, correlating the nanoparticle geometric effects, and mechanical behaviors based on continuum theories. The overall aspect ratio of dispersed tactoids obtained through HT model fitting is in reasonable agreement with digital electron microscope image analysis. Moreover, glass transition behaviors of the composites were characterized using broadband dielectric relaxation spectroscopy. The segmental relaxation behaviors indicate that the associated mechanical property changes are due to the continuum filler effect rather than the interfacial confinement effect.

M1.00090 Influence of Surface Coating of Magnetic Nanoparticles on Mechanical Properties of Polymer Nanocomposites  ECEM YARAR, GIZEM KARAKAS, Yeditepe University, DENIZ RENDE, RAHMI OZISIK, Rensselaer Polytechnic Institute, SEYDA MALTA, Yeditepe University — Polymer nanocomposites have emerged as promising materials due to improved properties when compared with conventional bulk polymers. Nanofillers are natural or synthetic organic/inorganic particles that are less than 100 nm in at least one dimension. Even the addition of trace amounts of nanofillers to polymers may lead to unique combinations of properties. Among variety of inorganic nanofillers, iron oxide magnetic nanoparticles are of great interest due to their unique physical and chemical properties, such as low toxicity, biocompatibility, large magnetization and conductivity, owing to their extremely small size and large specific surface area. In this study, approximately 8-10 nm magnetic nanoparticles coated with either citric acid or oleic acid are synthesized and blended with poly(methyl methacrylate) (PMMA) or poly(ethylene oxide) (PEO). The hydrophobicity/hydrophilicity of the polymer and the surface coating on the iron oxide nanoparticles are exploited to control the dispersion state of nanoparticles, and the effect of dispersion on mechanical and thermal properties of the nanocomposite are investigated via experimental methods such as dynamic mechanical analysis and differential scanning calorimetry.

This material is based upon work partially supported by the National Science Foundation under Grant No. CMMI-1538730 and TUBITAK 112M066

M1.00091 Wide Angle X-Ray Scattering Investigations on Irradiated iPP-VGCNF Nanocomposites  ARNOLD FONSECA, DORINA CHIPARA, KAREN LOzano, MIRCEA CHIPARA, The University of Texas Rio Grande Valley — Isotactic Polypropylene (iPP) has been loaded by various amounts of Vapor Grown Carbon Nanofiber (VGCNF), ranging between 0 and 20 % wt., via melt mixing. The as obtained nanocomposites were irradiated by \(^{60}\text{Co}\) source. Wide Angle X-Ray Spectroscopy has been used to quantify the changes in the crystalline structure and the degree of crystallinity of iPP-VGCNFs nanocomposites. The measurements have been carried out by a Bruker Discover 8 spectrometer. Additional measurements have been performed by Raman spectroscopy using a Renishaw InVia microscope system operating at 532 and 785 nm. The experimental spectra of the nanocomposite were fitted by assuming a superposition of extended Breit-Wigner-Fano line shapes. It is concluded that the observed modifications noticed in these nanocomposites are dominated by the radiation-induced degradation of the polymeric matrix. Dierential Scanning calorimetry data provided additional information regarding the effect of the nanofiller on the degree of crystallinity.

M1.00092 Designing a gel–fiber composite to extract nanoparticles from solution  YA LIU, University of Pittsburgh, OLGA KUKSENOK, Clemson University, ANNA BALAZS, University of Pittsburgh — Using DPD simulations, we proposed the design of a gel–fiber coating where the components of the system act in concert to extract particles from solution and localize these solids in the underlying gel layer. We model an array of flexible fibers that are embedded in a lower critical solution temperature (LCST) thermo-responsive gel, which swells at lower temperatures and collapses at higher temperatures. The system is immersed in a solution containing dispersed nanoparticles and this fluid is driven to flow by an imposed shear. When the gel is heated, it collapses to expose the fibers, and thereby, triggers the “catch” process. Namely, the fibers can act like “arms” that wrap around the nanoparticle and bring it from the outer solvent into the gel layer. Moreover, we show that depending on the flexibility and hydrophobicity of the fibers, as well as the imposed shear, we can position the nanoparticles at the desired height within the gel layer. Our approach can be utilized for the detection and separation of components in fluids and for the controlled insertion of nanoparticles within a hydrogel at a particular distance from the gel interface.

M1.00093 ABSTRACT WITHDRAWN
M1.00094 Viscoelastic Analysis of Thermally Stiffening Polymer Nanocomposites¹, ANDREW EHLERS*, DENIZ RENDE, Rensselaer Polytechnic Institute, ERKAN SENSES, PINAR AKCORA, Stevens Institute of Technology, RAHMI OZISIK, Rensselaer Polytechnic Institute — Poly(ethylene oxide), PEO, filled with silica nanoparticles coated with poly(methyl methacrylate), PMMA, was shown to present thermally stiffening behavior above the glass transition temperature of both PEO and PMMA. In the current study, the viscoelastic behavior of this nanocomposite system is investigated via nanoindentation experiments to complement on going rheological studies. Results were compared to neat polymers, PEO and PMMA, to understand the effect of coated nanoparticles.

¹This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730. *Undergraduate student.

M1.00095 Controlling the Degradation of Bioreosorbable Polymers², ISTVAN MORITZ, BRIAN CROWLEY*, ELIZABETH BRUNDAGE*, Materials Science and Engineering, Rensselaer Polytechnic Institute, DENIZ RENDE, Center for Materials, Devices and Integrated Systems, RENSSELAER POLYTECHNIC INSTITUTE — Biodegradable polymers play a vital role in the development of implantable materials that are used in surgical procedures, controlled drug delivery systems, and tissue engineering scaffolds. The half-life of common bioreosorbable polymers ranges from 3 to over 12 months and slow bioreosorption rates of these polymers restrict their use to a limited set of applications. The use of embedded enzymes was previously proposed to control the degradation rate of bioreosorbable polymers, and was shown to decrease average degradation time to about 0.5 months. In this study, electromagnetic actuation of iron oxide magnetic nanoparticles embedded in an encapsulant polymer, poly(ethylene oxide), PEO, was employed to initiate enzyme assisted degradation of bioreosorbable polymer poly(caprolactone), PCL. Results indicate that the internal temperature of iron oxide magnetic nanoparticle doped PEO samples can be increased via an alternating magnetic field, and temperature increase depends strongly on nanoparticle concentration and magnetic field parameters. The temperature achieved is sufficient to relax the PEO matrix and to enable the diffusion of enzymes from PEO to a surrounding PCL matrix. Current studies are directed at measuring the degradation rate of PCL due to the diffused enzyme.

²This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730. *Undergraduate student.

M1.00096 Interfacial slip in nano filled polymer blends, JOHN MIKHAIL, DI XU, JOSEPH ORTIZ, DILIP GERAPPPE, Stony Brook University — The ability to control the interfacial slip in polymer blends is key to strengthening the material. Here, we look at how nano fillers can be used to strengthen the interface. By designing nano fillers with the appropriate surface energy we show how nano fillers can localize at the interface between the two polymer blends. We examine the role that the aspect ratio of the nano filler has on its ability to reduce the interfacial slip, and look to understand the mechanisms by which the slip is reduced. We look for network formation near the interface as a possible strengthening mechanism.

M1.00097 Nanocellulose Composite Materials Synthesizes with Ultrasonic Agitation, TIMOTHY KIDD, ANDREW FOLKEN, BYRON FRITCH, DEREK BRADLEY, University of Northern Iowa — We have extended current techniques in forming nanocellulose composite solids, suspensions and aerogels to enhance the breakdown of cellulose into its molecular components. Using only mechanical processing which includes ball milling, using a simple mortar and pestle, and ultrasonic agitation, we are able to create very low concentration uniform nanocellulose suspensions in water, as well as incorporate other materials such as graphite, carbon nanotubes, and magnetic materials. Of interest is that no chemical processing is necessary, nor is the use of nanoparticles, necessary for composite formation. Using both graphite and carbon nanotubes, we are able to achieve conducting nanocellulose solids and aerogels. Standard magnetic powder can also be incorporated to create magnetic solids. The technique also allows for the creation of an extremely fine nanocellulose suspension in water. Using extremely low concentrations, less than 1% cellulose by mass, along with careful control over processing parameters, we are able to achieve highly dilute, yet homogeneous nanocellulose suspensions. When air dried, these nanocellulose solids have a strength profile similar to those created with more typical starting cellulose concentrations (2-10%). However, when freeze-dried, these dilute suspensions form aerogels with a new morphology with much higher surface area than those with higher starting concentrations. We are currently examining the effect of this higher surface area on the properties of nanocellulose aerogel composites and how it influences the impact of incorporating nanocellulose into other polymer materials.

M1.00098 Predicting $\chi$ for polymers with stiffness mismatch from simulations, DANIEL KOZUCH, WENLIN ZHANG, ENRIQUE GOMEZ, SCOTT MILNER, Department of Chemical Engineering, Penn State University — The Flory-Huggins $\chi$ parameter describes the excess free energy of mixing and governs phase behavior for polymer blends and block copolymers. For chemically distinct polymers, the value of $\chi$ is typically determined through the use of bead-spring models, or through the use of equilibrium thermodynamics. More recently, the non-ideal packing and thermodynamic interactions of chains within a polymer blend, $\chi$, arising from non-ideal local packing, becomes more significant. Using polymer field theory, Fredrickson, Liu, and Bates predict that a difference in backbone stiffness can result in a positive $\chi$ for chains consisting of chemically identical monomers. To quantitatively investigate this phenomenon, we perform molecular dynamic (MD) simulations for bead-spring chains which differ only in stiffness. From the simulations, we apply a novel thermodynamic integration to extract $\chi$ as low as $10^{-3}$ per monomer for blends with mild stiffness mismatch. By introducing a standardized effective monomer, we map real polymers to our bead-spring chains and show that the predicted entropic portion of $\chi$ are consistent with experimental data.

M1.00099 Comparative Study of Silk-Silk Alloy Materials, YE XUE, Rowan University; Nanjing University, DAVE JAO, Rowan University, WENBING HU, Nanjing University, NATHAN WOLF, ÉVÀ-MARIE ROCKS, XIAO HU, Rowan University — Silk fibrin materials can be used for various kinds of biomedical applications. We report a comparative study of silk-silk blend materials using thermal analysis and infrared spectroscopy. Four groups of silk-silk blend films: Mori-Tussah, Mori-Muga, Mori-Eri and Mori-Thai, were fabricated from aqueous solutions and blended at different weight ratios, respectively. These silk-silk blend systems exploit the beneficial material properties of both silks. DSC and temperature-modulated DSC were used to measure the transition temperatures and heat capacity of these water-based silk-silk blend films. Fourier transform infrared spectrometer was used to characterize secondary structure of these protein crystalline structures of silk-silk blends. This study demonstrates that Mori silk is fully miscible with Tussah, Muga, Eri and Thai silk at different weight ratios without phase separation. Glass transition temperatures, degradation temperatures and the contents of alpha-helix and random coils of those silk-silk blend films can be controlled by changing the contents of different silks in the blend system. The features of Mori silk combined with the attributes of Tussah, Muga, Eri and Thai silk offer a useful suite of materials for a variety of applications in the future.

M1.00100 Compatibility and Impact Resistance of Biodegradable Polymer Blends Using Clays and Natural Nanotubes, YICHEN GUO, XUE YUAN, XIANGHAO ZUO, MIRIAM RAFAILOVICH, Stony Brook University — Montmorillonite clays and Halloysite nanotubes (HNTs) were modified by surface adsorption of resorcinol di (phenyl phosphate) (RDP) oligomers. Biodegradable poly(lactic acid) (PLA) and poly (butylene adipate-co-butylene terephthalate) (PBAT) polymers were blended together with RDP coated clays and tubes. TEM images of thin sections indicated that even though both RDP coated clay nanotubes and platelets located on the interfacial region between two immiscible polymers, only the platelets, having the larger aspect ratio, were able to reduce the PBAT domain sizes. The ability of clay platelets to partially compatibilize the blend was further confirmed by the dynamic mechanical analysis (DMA) which showed that the glass transition temperatures of two polymers tended to shift closer. Izod impact testing demonstrated that the rubbery PBAT phase greatly increased the impact strength of the unfilled blend, but addition of only 5% of clay filler decrease the impact strength by nearly 50% while a small increase was observed with nanotubes at that concentration. A simple model is proposed. The clay platelets are observed to cover the interfacial area. Although they are effective at reducing the interfacial tension, they block the entanglements between two polymer phase and increase the overall brittleness. On the other hand, the HNTs are observed to lie perpendicular to the interface, which makes them less effective in reducing interfacial tension, but far more effective at retaining micro-crack propagation.

M1.00101 Comparative Study of Silk-Silk Alloy Materials, YE XUE, Rowan University; Nanjing University, DAVE JAO, Rowan University, WENBING HU, Nanjing University, NATHAN WOLF, ÉVÀ-MARIE ROCKS, XIAO HU, Rowan University — Silk fibrin materials can be used for various kinds of biomedical applications. We report a comparative study of silk-silk blend materials using thermal analysis and infrared spectroscopy. Four groups of silk-silk blend films: Mori-Tussah, Mori-Muga, Mori-Eri and Mori-Thai, were fabricated from aqueous solutions and blended at different weight ratios, respectively. These silk-silk blend systems exploit the beneficial material properties of both silks. DSC and temperature-modulated DSC were used to measure the transition temperatures and heat capacity of these water-based silk-silk blend films. Fourier transform infrared spectrometer was used to characterize secondary structure of these protein crystalline structures of silk-silk blends. This study demonstrates that Mori silk is fully miscible with Tussah, Muga, Eri and Thai silk at different weight ratios without phase separation. Glass transition temperatures, degradation temperatures and the contents of alpha-helix and random coils of those silk-silk blend films can be controlled by changing the contents of different silks in the blend system. The features of Mori silk combined with the attributes of Tussah, Muga, Eri and Thai silk offer a useful suite of materials for a variety of applications in the future.
M1.00101 Hybrid Simulation Strategy for Simulating Self-Assembled Morphologies at the Atomicistic Length Scales

1. VAIDYANATHAN SETHURAMAN, VENKAT GANESAN, Univ of Texas, Austin — In the context of lithium-ion batteries, an enhancement in both ionic conductivity and mechanical properties, were observed for block copolymer electrolytes with increasing MW. On the contrary, when homopolymers were used as electrolytes, the ionic conductivity decreased with increasing MW. However, the origins of such increase in conductivity are unclear and are speculated to be tied to both the morphology and the atomistic details of the copolymer themselves. Motivated by such issues, we present a strategy to create ordered morphologies of block copolymers at the atomicistic level using a combination of coarse-graining and inverse coarse-graining techniques. A mapping which is developed using the long-ranged structural mapping in the disordered phases will be utilized to generate self-assembled morphologies. In particular we focus on generating self-assembled morphologies of PS-PEO at the atomicistic length scales. Statics and dynamics of such self-assembled morphologies will be presented and the effect of self assembly on the transport properties of ions will also be explored.

1 Funded by NSF

M1.00102 Controlling Miscibility in Polyethylene-Polynorbornene Block Copolymers via Side-Group Chemistry.

1. WILLIAM MULHEARN, RICHARD REGISTER, Princeton University — Block copolymers containing a crystallizable block, such as polyethylene (PE), and an amorphous block with high glass transition temperature (T_g) are an interesting class of materials since the rigid glassy block can improve the mechanical response of the article under strain by reinforcing the crystal fold surface. However, to prepare an easily processable PE-containing block copolymer it is necessary to avoid microphase separation in the melt by selection of amorphous blocks with weak repulsive interactions against PE (low Flory interaction parameter χ or interaction energy density λ). Most such low-χ polymers are chemically similar to PE, such as copolymers of ethylene and a small amount of an α-olefin, and therefore exhibit similarly low glass transition temperatures. This work investigates a series of low- and high-T_g polymers based on substituted norbornene monomers, polymerized via ring-opening metathesis polymerization (ROMP). Hydrogenated polynorbornene derivatives possess a wide range of glass transition temperatures, and miscibility with PE can be readily tuned by the choice of substituents on the monomers (e.g. aromatic vs. aliphatic groups). Two species investigated, hydrogenated poly(cyclohexyl norbornene) and hydrogenated poly(norbornyl norbornene), have high T_g and also remain miscible with polyethylene to high molecular weight. Furthermore, we developed a set of mixing rules to quantitatively predict the solubility behavior of substituted ROMP polynorbornenes as a function of their side-groups.

M1.00103 Influence of Homopolymers on the Microdomain Behavior of Block Copolymers in 2D Confinement

1. YOUNGKEOL KIM, SUNGYOUL HWANG, GUIDUK YU, KOOKHEON CHAR, Seoul Natl Univ — Constraints imposed by nanometer scale confinement lead to changes in bulk equilibrium behavior of block copolymers (BCPs). Cylindrical pores with diameters corresponding to the length equivalent of several copolymer chains have been employed to investigate the influence of two-dimensional confinement on the behavior of BCPs. In this study, we expand the scope to homopolymer-BCP binary blends. Given fraction of homopolymers, the phase behavior of blends is dependent on molecular weight (Mw) of homopolymers. Lamella- and cylinder-forming poly(styrene-butadiene) (PS-b-PBD) and PS homopolymers (hPS) were drawn into the pores of anodized aluminum oxide (AAO) membranes in the melt by capillary forces. Based on the detailed observation of the morphologies within porous columns, we analyzed the structural transition of BCPs induced by the presence of hPS and confinement. The effect of hPS on the micro-domain of BCPs is greatly accentuated in nanoscale confinement compared to the bulk state due to the entropic loss of polymer chains. Pore diameters of AAO and Mw of the PS-b-PBD are also controlled so as to examine the effects of confinement on the phase transition of PS-b-PBD/hPS blends.

M1.00104 Tunable Surface Energy Interlayer Coating to Control the Phase Behavior of Block Copolymers in 2D Confinement

1. SUNGYOUL HWANG, YOUNGKEOL KIM, DOKYEONG KWON, KOOKHEON CHAR, Seoul Natl Univ — There have been many studies to investigate the phase behavior of block copolymers (BCPs) in cylindrical confinement. In the nanometer scale 2D confinement, the phase behavior of BCPs is mainly dependent upon commensurability and interfacial interaction. However, most studies have focused only on the effects of commensurability on the microdomains of BCP. In this study, we employed organosilicate (OS) which has tunable surface energy upon adjusting curing temperature as interlayer to examine the phase behavior of BCPs as a function of interfacial energy. The OS interlayer was coated in the inner surface of anodized aluminum oxide (AAO) pores by template-wetting method and cured in a range of temperature to control the surface energy of the interlayer. Lamellae-forming poly(styrene-b-methyl methacrylate) (PS-b-P(MMA)) (SMA) in the melt was injected into the OS-coated AAO pores by capillary forces. With the detailed analysis, we note that the self-assembly of SMA within 2D confinement is competitively affected by both entropic and enthalpic effects as the contact interfacial energy is varied. Simple by controlling the curing temperature of the OS interlayer, various morphologies arising from both preferential and neutral wetting were identified.

M1.00105 Bottlebrush Copolymer Morphology Transition: Influence of Side Chain Length and Block Volume Fraction

1. YUE GAI, DONG-PO SONG, JAMES WATKINS, Univ of Mass - Amherst — Brush block copolymers synthesized via living ring-opening metathesis polymerization (ROMP) offer unique advantages as templates for functional hybrid materials. Unlike linear block copolymer, the bottlebrush polymer phase transition not only depends on volume fractions of the two blocks but also on side chain length. Here we report the morphology transitions of BCP-PEO bottlebrush copolymer (BBBCP) as a function of PEO side chain length and block volume fraction. For the BBBCPs with similar side chain lengths, highly ordered lamellar morphologies were observed with PEO volume fractions in a wide range from 32 vol% to 72 vol%, which is significantly different from that of traditional linear block copolymers. This study will lay the groundwork for nanostructure fabrications using the BBBCPs and provides new insights into the phase behavior of the new type of materials.

1 This work was supported by NSF center for Hierarchical Manufacturing at the University of Massachusetts, Amherst.

M1.00106 Microwave Irradiation on Graphene Dispersed Within Polymeric Matrices.

1. JORGE CISNEROS, BRIAN YUST, MIRCEA CHIPARA, Univ of Texas Rio Grande Valley — Graphene is a two dimensional nanomaterial with high thermal and electric conductivity and Young modulus. These features make graphene an ideal reinforcement for polymeric matrices. However, the mechanical features of polymer-carbon nanostructured composites are limited by the dispersion of the filler and by the delamination or microcracks initiated at the interface between the polymer matrix and nanofiller. This last weakness can be addressed by improving the interface via chemical and physical methods. Microwave heating of graphite is a very efficient approach if the polymeric matrix does not also have a strong absorption. During the irradiation, the nanofiller is preferentially heated; the local melting of the polymer at the interface improves the interface by filling the microcracks and delaminations. Nanocomposites of polystyrene-poly(ethylene-ran-butylene)-polystyrene loaded by various amounts of graphene ranging from 0 % to 20 % wt. have been prepared by solution mixing using chloroform as solvent. The as obtained nanocomposites have been subjected to microwave irradiation in an Anton Paar Monowave 300 system operating at 75 W, for various irradiation times 5, 10, 15, 30, 45, and 60 minutes. The effect of microwave irradiation has been studied by Raman spectroscopy.
M1.00107 Acoustic and Ultrasonic Spectral Evolution in Pre- and Post-Damage Self-Healing Poly (Ethylene Co-Methacrylic Acid) Ionomer Samples, JONATHAN BUCKLEY, KENNETH PESTK A II, Longwood University, STEPHEN KALISTA, Department of Biomedical Engineering, Rensselaer Polytechnic Institute — We measured the pre- and post-damage resonant spectra of several self-healing ionomer samples composed of poly (ethylene co-methacrylic acid) (EMAA). The post-damage results indicate significant time-dependent variation in the acoustic and ultrasonic resonant spectral waveforms of these self-healing samples. These results are consistent with other recent experiments that demonstrate time evolution of resonant frequencies and associated quality factors within samples of post-damage EMAA ionomers. However, in our experiments it was found that, in some circumstances, the quality factors and associated resonant frequencies can exhibit time-dependent variation both before and after external damage. By quantifying time-dependent variations in the spectra of undamaged samples, including quality factor, resonant frequency and spectral waveform, we demonstrate a method to isolate changes in the resonant spectra that are present solely due to the post-damage healing behavior of these EMAA ionomers.

M1.00108 Effect of charge density in chain extension reactions involving complexes of 4, 4'-diaminodiphenylmethane and various alkali metal salts, SUBRAJEET DESHMUKH, KATHERINE CARRASQUILLO, FANG CHANG, TSAI, LIN A WU, SHAW LING HSU, University of Massachusetts Amherst, UNIVERSITY OF MASSACHUSETTS AMHERST TEAM — Controlling the reaction of polyethylene in disocyanate (MDI)-terminated polymer prepolymer and 4, 4'-diaminodiphenylmethane (MDA) is extremely important in many large scale applications. The ion-diamine complex has the advantage of blocking the instantaneous reaction between the diamine and isocyanate from taking place. We synthesized the complexes of MDA with various alkali metal salts. These complexes create a barrier between the diamine and isocyanate thus preventing the premature reaction. We compared the complexes in terms of their dissociation and the subsequent curing with the prepolymer. Charge density had a tremendous effect. DSC showed that Na complexes dissociated at a lower temperature and needed less energy to dissociate than the Li complexes. The effect of change in cation on complex dissociation was more pronounced compared to the change in anion. Also, the ionic liquid greatly altered the dissociation behavior. Temperature and time resolved IR spectroscopy was used to monitor the urea and NH band. By DSC and IR, we showed that NaCl complex is best suited for the curing of prepolymer with regards to curing temperature and energy.

M1.00109 Structural dynamics in polystyrene-b-polyisoprene copolymers with varying molecular architectures, THOMAS KINSEY, MAXIMILIAN HERES, JIMMY MAYS, ROBERTO BENSON, JOSHUA SANGORO, Univ of Tennessee, Knoxville — A series of polystyrene-polyisoprene block copolymers with different molecular architectures are investigated by broadband dielectric spectroscopy and temperature modulated differential scanning calorimetry. The influence of copolymer composition on segmental and normal mode relaxation dynamics is analyzed. These results are discussed with respect to the current understanding of copolymer dynamics and interactions.

M1.00110 How to Improve Ion Transport in Polymer Nanocomposites and Interactions, SANTHOSH MOGURAMPALLY, VENKAT GANESAN, Univ of Texas, Austin — We present different strategies to enhance ion conducting properties of polymer nanocomposites electrolytes and their implications by varying the surface chemistries of the nanoparticles and interactions between nanoparticle and components of polymer-salt mixture. Our molecular dynamics simulations suggest that the ionic mobilities and conductivities correlate with the comparison of the changes in polymer segmental dynamics and the modifications of the local environment of ion species arising from the introduction of nanoparticles. In the presence of α, β and γ-Al2O3 nanoparticles, we observe a monotonic decrease of ionic conductivities and mobilities with the nanoparticle loading due to the corresponding slowing of polymer dynamics. However, with the introduction of the repulsive interactions between nanoparticle and components of polymer-salt mixture, we find an increase in the mobility and conductivity of the polymer nanocomposites. However, the repulsive interactions seem to decrease the elastic moduli in contrast to the moduli enhancing effects by attractive interactions.

M1.00111 STRUCTURE OF ANION-CONDUCTING POLYMERS FROM WAXS AND MD SIMULATIONS, BARBARA FRISKEN, SEPEHR TAHMASEBI, ERIC SCHIBLI, STEVEN HOLDCROFT, Simon Fraser University — The structure of novel polymers for anion exchange membranes (AEMs) is investigated using wide angle X-ray scattering (WAXS) combined with molecular dynamics (MD) simulations using a united-atom force field model based on the DREIDING force field. The polymers being studied are poly(benzimidazole) (PBI) derivatives including poly(dimethylbenzimidazole) (PDIMBI), mesitylene poly(benzimidazole) (mes-PBI), and mesitylene poly(dimethylbenzimidazole) (mes-PDMIBI). WAXS reveals an amorphous structure with two main length scales. By comparing simulation results to WAXS data, we attribute features observed in the scattering data to side-to-side spacing between polymer chains and to the parallel-ring stacking of the benzimidazole rings. Overall, we are able to validate the interpretation of scattering data by combining MD simulations and scattering experiments.

M1.00112 Charge Transport and Dynamics in Confined Phosphonium-based Ionic Liquids1, TYLER COSBY, University of Tennessee, Knoxville, KATSUHIKO TSUNASHIMA, National Institute of Technology, Wakayama College, JOSHUA SANGORO, University of Tennessee, Knoxville — Charge transport and structural dynamics in a homologous series of phosphonium-based ionic liquids confined in silica nanopores are investigated by broadband dielectric spectroscopy and Fourier transform infrared spectroscopy. The impact of alkyl chain length and hydrophobic aggregation on the physicochemical properties as well as the interplay between confinement effects and pore-wall interactions through silica surface silanization are investigated. The results are discussed within the framework of current understanding of confinement effects in liquid systems, especially in comparison to imidazolium-based ionic liquids.

M1.00113 Charge Transport and Dynamics in Confined Ammonium and Phosphonium-based Ionic Liquids, MATTHEW HARRIS, TYLER COSBY, Univ of Tennessee, Knoxville, KATSUHIKO TSUNASHIMA, National Institute of Technology, Wakayama College, JOSHUA SANGORO, Univ of Tennessee, Knoxville — Charge transport and structural dynamics in a homologous series of ammonium and phosphonium ionic liquids confined in silica nanopores are investigated by broadband dielectric spectroscopy and Fourier transform infrared spectroscopy. The impact of the central atom of the cation on the physicochemical properties as well as the interplay between confinement effects and pore-wall interactions through silica surface silanization are investigated. The results are discussed within the framework of current understanding of confinement effects in liquid systems, especially in comparison to imidazolium-based ionic liquids.

M1.00114 Amphiphilic Zwitterionic Coatings for Marine Anti-Biofouling Applications, EDWIN WALKER JR, C. K. PANDIYARAJAN, KIRILL EFIMENKO, JAN GENZER, North Carolina State Univ — Marine biofouling is a problem plaguing the surfaces of cargo ships, military ships and submarines. Previous approaches have relied primarily on the use of Cu-based coatings, which have deleterious effects on the marine environment. We studied the resistance of the coatings towards non-specific protein adsorption using fibrinogen and BSA.

1 NSF DMR Polymers Program
M1.00115 How does the molecular network structure influence PDMS elastomer wettability?  
MATTHEW MELILLO, JAN GENZER, North Carolina State University — Poly(dimethylsiloxane) (PDMS) is one of the most common elastomers, with applications ranging from medical devices to absorbents for water treatment. Fundamental understanding of how liquids spread on the surface of and absorb into PDMS networks is of critical importance for the design and use of another application - microfluidic devices. We have systematically studied the effects of polymer molecular weight, loading of tetra-functional crosslinker, end-group chemical functionality, and the extent of dilution of the curing mixture on the mechanical and surface properties of end-linked PDMS networks. The gel and sol fractions, storage and loss moduli, liquid swelling ratios, and water contact angles have all been shown to vary greatly based on the aforementioned variables. Similar trends were observed for the commercial PDMS material, Sylgard-184. Our results have confirmed theories predicting the relationships between modulus and swelling. Furthermore, we have provided new evidence for the strong influence that substrate modulus and molecular network structure have on the wettability of PDMS elastomers. These findings will aid in the design and implementation of efficient microfluidics and other PDMS-based materials that involve the transport of liquids.

M1.00116 The effects of elastocapillary length on the surface creasing instability of hydrogels  
TESTU OUCHI, Univ of Mass - Amherst, QIHAN LIU, ZHIGANG SUO, Harvard University, RYAN HAYWARD, Univ of Mass - Amherst — Creasing is a mode of surface instability induced by compressing elastomers or gels. Formation of creases is known to proceed by a nucleation and growth process, and the critical nucleus size is thought to be determined by the elastocapillary length (defined by the ratio of surface tension to elastic modulus). Here, we vary the elastocapillary length over the range of 0.008 to 0.4 mm by preparing a series of soft hydrogels with different compositions and contacting them with humidified air. By rapidly applying compression, we are able to achieve strains that exceed the Maxwell strain (where creases become favorable compared to a flat surface) by more than 0.10, and which approach Biot’s prediction for linear instability of a compressed half-space. Regardless of the conditions, however, we observe formation of creases only by nucleation and growth, although the density of nucleation sites is found to be sensitive to elastocapillary length. Interestingly, fast propagation of creases (at velocities similar to the speed of sound in the material) are found at strains approaching Biot’s point.

M1.00117 Computer Simulations of Bottlebrush Melts and Soft Networks  
ZHEN CAO, Univ of Akron, JAN-MICHAEL CARRILLO, Oak Ridge National Laboratory. SERGEI SHEIKO, Univ of NC - Chapel Hill, ANDREY DOBRYNIN, Univ of Akron — We have studied dense bottlebrush systems in a melt and network state using a combination of the molecular dynamics simulations and analytical calculations. Our simulations show that the bottlebrush macromolecules in a melt behave as ideal chains with the effective Kuhn length bK. The bottlebrush induced bending rigidity is due to redistribution of the side chains upon backbone bending. Kuhn length of the bottlebrushes increases with increasing the side-chain degree of polymerization nsc as bK(nsc) ∝ nsc 0.46. This model of bottlebrush macromolecules is extended to describe mechanical properties of bottlebrush networks in linear and nonlinear deformation regimes. In the linear deformation regime, the network shear modulus scales with the degree of polymerization of the side chains as G0 ∝ (nsc + 1)−1 as long as the ratio of the Kuhn length to the size of the fully extended bottlebrush backbone between crosslinks, Rmax, is smaller than unity, bK / Rmax << 1. Bottlebrush networks with bK / Rmax ∝ 1 demonstrate behavior similar to that of networks of semiflexible chains with G0 ∝ nsc 0.5. In the nonlinear deformation regime, the deformation dependent shear modulus is a universal function of the first strain invariant I1 and bottlebrush backbone deformation ratio β describing stretching ability of the bottlebrush backbone between crosslinks.

M1.00118 Modeling polymer gel that strengthen under tension  
SANTIDAN BISWAS, VICTOR V. YASHIN, ANNA C. BALAZS, Univ of Pittsburgh — We develop a constitutive model of a responsive polymer gel, which can reversibly form additional crosslinks when under tension. We assume that the polymer chains incorporate the folded domains encompassing the reactive functional groups (cryptic sites). Under extension of the network, the domains unfold and expose the cryptic sites, which can then form labile bonds with the linker chains grafted to the network. Once the deformation is removed, the linkers detach from the cryptic sites, and unfolded domains go back to the folded configuration thus hiding the cryptic sites. The gel behavior under applied force is described by the equations of elasticity of the polymer network coupled to the kinetic equations for the unfolding and binding transitions. The developed model could be used for designing new polymer gel-based materials that exhibit self-strengthening in response to a mechanical action.

M1.00119 Modeling thermal-mechanical behavior of networks with reconfigurable crosslinks  
JEH-CHANG YANG, YUAN MENG, MITCHELL ANTHAMATTEN, University of Rochester — Actively moving polymers nearly always involve the storage or release of mechanical energy using external stimuli. Thermomechanical experiments were conducted on well-defined chemical networks bearing both permanent and light-responsive covalent junctions. Experimental data include stress relaxation and mechanical creep during photoinduced network reconfiguration as well as equilibrium stress-strain behavior of reprogrammed networks. Physical models of elastic networks were applied to describe thermomechanical behavior during and after bond re-formation while under external stress. The role of dangling ends in influencing competitive network mechanics is evaluated to explain observed phenomena and discrepancies between theory and data. Understanding how process path is related to the equilibrium thermomechanics of such reprogrammed networks is important to engineering shape actuator driven by crystallization.

M1.00120 Imparting large macroscopic changes with small changes in polypeptide composition  
MICHELLE SING, GARETH MCKINLEY, BRADLEY OLSEN, Massachusetts Institute of Technology — Block copolymers composed of polypeptides provide an excellent platform for exploring the underlying physics surrounding macroscopic associative network behavior. Previous work in our group has elucidated a difference in the mechanical properties of two nearly identical elastin-like polypeptide (ELP) endblocks. In poly(ELP)s, this substitution is known to result in tighter beta turns. These beta turns exhibit slower responses to changes in temperature within the material. Under shear, the modulus for the alanine-containing ELP triblock is almost three times higher than the glycine-containing ELP. Additionally, preliminary tensile tests show higher stress and strain at break for the alanine ELP triblock. We are able to explain the reasons for this behavior using a variety of spectroscopic and analytical techniques. Small angle neutron and x-ray scattering indicate differences in ordering between the alanine and glycine containing ELP materials both in shear and in stagnant flow.

M1.00121 Effect of Temperature and Strain on a Self–assembled Gel  
SATISH MISHRA, SATANU KUNDU, Mississippi State University — Gels are widely used in food industry and biomedical field. For physically associating gels, mechanical properties depend on the nature of association between the polymer and the solvent. A thermoreversible, physically associating gel is considered here, which consists of 10% (v/v) poly (methyl methacrylate) - poly (n-butyl acrylate) - poly (methyl methacrylate) in butanol, a midblock selective solvent. Below gelation temperature, the end blocks collapse and form aggregates, and the mid-blocks act as bridges between those aggregates. Rheo-SANS experiments were conducted on these samples where small angle neutron scattering (SANS) and shear-rheology experiments are combined. SANS data were collected over a wide temperature range, from 65C to -10C with and without strain. Near the gelation temperature, SANS data can be fitted with hard sphere model. However, with decrease of temperature, structural changes, due to clustering of aggregates, are observed. The SANS and rheological results in combination provide insight in structural changes of the gel with strain and temperature, respectively.
M1.00122 Rubber Elasticity for percolation network consisting of Gaussian Chains, KENGO NISHI, Georg-August-Universitét Göttingen, MITSUHIRO SHIBAYAMA, TAKAMASA SAIKAI, The University of Tokyo — A theory describing the elastic modulus for percolation networks of Gaussian chains on general lattices such as square and cubic lattices is proposed and its validity is examined with simulation and mechanical experiments on well-defined polymer networks. The theory was developed by generalizing the effective medium approximation for Hookean spring network (EMA) to Gaussian chain networks. From EMA theory, we found that the ratio of the elastic modulus at pC to that at p = 1G0 must be equal to \(G/G_0 = (p - 2f)/(4 - 2f)\) if the position of sites can be determined so as to meet the force balance, where \(f\) is the degree of cross-linking reaction. However, the EMA prediction cannot be applicable near its percolation threshold because EMA is a mean field theory. Thus, we combine real-space renormalization and EMA, and propose a theory called real-space renormalized EMA, i.e., REMA. The elastic modulus predicted by REMA is in excellent agreement with the results of simulations and experiments of near-ideal diamond lattice gels.

Please set this talk on Mon, Tue, or Wed (March 14-16) just after its accompanying talk, MAR16-2015-000773.

M1.00123 Nonlinear Stress Relaxation of “Quasi-monodisperse” Polyisoprene and Poly(p-tert-butylstyrene), HIROSHI WATANABE, YUMI MAKINO, KEIKO SHIBAIHARA, GABRIEL ARECHEDERRA, JAMIE KROPKA, Sandia National Laboratories — The observance of an increase in glassy polymer relaxation rates under a mechanical deformation is often referred to as deformation induced mobility (DIM). It has been argued that stress relaxation experiments can provide indirect evidence of this phenomenon. Recently, stress relaxation experiments have been interpreted as demonstrating a mobility decrease with increased deformation when very slow strain rates, \(1.2 \times 10^{-4} \text{s}^{-1}\), are used to apply the deformation. This would suggest against generality of DIM and would not agree with expected surface tension changes associated with each photochemical transformation. We believe this patterning methodology will be potentially useful out of those regions can be directed with precision. To this end, we describe here a photopolymer whose melt-state surface tension can be selectively raised or lowered in light exposed regions depending on the wavelength and dose of applied light. The direction of Marangoni flow into or out of irradiated regions agrees with expected surface tension changes associated with each photochemical transformation. We believe this patterning methodology will be potentially useful for high throughput fabrication environments such as roll-to-roll processing that can exploit contact-free and solvent-free topography development.

M1.00124 Bidirectional Control of Flow in Thin Polymer Films by Photochemically Manipulating Surface Tension, CHAE BIN KIM, DUSTIN JANES, SUNSHINE ZHOU, AUSTIN DULANEY, CHRISTOPHER ELLISON, The University of Texas at Austin — The Marangoni effect causes transport of liquids in response to surface tension gradients. In a thin polymer film, such flow results in formation of topographic features that could be exploited as a practically useful route to manufacture patterned surfaces. An especially versatile material for this application should be able to be spatially programmed to possess regions of higher or lower relative surface tension so that the direction of flow into or out of those regions can be directed with precision. To this end, we describe here a photoresponsive liquid whose melt-state surface tension can be selectively raised or lowered in light exposed regions depending on the wavelength and dose of applied light. The direction of Marangoni flow into or out of irradiated regions agrees with expected surface tension changes associated with each photochemical transformation. We believe this patterning methodology will be potentially useful for high throughput fabrication environments such as roll-to-roll processing that can exploit contact-free and solvent-free topography development.

M1.00125 Dynamics of associating polymers and the sticky Rouse model: a study by combined dielectric and dynamic mechanical techniques, YANGYANG WANG, Oak Ridge National Laboratory, TYLER COSBY, JOSHUA SANGORO, University of Tennessee, Knoxville — Reversible association through non-covalent bonding is ubiquitous in the soft matter world. Despite decades of studies, the dynamics of associating polymers have not been well understood. Here we examine the dynamics of butadiene- and isoprene-based model polymeric systems with pairwise association through hydrogen bonding. Compared to ionomers, where reversible crosslinks are typically not well defined, these hydrogen bonding polymers are associated through strictly binary contacts and thus provide a better opportunity to test theoretical ideas. By combining dielectric spectroscopy and dynamic mechanical measurement, we are able to identify both chain and junction dynamics and analyze their motional coupling mechanism. The results are discussed in the context of the sticky Rouse model.

M1.00126 Evolution of Yield Stress during Structural Relaxation for the Epoxy 828DEA, GABRIEL ARECHEDERRA, JOHN MCCOY, New Mexico Tech, JAMIE KROPKA, Sandia National Laboratories — The evolution of yield stress from structural relaxation of diethanolamine cured diglycidyl ether of bisphenol-A, 828DEA, was tracked using uniaxial compression experiments. Samples were aged isothermally, and the progression of the fictive temperature in order to interpret the evolution of yield stress.


M1.00127 Can Stress Relaxation Experiments be Used to Assess Deformation Induced Mobility in Glassy Polymers?, JAMIE KROPKA, KEVIN LONG, Sandia National Laboratories — The observance of an increase in glassy polymer relaxation rates under a mechanical deformation is often referred to as deformation induced mobility (DIM). It has been argued that stress relaxation experiments can provide indirect evidence of this phenomenon. Recently, stress relaxation experiments have been interpreted as demonstrating a mobility decrease with increased deformation when very slow strain rates, \(1.2 \times 10^{-4} \text{s}^{-1}\), are used to apply the deformation. This would suggest against generality of DIM and would not agree with expected surface tension changes associated with each photochemical transformation. We believe this patterning methodology will be potentially useful for high throughput fabrication environments such as roll-to-roll processing that can exploit contact-free and solvent-free topography development.

M1.00128 Chain networking revealed by molecular dynamics simulation, YEXIN ZHENG, MESFIN TSIGE, SIH-QING WANG, Department of Polymer Science, University of Akron — Based on Kremer-Grest model for entangled polymer melts, we demonstrate how the response of a polymer glass depends critically on the chain length. After quenching two melts of very different chain lengths (350 beads per chain and 30 beads per chain) into deeply glassy states, we subject them to uniaxial extension. Our MD simulations show that the glass of long chains undergoes stable necking after yielding whereas the system of short chains is unable to neck and breaks up after strain localization. During ductile extension of the polymer glass made of long chain significant chain tension builds up in the load-bearing strands (LBSs). Further analysis is expected to reveal evidence of activation of the primary structure during post-yield extension. These results lend support to the recent molecular model and are the simulations to demonstrate the role of chain networking. This work is supported, in part, by a NSF grant (DMR-EAGER-1444859)

M1.00129 How plasticizer makes a ductile polymer glass brittle?1, YUE ZHAO, XIAOXIAO LI, SHI-QING WANG, Univ of Akron — During uniaxial extension, a polymer glass of high molecular weight is ductile at high temperatures (still below Tg) and turns brittle when the temperature is sufficiently lowered. Incorporation of small-molecular additives to polymer glasses can speed up segmental relaxation considerably. The effect of such plasticization should be to make the polymers more ductile. We examined the effect of blending a few weight percent of either triphenyl phosphate (TPP) or a mineral oil to a commercial-grade PS and PMMA. Our Instron tests show that the plasticized PS is less ductile. Specifically, at 70 oC, the original PS is ductile at an extensional rate of 0.02 s-1 [1] whereas the PS with 4 wt. % TPP turns brittle. Mechanical spectroscopic measurements show that the alpha relaxation time is shortened by more than two orders of magnitude with 4 wt. % TPP. On the other hand, such anomalous behavior did not occur in PMMA. We need to go beyond the conventional description to rationalize these results. [1] Li, X.; Wang, S. Q. ACS Macro Letters 2015, 1110-1113.

M1.00130 Surface diffusion of molecular glasses: Material dependence and impact on physical stability1, SHIGANG RUAN, WEI ZHANG, LIAN YU, University of Wisconsin-Madison — Surface diffusion coefficients have been measured for molecular glasses tris-naphthylbenzene (TNB) and PMMA oligomers by surface grating decay. Surface diffusion on TNB is vastly faster than bulk diffusion, by a factor of 107 at Tg, while the process is very slow on PMMA. Along with the previous results on o-terphenyl, nifedipine, indomethacin, and polystyrene oligomers, we find that surface diffusion slows down with increasing molecular size and intermolecular forces, whereas bulk diffusion has a weaker material dependence. The molecular glasses studied show fast crystal growth on the free surface. A general correlation is observed between the coefficient of surface diffusion and the velocity of surface crystal growth, indicating surface crystallization is supported by surface mobility. (Zhu, L., et al. Phys. Rev. Lett. 106 (2011): 256103; Zhang, W., et al. J. Phys. Chem. B 119 (2015): 5071-5078)

M1.00131 Liquid Crystalline Phases of Polymer Brushes1, KIANA AMINI, NASSER ABUKHDEIR, MARK MATSEN, University of Waterloo — The phase behavior of liquid-crystal polymeric brushes in solvent are investigated using self-consistent field theory. The polymers are modeled as freely-jointed chain consisting of N rigid segments. The isotropic interactions between the polymer and the solvent are treated using the standard Flory-Huggins theory, while the anisotropic liquid-crystalline (LC) interactions between rigid segments are taken into account using the Mayer-Saupe theory. For weak LC interactions, the brush exhibits the conventional parabolic-like profile, while for strong LC interactions, the polymers crystallize into a dense brush with a step-like profile. At intermediate interaction strengths, we find the microphase-segregated phase observed previously for lattice-model calculations in this phase, the brush exhibits a crystalline layer next to the grafting surface with an external layer similar to the conventional brush.

M1.00132 Thermal Characterization of Thermotropic Nematic Liquid-Crystalline Elastomers, DAVID THOMAS, MATT CARDARELLI, Tufts University, ANTONI SANCHEZ-FERRER, ETH Zurich, BADEL L. MBANGA, TIMOTHY J. ATHERTON, PEGGY CEBE, Tufts University — Nematic Liquid-Crystalline Elastomers (LCEs) are weakly crosslinked polymeric networks that exhibit rubber elasticity and liquid-crystalline orientational order due to the presence of mesogenic groups. Three end-on side-chain nematic LCEs were investigated using real-time synchrotron wide-angle X-ray scattering (WAXS), differential scanning calorimetry (DSC), and thermogravimetry (TG) to correlate thermal behavior with structural and chemical differences among them. The elastomers differed in crosslinking density and mesogen composition. Thermally reversible glass transition temperature, Tg, and nematic-to-isotropic transition temperature, Tni, were observed upon heating and cooling for all samples. By varying the heating rate, Tg and Tni were determined at zero heating rate. The temperature dependence of the orientational order parameter was determined from the anisotropic azimuthal angular distribution of the equatorial reflection seen during real-time WAXS experiments. Our results show that the choice of crosslinking unit, its shape, density, as well as the structure of co-monomers, all influence the temperature range over which the thermal transitions take place.

M1.00133 Crystal Growth Theory for Random Copolymers of Crystallizable and Non-crystallizable Units, HERVE MARAND, HADI MOHAMMADI, Virginia Tech, Department of Chemistry — While the presence of randomly distributed non-crystallizable units (e.g. short branches in metalloocene linear low density polyethylene) has been carefully considered in the thermodynamics of copolymers crystallization, it has been mostly ignored in the analysis of crystal growth rate data. In this work, we present an extension of the Lauritzen-Hoffman (LH) secondary nucleation theory that considers crystal growth processes for random copolymers of crystallizable and non-crystallizable units. Concentrating on the distribution of crystallizable unit sequence lengths rather than the whole polymer chain, rate equations in the LH theory are modified to account for the population of crystallizable sequences able to form a specific number of folds. We then calculate the flux over the nucleation barrier for each lamellar thickness, the secondary nucleation rate, i, the substrate completion rate, g, and derive the crystal growth rate, G, as a function of crystallization temperature. The model also allows prediction of the lamellar thickness distribution as a function of crystallization temperature. In qualitative agreement with literature data, our model predicts lower crystal growth rates and higher average lamellar thicknesses for m-LLDPE than for linear polyethylene at the same undercooling.

M1.00134 Flow-induced Crystallization of Long Chain Aliphatic Polyamides under a Complex Flow Field1, XIA DONG, YUNYUN GAO, LILI WANG, DUJIN WANG, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry CAS — The present work deals with the flow-induced multiple orientations and crystallization structure of polymer melts under a complex flow field. This complex flow field is characteristic of the consistent coupling of extensional pulse and closely followed shear flow in a narrow channel. Utilizing an ingeniously combination of an advanced micro-injection device and long chain aliphatic polyamides, the flow-induced crystallization of advanced polymer morphology was well preserved for ex-situ synchrotron micro-focused wide angle X-ray scattering as well as small angle X-ray scattering. The experimental results clearly indicate that the effect of extensional pulse on the polymer melt is restrained and further diminished due to either the transverse tumble of fountain flow or the rapid retraction of stretched high molecular weight tails. However, the residual shish-kebab structures in the core layer of the far-end of channel suggest that the effect of extensional pulse should be considered in the small-scaled geometries or under the high strain rate condition.

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1This work was supported by NSERC of Canada.


1This work was supported by NSERC of Canada.
M1.00135 Effects of mechanical strain and heat on the strain-induced crystalline $\beta$ to $\alpha$ structural transition of syndiotactic polystyrene. - FUJUAKI ENDO, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University - The polymorphic behavior of syndiotactic polystyrene (sPS) during the $\beta$ to $\alpha$ form transition was investigated. sPS presents complex polymorphism with five crystalline forms. Quite a few crystalline structural transitions have also been reported, including our recent discovery of the structural transition from $\beta$ to $\alpha$ forms induced by tensile deformation at around 200°C. In this study, we analyzed the individual effects of mechanical strain and heat on the $\beta$ to $\alpha$ crystalline structural transformation caused by the mechanical deformation. sPS film samples containing $\beta$ form crystals were prepared and stretched at 130°C (near the glass transition temperature of sPS), followed by the annealing process of the samples below the melting temperature. X-ray analyses revealed that the stretched sample possessed mesomorphic $\alpha$ forms, indicating that the mechanical strain could invoke the destruction of $\beta$ form crystals by producing mesomorphic $\alpha$ forms. Interestingly, the annealed samples exhibited sharp X-ray reflections typical of $\alpha$ forms, which became even sharper by the increase in the annealing temperature. It was therefore concluded that the heat could induce the structural transitions from mesomorphic $\alpha$ forms to perfect $\alpha$ forms.

M1.00136 Tracing Poly(ethylene-oxide) Crystallization using Atomic Force Microscopy - XAVIER CAPALDI, SAMUEL MANUEL, None - The early stages of nucleation and crystallization of Poly(ethylene-oxide) have been studied using Atomic Force Microscopy equipped with a heating and cooling stage. Effects of molecular weight and sample preparation techniques were studied using amplitude and frequency modulation. Mapping the viscoelastic behavior at different temperatures and has enabled the development of a relatively new technique for following the evolution of crystallization and melting of a semi-crystalline polymer.

M1.00137 Viscoelastic Properties of Fluorinated Ethylene-Propylene (FEP) Random Copolymers - MEGAN CURTIN*, BENJAMIN WRIGHT*, Chemical and Biological Engineering, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute - Fluorinated ethylene-propylene (FEP) random copolymers contain tetrafluoroethylene (TFE) and hexafluoropropylene (HFP) repeat units. FEP is an excellent alternative to poly(tetrafluoroethylene), PTFE, which cannot be melt processed due to its high molecular weight and extensive crystallinity. On the other hand, FEP is a meltprocessable polymer and offers similar if not the same properties as PTFE. Many studies have been performed on FEP over the years, however, the properties of these polymers strongly depend on the HFP concentration and molecular weight (distribution). Just like PTFE, FEP cannot be dissolved in many solvents, therefore, obtaining molecular weight distribution of these polymers is not possible with commonly used methods. In the current study, we perform rheological analysis of various FEPs and obtain their molecular weight distributions by employing the Tuminello method.

M1.00138 Thermal Properties of Trogamid by Conventional and Fast Scanning Calorimetry - PEGGY CEBE, JOHN MERFELD, BIN MAO, Tufts University, ANDREAS WURM, EVGENY ZHURAVLEV, CHRISTOPH SCHICK, University of Rostock - We use conventional slow scan rate differential scanning calorimetry, and fast scanning chip-based calorimetry (FSC), to investigate the crystallization and melting behavior of Trogamid, a chemical relative of nylon. Fundamental thermal properties of Trogamid were studied, including the melt crystallization kinetics, heat of fusion, and the solid and liquid state heat capacities. Using slow scan DSC (at 5 K/min), Trogamid displays a glass transition relaxation process at ~133°C, melting endotherm peak at 250°C, and is stable upon repeated heating to 310°C. When using slow scan DSC, the isothermal melt crystallization temperatures were restricted to 225°C or above. Trogamid crystallizes rapidly from the melt and conventional calorimetry is unable to cool sufficiently fast to prevent nucleation and crystal growth prior to stabilization at lower crystallization temperatures. Using FSC we were able to cool nano-gram sizes samples at 2000 K/s to investigate a much lower range of melt crystallization temperatures, from 205-225°C. The experimental protocol for performing FSC on semicrystalline polymers to obtain liquid state heat capacity data will be presented.

M1.00139 Polymer crystallization in thin films: morphology and physical properties - GIOVANNI KELLY, JULIE ALBERT, Tulane University - Polymer crystallization has been studied both computationally and experimentally for decades, elucidating many of the mysteries surrounding crystallization kinetics and thermodynamics. However, many unanswered questions remain pertaining to the relationships between crystallization phenomena and material properties needed for specific applications that range from drug delivery and tissue engineering to optical devices and mechanically robust membranes. One of the especially interesting facets of polymer crystallization is the behavior observed when these long chain molecules are spatially confined in thin and ultrathin films. Confined geometry leads to chain configurations, and therefore thermal, mechanical, and optical properties, sometimes far removed from reported bulk values. This project aims to study the phenomena exhibited by linear semi-crystalline polymers in thin films as well as the way in which blending with homopolymers, block copolymers, and novel polymer chain architectures affect morphology, biodegradation, optical, thermal, and mechanical properties.

M1.00140 Morphological Evolution During Tensile Deformation in Semi-Crystalline Precise Functional Copolymers via Fitting of In Situ Xray Scattering - EDWARD B. TRIGG, L. ROBERT MIDDLETON, University of Pennsylvania, BRIAN S. AITKEN, University of Florida, JASON AZOULAY, DUSTIN MURTAGH, Sandia National Laboratories, KENNETH B. WAGENER, University of Florida, JOSEPH CORDARO, Sandia National Laboratories, KAREN I. WINEY, University of Pennsylvania - Morphological evolution during tensile deformation of semi-crystalline polymers is often described qualitatively. The layered crystalline structures of precise copolymers, in which functional groups are bonded at precise intervals along the polymer backbone, allow for quantitative fitting of oriented X-ray scattering peaks to provide additional information. The crystallites in precise poly(ethylene-co-acrylic acid) align with the acid group layers' normal vector parallel to the tensile direction, while those in precise poly(ethylene-co-imidazolium bromide) align with the layers' normal vector perpendicular to the tensile direction. We present fits of in situ X-ray scattering during tensile deformation of semi-crystalline precise copolymers, to quantify the size, shape, and degree of orientation of the crystallites during the deformation process. Mathematical descriptions of the X-ray scattering in these two cases are explored, and a physical explanation for the difference in alignment direction is proposed.

M1.00141 Probing polyethylene crystallization via simultaneous Raman scattering, rheology and microscopy - KALMAN MIGLER, ANTHONY KOTULA, ANGELA HIGHT WALKER, NIST - The structure and rheology of polyolefins during crystallization is of critical importance to the polymer processing industry. Here we present simultaneous Raman scattering, rheological and optical microscopy measurements of crystallizing high density polyethylenes during quiescent and slow flow conditions. Raman scattering measurements during quiescent crystallization allow us to quantify three different mass fractions of chain conformers: an amorphous fraction, an orthorhombic crystalline fraction, and a fraction of chains that contain many consecutive trans bonds but are not part of the orthorhombic crystal. These non-crystalline consecutive trans (NCCT) conformers are generated as a precursor to crystallinity. Slow steady shear rates (1 s⁻¹) applied during isothermal crystallization experiments dramatically increase the crystallization rate as well as the amount of NCCT conformers produced. Optical measurements of sheared samples during crystallization reveal the formation of fiber structures that compositionally contain more NCCT conformers than the surrounding melt. The increase in the complex shear modulus commonly measured for crystallizing polyethylenes correlates with the growth of chain conformers and the appearance of spherulites within the melt.
M1.00142 Molecular simulations of the formation of semi-crystalline structure from supercooled polyethylene melt. PENG YI, Johns Hopkins Univ — Formation of semi-crystalline structure is important for industrial processing, but it is scientifically poorly understood due to the strong anisotropy and the conformational flexibility of polymer chains. In this work we report the results of molecular dynamics simulations of homogeneous crystallization from polyethylene melts. A realistic united atom model was used. At room temperature (~30% supercooling), the crystal nucleation and growth lead to a stable semi-crystalline structure, with crystal lamellae separated by amorphous regions. Entanglement in the amorphous region prevents further crystal growth. The crystal-amorphous interface migrates with changing annealing temperature. Chain segments in the amorphous region adopt loop, bridge and tail conformations. Their populations and lengths were calculated and analyzed.

M1.00143 Engineering Multi-scale Electrospin Structure for Integration into Architected 3-D Nanofibers for Cimex Annihilation: Fabrication and Mechanism Study. SHAN HE, LINXIN ZHANG, Stony brook university, YING LIU, Advanced Energy Research and Technology Center, MIRIAM RAFAILOVICH, Stony Brook University, GARCIA CENTER FOR POLYMERS AT ENGINEERED INTERFACES TEAM — In this study, engineered electrospin scaffolds with fibers oriented with designed curvature in three dimensions (3D) including the looped structure were developed based on the principle of electrostatic repulsion. Here we illustrate that 3D electrospin recycled polystyrene fibers could closely mimic the unique architectures of multi-direction and multi-layer nano-spiralweb. In contrast to virgin PS, the recycled PS (Dart Styrofoam) are known to contain zinc stearate which acts as a surfactant resulting in higher electrical charge and larger fiber curvature, hence, lower modulus. The surfactant, which is known to decrease the surface tension, may have also been effective at decreasing the confinement of the PS, where chain stretching was shown to occur, in response to the high surface tension at the air interface. Three dimensional flexible architecture with complex structures are shown to be necessary in order to block the motion of Cimex lectularius. Here we show how an engineered electrospin network of surfactant modified polymer fibers with calculated dimensions can be used to immobilize the insects. The mechanical response of the fibers has to be specifically tailored so that it is elastically deformed, without fracturing or flowing. Carefully controlling and tailoring the electrospinning parameters we can now utilize architected 3D nanofiber to create an environmental-friendly Cimex immobilization device which can lead to annihilation solution for all the other harmful insects.

M1.00144 From Non-equilibrium to Equilibrium: Micellar Kinetics seen by Time-resolved Small-angle Scattering. REIDAR LUND, Department of Chemistry, University of Oslo — The kinetic pathways of self-assembled nanostructures are not fully understood. Time-resolved small-angle X-ray/neutron scattering (TR-SAXS/SANS) is a powerful technique that allows kinetics processes such as nucleation processes and morphological transitions to be followed with structural resolution over time scales starting from milliseconds. Neutrons offer the additional advantage of facile contrast variation through H/D substitution schemes, which also allow equilibrium processes such as molecular exchange and diffusion to be studied. Here we will highlight the current capabilities of TR-SAS and show results on the kinetics of polymeric micelles. We will address how the understanding of kinetic pathways can be used control the nanostructure.


M1.00145 Characterization and Molecular Simulation of Poly(p-phenylene/m-phenylene) Copolymers. ROBERT BUBECK, Michigan State University, STEVEN KEINATH, Michigan Molecular Institute - Retired — Characterization and molecular simulation of the molecular structure and microstructure of poly(p-phenylene/m-phenylene) copolymers were carried out. Tensile modulus, yield stress, and entanglement molecular weight were modeled as amorphous polymers as a function of m-phenylene content. Significant biphasic character, however, was observed for two copolymers in the melt near 300°C using variable temperature synchrotron-based WAXS. The biphasic nature of the melt may be a contributor to difficulty in melt processing. Precise experimental determinations of entanglement molecular weights were frustrated by the occurrence of significant amounts of nematic mesophase order in the rubbery and melt regimes of two commercial poly(p-phenylene/m-phenylene) examples. Nonetheless, entanglement molecular weights obtained by molecular modeling can be useful for experimental guidance because the level of order in the glassy phase near ambient temperature was found to be low (5 %) regardless of melt processing history. Based on both the modeling and WAXS measurements, it is believed that increasing m-phenylene content reduces modulus, and improves toughness and processibility.

1 Beamtine at the Cornell High Energy Synchrotron Source is gratefully acknowledged.

M1.00146 Thermal Conductivity behavior of MWCNT based PMMA and PC composites. GIRLIA DUBEY, York College-CUNY, NY11451, PRASHANT JINDAL, University Institute of Engineering & Technology, Panjab University,160014, India, RAJIV BHANDARI, NEHA DHIMAN, CHETAN BAJAJ, VIJAY JINDAL, Department of Physics, Panjab University, Chandigarh 160014, India — Poly methyl methacrylate (PMMA) and Polycarbonate (PC) are low cost polymer materials which can be easily transformed into desired shapes for various applications. However they have poor mechanical, thermal and electrical properties which are required to be enhanced to widen their scope of applications specifically where along with high strength, rapid heat transfer is essential. Multi Walled Carbon nanotubes (MWCNTs) are excellent new materials having extraordinary mechanical and transport properties. We will report results of fabricating composites of varying compositions of MWCNTs with PMMA and PC and their thermal conductivity behaviour using simple transient heat flow methods. The samples in disk shapes of around 2 cm diameters and 0.2 cm thickness with MWCNT compositions varying up to 10 wt% were fabricated. We found that both PMMA and PC measured high thermal conductivity with increase in the composition of CNTs. The thermal conductivity of 10wt% MWCNT/PMMA composite increased by nearly two times in comparison to pure PMMA.
M1.00147 Rheological Properties of a Polybutadiene/Clay Nano-Composite Crosslinked via Thiol-ene Click Chemistry, VIJESH TANNA, H. HENNING WINTER, Univ of Mass - Amherst — We have created an industrially feasible processing method to create a novel polybutadiene/clay nanocomposite. The fabrication step was designed such that the final composite would be chemically crosslinked with in-diffused clay sheets dispersed randomly throughout the polymer matrix. Due to the polybutadiene’s high functionality, the composite’s storage modulus was shown to increase by several orders of magnitude due to crosslinking. In addition, the effect of reinforcements due to clay was shown to double the storage modulus of the composite due to the high elasticity of individual clay sheets. Surprisingly, we observed a critical crossover frequency, \( \omega_c \), below which the mechanical properties, complex modulus, of the neat crosslinked polymer slightly exceed that of the composite. This transition may be due to the large lateral dimensions of the individual clay sheets, hundreds of microns, preventing a small number of crosslinks from forming. We have shown that reinforcement from both chemical crosslinks and clay significantly improves the mechanical properties of the polybutadiene/clay composite and have quantified this reinforcement over a wide range of temperatures and frequencies.

M1.00148 Quantum Molecular Dynamics Validation of Nanocarbon Synthesis by High-Temperature Oxidation of Nanoparticles\(^1\), CHUNYANG SHENG, KENICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, Collaboratory for Advanced Computing and Simulations, KOHEI SHIMAMURA, FUYUKI SHIMOJO, Department of Physics, Kumamoto University, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, DEPARTMENT OF PHYSICS, KUMAMOTO UNIVERSITY COLLABORATION, CACS USC COLLABORATION — High-temperature oxidation of silicon-carbide nanoparticles (nSiC) underlies a wide range of technologies from high-power electronic switches for efficient electrical grid, thermal protection of space vehicles, to self-healing ceramic nanocomposites. Here, multimillion-atom reactive molecular dynamics simulations validated by \( \text{ab initio} \) quantum molecular dynamics simulations predict unexpected condensation of large graphene flakes during high-temperature oxidation of nSiC. In the validation process Small nSiC in oxygen environment is chosen to perform QMD simulation, then the QMD results provide the number of Si-O and C-O bonds as a function of time and high temperature, Same RMD simulation is simultaneously performed. We compare the time evolution of different bonds, and observe the condensation of large number of C-cluster nuclei into larger carbon clusters. We further provide the QMD simulation results as an input to a genetic algorithm, which trains the RMD force field parameters, the output force field produce results that are closer to the ground truth QMD simulation results.

\(^1\)This research was supported by the Department of Energy (DOE)

M1.00149 Role of Entropic Barriers in Controlling Polymer Diffusion in Polystyrene Nanocomposites, PHILIP GRIFFIN, WEI-SHAO TUNG, University of Pennsylvania, JEFFREY METH, Dupont, NIGEL CLARKE, University of Sheffield, RUSSELL COMPOSTO, KAREN WINEY, University of Pennsylvania — Polymer diffusion in polymer nanocomposites (PNCs) is significantly modified relative to the neat state. While it is suspected that nanoparticle-induced confinement plays a key role in the diffusion process, a detailed understanding of this process remains nonetheless elusive. We present recent studies of the temperature dependent polymer center-of-mass tracer diffusion coefficient in an athermal PNC comprising polystyrene and phenyl-capped, spherical silica NPs using elastic recoil detection. We find that the polymer tracer diffusion coefficient in the PNC relative to the bulk decreases with increasing nanoparticle concentration and is unexpectedly more strongly reduced at higher temperatures. This unusual temperature dependence of polymer diffusion in PNCs cannot be explained by the reptation model or a modified version incorporating an effective tube diameter, but instead it is the direct result of entropic free energy barriers imposed on polymer chains under confinement.

M1.00150 Morphology and Transport Properties of Novel Polymer Nanocomposites Resulted from Melt Processing of Polyvinylacetate Substrates Coated with Layer-by-Layer Assemblies, IMAN SOLTANI, RICHARD J. SPONTAK, North Carolina State Univ — Novel polymer nanocomposites (PNCs) were processed through layer-by-layer (LBL) deposition of clay and polyethylene terephthalate ionomer layers on polyvinylacetate (PVAc) substrates, followed by repetitive melt pressing of coated samples to crush LBL assemblies into the polymeric matrix. The increase in the clay content in resulted PNCs prepared through similar LBL coatings, relative to previously studied hydrophobic polystyrene-based nanocomposites, postulated superiority of PVAc, with relatively higher hydrophilicity, to interact with LBL assemblies. Also, these PNCs showed relatively good barrier improvement against transport of oxygen and carbon dioxide gases, proposing the scavenging effect of LBL assemblies crushed portions as highly tortuous labyrinths with high aspect ratios, comprising edge-edge flocculated exfoliated clay platelets, observed through transmission electron micrographs. However, combinative morphological investigations through optical microscopy, x-ray diffractometry, and transmission electron microscopy proposed low global dispersion of clay throughout polymeric matrix, conjecturing insufficient intensity of stress applied through cyclic melt pressing, and/or slight thermal degradation of samples via extended times of processing at high temperatures.

M1.00151 Polymer Dynamics by Dielectric Spectroscopy, JENNIFER ZEHNER, KARIN BICHLER, GERALD SCHNEIDER, Louisiana State University Chemistry Department — Theoretical modeling of polymer dynamics is fundamentally important to describe experimental results and to develop new materials. There are many different processes in polymers covering a very broad time range. Dielectric spectroscopy is able to cover a broad frequency range, around 10 decades. Thus many different processes can be studied and it provides a unique means to explore the processes and the time-scales. In our presentation, we emphasize how the line-structures permits to derive information on certain mechanisms. We use entangled melts and demonstrate the influence of entanglements, contour length-fluctuations and constraint release on the spectra and describe it by a theory. Furthermore, we compare it to rheology experiment and demonstrate those parts which are complimentary. We use this knowledge to achieve an advanced understanding of polymer dynamics in nanocomposites.

M1.00152 Polymer Dynamics in Blends, KARIN BICHLER, JENNIFER ZEHNER, GERALD SCHNEIDER, Louisiana State University Chemistry Department — Depending on their miscibility mixtures of polymers or polymers and nanoparticles tend to phase separate. Such systems are of fundamental interest. For example, in case of a blend of two polymer melts a dynamic asymmetry may be generated. It could slow down the chains in one phase or accelerate the chains in the other phase. Due to their heterogeneity these systems are of fundamental interest. Using a certain technique it is very challenging to access all of the information necessary to understand the materials and the interplay between different phases. In order to enhance our understanding, we apply dielectric spectroscopy, scattering experiments and atomic force microscopy to reveal both structure and dynamics and to unravel the fascinating processes.

M1.00153 Nonadiabatic Dynamical Studies of Lead Chalcogenide Quantum Dots (Pb\(_{16}\)X\(_{16}\); \( X = S, Se, Te \)) Passivated with thin Cadmium Chalcogenide Shells, PATRICK TAMUKONG, SVELTANA KILINA, North Dakota State University — DFT and TD-DFT studies of Pb\(_{16}X_{16}/Cd_{2}Y_{2}\) (\( X = S, Se, Te \)) core/shell quantum dots (QDs) have been performed to assess their ground (i.e., the optimized geometries, density of states, projected density of states, and optical absorption spectra), and excited state properties. Most of the heterostructures were analyzed for the first time (e.g., Pb\(_{16}S_{16}/Cd_{2}Te_{2}\) and Pb\(_{16}S_{16}/Cd_{2}Se_{2}\)). The thin shell core/shell QDs proved to be largely borderline type II with much similarly between QDs containing Cd\(_{2}S_{2}\) and Cd\(_{2}Se_{2}\) shells, whereas core/shell QDs with a Cd\(_{2}Te_{2}\) shell appeared to be borderline type-I. Nonadiabatic DFT-based dynamics, coupled with the surface hopping method, have been done to investigate fates of excited electrons or holes in these systems.
M1.00154 Emergent Magnetism in Mesoporous Materials, SHER ALAM, KEK Accelerator Lab, AJAYAN VINU, University of Queensland — We discuss the emergence of magnetism in Mesoporous Materials. We have obtained experimental results showing a variety of magnetic behaviors arising, by using different types of mesoporous or nanoporous templates. Since the templates allow different magnetic properties to arise naturally we have dubbed this as dynamic templating method. Our procedure and realization incidentally demonstrates the idea of Nanoarchitecronics proposed by Aono, as a MANA concept. Which, simply means to allow different nano-blocks to interact to obtain a certain desired structure and properties.

M1.00155 Using Self-Similarity to Simulate Meniscus Evolution Around TMV Due to Surface Diffusion, RICHARD POTTER, YUE ZHANG, ZAHRA FAKHRRAI, Univ of Pennsylvania — It has been hypothesized that enhanced surface diffusion allows the formation of stable molecular glasses during physical vapor deposition. The improved properties of these glasses, such as increased density and kinetic stability can help improve material properties in pioneering fields of technology such as organic electronics and pharmaceutical drug delivery. While surface diffusion has been measured previously on the surfaces of organic glasses, direct measurements on the surface of vapor-deposited stable glasses has proven more challenging. This research focuses on a straightforward method for measuring the surface diffusion coefficients of molecular glasses through the use of tobacco mosaic virus (TMV) nanorods as probe particles. In conjunction, mathematical models based on the thin film equation were used to simulate fast meniscus formation around the nanorods on the glassy surface. The evolution of the meniscus is self-similar, which allows quick quantification of the diffusion coefficient, by solving the time evolution for a single experiment. Experimental data were compared and fit to these simulations to derive a quantity for the surface diffusion coefficient, D. 

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M1.00156 Interfacial damping properties of polymeric composites: Effect of interfacial strength, YAPING HUANG, Nanyang Institute of Technology — Experimental studies on interfacial properties of polymeric composites, such as glass transition temperature, showed that the interfacial strength was critical. Numerical studies could also predict interfacial properties based on interfacial strength. In this study, interfacial damping properties and interfacial strength of fiber based polymeric composites were measured by dynamic mechanical tests and micro-bond tests, respectively, with the objective of quantitative analysis. Properties of polymers, varying from polar to non-polar, from amorphous to semi-crystalline, from low molecular weight to high molecular weight, were investigated. The results showed supportive predictions about interfacial damping properties of fiber based polymeric composites.

M1.00157 Equilibrium flattening process of irreversibly adsorbed polymer chains on a solid, MANI SEN, Materials Science and Engineering (MSE), Stony Brook University (SBU), NY, NAISHENG JIANG, MAYA ENDOH, TADANORI KOGA, MSE, SBU, DAISUKE KAWAGUCHI, KEIJI TANAKA, Kyushu University, Japan — We here report the equilibrium process of adsorbed polymer chains on a solid by sum frequency generation (SFG) spectroscopy. Polystyrene (PS, Mw = 290 kDa) thin films prepared onto quartz prisms (a weakly attractive system) were used as a model system. Spin-cast PS 50 nm films on quartz surface (QS) were annealed at 150°C for 100 h and subsequently rinsed with chloroform to derive the “flattened chains” that lie flat onto the substrate surface. The SFG results for the “matured” flattened chains after annealing for 96 h revealed the strong interfacial orientation of the backbone chains and weak orientation of PS phenyl rings at the QS which is in contrast to a PS spin-cast film annealed at 150°C for 1 h: the phenyl rings were strongly directed toward the QS, while the backbone chains were weakly oriented toward the QS. We postulate that the increase in the number of solid/segment contacts of the backbone chains is the driving force for this equilibrium flattening process. We will also discuss the generality of this flattening process by using solvent-cast PS thin films where the chains are randomly oriented near the QS.

3 Acknowledgement: NSF Grant No. CMMI-1332499.

M1.00158 Phase Transitions of 2-Decanol in Nano Pores, SAMUEL AMANUEL, JASON TURNER, CALEB NOVINS, ALEXANDER CLAIN, Dept. of Phys & Astro., Union College — We studied the melting of 2-decanol confined in nano pores, 10-100 nm, using a power-compensated Differential Scanning Calorimeter (DSC). The melting temperature of the nano confined 2-decanol decreases as pore size decreases and a linear relationship is observed between the melting temperature and the inverse of the pore size. This is in agreement with the Gibbs-Thomson prediction. In addition, the apparent heat of fusion of the 2-decanol confined in the nano pores appears to decrease as the size of the pores decreases. However, the apparent heat of fusion of the nano confined 2-decanol may not necessarily be its true heat of fusion. Annealing, for instance, increases the apparent heat of fusion by as much as 26%. A correction or alternate procedure should be employed to extract the true heat of fusion from DSC measurements, especially when the physical size of the sample is in nano scale or the sample possesses a large surface area to volume ratio.

1 This work was partially supported by NSF-DMR: 1229142.

M1.00159 Heat of fusion of primary alcohol confined in Nano pores, HARRISON GRiffin, SAMUEL AMANUE, Dept. of Phys. & Astro., Union College — Melting behavior of physically confined 1-decanol in nano porous silica was probed using a Differential Scanning Calorimeter (DSC). In agreement with the Gibbs-Thomson prediction, we observe that the melting temperature of the confined 1-decanol scales inversely with the physical size of the pores. Contrary to the assumption used in developing the Gibbs-Thomson equation however, the apparent heat of fusion decreases as the the pore size decreases. Previously, several models have been proposed where the interfacial layer/s of molecules do not participate in the phase transition and thereby would not contribute to the heat of fusion. While these could reconcile the seeming contradiction, annealing the nano confined materials enables some of the interfacial layers to be incorporated into an existing crystal. This leads to an increase in the apparent heat of fusion and a systematic relationship exists between the annealing temperature and the increase in the apparent heat of fusion.

2 This work was partially supported by NSF-DMR: 1229142.

M1.00160 Structure and Dynamics of Polymers in Cylindrical Nanofluidization: A Molecular Dynamics Study, JAMES PRESSLY, ROBERT RIGGLEMAN, KAREN WINEY, Univ of Pennsylvania — The structure and dynamics of polymers under nanofluidization is critical for understanding how polymers behave in applications from hydraulic fracturing to fabricating integrated circuits. We previously used simulations to explore the effect of the diameter of cylindrical pores (d = 10-40σ, where σ is the unit length in reduced units) on polymer end-to-end distance (Rg,perp, Rg,par), entanglement density, melt diffusion coefficient (D), and local relaxation time (τperp, τpar) at fixed polymer chain length (N = 350). These studies found D, Rg,par, and τperp increased with increasing confinement while entanglement density, Rg,perp, decreased. Experiments also found that D increased but to a lesser extent. Here, we examine the molecular weight dependence of these properties using N = 25, 50, 100, 200, 350, and 500 confined to pores of diameter 14σ to examine a range of confinements. Our preliminary results show that as N increases D and Rg,par, increase as well, relative to the unconfined state, while entanglement density and Rg,perp decrease, consistent with our previous work. Interestingly, τ is shown to be independent of chain length indicating the impact of confinement imposed by reducing pore diameter is distinct from that imposed by increasing chain length.
M1.00161 Man-made Earthquakes & Multifractals in Neutral Fluid Turbulence/Injection

WH. MAKSOED1, Prodi of Physics UI, Depok 16424—INDONESIA — Man-made earthquakes coincide with induced seismicity “typically minor earthquakes & tremors that are caused by human activity that alters the stresses & Strains on the earth crust” [Wikipedia: “induced seismicity”]. For these, RD Andrews wrote: “Based on observed seismicity rate & geographical trends following major oil & gas plays with large amounts of produced water, the rates & trends in seismicity are very unlikely to represent a naturally occurring process”. “The Prague, Oklahoma, earthquake sequence of 2011, along the Wilzetta faults zone, included the significant foreshock, a main shock of magnitude 5.7, it has been suggested that this sequence represent earthquakes triggered by fluid injection/natural fluid turbulence shows multifractal characteristics”, of [405]→325-7968 of Dr. G. Randy Keller to UI tuitions of @ Rp. 29, 405, 000.00.

1 Acknowledgements to HE. Mr. H. TUK SETYOHADI, Jl. Sriwijaya Raya 3, South-Jakarta, INDONESIA
2of Rabi & Heisenberg hamiltonian oughts to relates to Chris King:“Neurofractal dynamics”

M1.00162 FLUIDS —

M1.00163 Chemically generated convective transport in microfluidic system, OLEG SHKLYAEV, Department of Chemical Engineering, The University of Pittsburgh, SAMBEETA DAS, AYUSMAN SEN, Department of Chemistry, The Pennsylvania State University, HENRY SHUM, ANNA BALAZS, Department of Chemical Engineering, The University of Pittsburgh, AYUSMAN SEN, Department of Chemistry, The Pennsylvania State University — High precision manipulation of small volumes of fluid, containing suspended micron sized objects like cells, viruses, and large molecules, is one of the main goals in designing modern lab-on-a-chip devices which can find a variety of chemical and biological applications. To transport the cargo toward sensing elements, typical microfluidic devices often use pressure driven flows. Here, we propose to use enzymatic chemical reactions which decompose reagent into less dense products and generate flows that can transport particles. Density variations that lead to flow in the assigned direction are created between the place where reagent is fed into the solution and the location where it is decomposed by enzymes attached to the surface of the microchannel. When the reagent is depleted, the fluid motion stops and particles sediment to the bottom. We demonstrate how the choice of chemicals, leading to specific reaction rates, can affect the transport properties. In particular, we show that the intensity of the fluid flow, the final location of cargo, and the time for cargo delivery are controlled by the amount and type of reagent in the system.

M1.00164 Flow reversal in enzymatic microfluidic pumps, HENRY SHUM, University of Pittsburgh, ISAMAR ORTIZ-RIVERA, ARJUN AGRAWAL, AYUSMAN SEN, Pennsylvania State University, ANNA BALAZS, University of Pittsburgh — A chemical reaction occurring at an enzyme-covered patch in a closed fluid chamber generates local solute concentration gradients and, hence, fluid density gradients. This has recently been shown to drive fluid flows with speeds of the order of microns per second. We develop and analyze a model that accounts for fluid density changes due to consumption of the reaction substrate and accumulation of products for such a fluid pump based on the enzyme urease. Hydrolysis of urea by urease produces ammonium bicarbonate, which leads to a net increase in solution density. Higher density fluid is expected to sink and spread horizontally away from the pump. Modeling reveals, however, that the local fluid density is not necessarily greatest near the pump and fluid flow can even reverse in direction after some time. The qualitative behavior depends on two dimensionless parameters, the ratio of solutal expansion coefficients and the ratio of diffusion coefficients for the reaction substrate and product. The predicted reversal of pumping direction is experimentally verified and we show that the direction of pumping also depends on the amount of enzyme present on the patch. A better understanding of these pumps will aid in the design of responsive, chemically powered microfluidic flow control.

M1.00165 Phase transitions analogy for cavity flows, PETRU FODOR, MIRON KAUFMAN, Physics, Cleveland State University — The fluid flow in cavity type systems, in which one of the walls is moving while the others are stationary, is analyzed using computational modeling, under the assumption of no-slip boundary conditions. By iteratively adapting the mesh used, we are able to map with high spatial resolution the complex fluid structures that form at the two types of corners of the cavity, i.e. (i) corners defined by stationary walls, and (ii) corners defined by a stationary and the moving wall, respectively. For the structures that form in the vicinity of the fixed points defined by the corners, we observe that the flow magnitudes and spatial distributions follow scaling laws similar with critical phenomena. In particular, the behavior at the first type of corner is analogous to a to a first-order transition (discontinuity) point, while the behavior at the second one is analogous to a thermodynamic critical point (second-order transition). These results provide a unique insight into the solution to Navier-Stokes equations for cavity flows.

M1.00166 A Statistical investigation of sloshing parameters for multiphase offshore separators, MD MAHMUD1, Lamar University, RAFIGUL KHAN2, Cameron Corp, QIANG XU1 Lammar University — Liquid sloshing in multiphase offshore separators has been the subject of intense investigations for last several decades both by experiments and simulations. Large number scientists have worked to minimize sloshing impacts and others have developed new methods to describe the sloshing patterns. In addition, complex mathematical models are developed to characterize sloshing phenomenon. However, a comprehensive statistical study of the input parameters and output results is yet to be done. In this study, statistical approaches will be considered to determine the significant parameters for liquid sloshing. The factor analysis and principal component analysis techniques are considered to identify the significant parameters for liquid sloshing. Numerical experiments are carried out through Computation Fluid Dynamics (CFD) technique using ANSYS Fluent software. The input parameters considered here are liquid depth/length ratio, acceleration, wave frequencies, amplitudes in various sea state and type of corners. The measured variables include hydrodynamic force, pressure, moments, turbulent kinetic energy, height of interfaces. Mathematical correlations may be developed from the data analysis.

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M1.00167 Efficient Combustion Simulation via the Adaptive Wavelet Collocation Method, KEVIN LUNG, ERIC BROWN-DYMOKOSKI, VICTOR GUERRERO, ERIC DORAN, KEN MUSETH, JO BALME, BOB URBBERGER, ANDRE KESSLER, STEPHEN JONES, BILLY MOSES, ANTHONY CROGNALE, Space Exploration Tech (SpaceX) — Rocket engine development continues to be driven by the intuition and expertise of designers, progressing through extensive trial-and-error test campaigns. Extreme temperatures and pressures frustrate direct observation, while high-fidelity simulation can be impractically expensive owing to the inherent multi-scale, multi-physics nature of the problem. To address this cost, an adaptive multi-resolution PDE solver has been developed which targets the high performance, many-core architecture of GPUs. The adaptive wavelet collocation method is used to maintain a sparse-data representation of the high resolution simulation, greatly reducing the memory footprint while tightly controlling physical fidelity. The tensorial, stencil topology of wavelet-based grids lends itself to highly vectorized algorithms which are necessary to exploit the performance of GPUs. This approach permits efficient implementation of direct finite-rate kinetics, and improved resolution of steep thermodynamic gradients and the smaller mixing scales that drive combustion dynamics. Resolving these scales is crucial for accurate chemical kinetics, which are typically degraded or lost in statistical modeling approaches.
M1.00168 Dual-Mode Measurement and Theoretical Analysis of Evaporation Kinetics of Binary Mixtures1, HANYU SONG, Mechanical Engineering, University of Connecticut, CHI-RUEI HE, Chemical Engineering, National Chung Hsing University, CARL BASDEO, JI-QIN LI, DEZHUIANG YE, Mechanical Engineering, University of Connecticut, DEVENDRA KALONIA, School of Pharmacy, University of Connecticut, SI-YU LI, Chemical Engineering, National Chung Hsing University, TAI-HSI FAN, Mechanical Engineering, University of Connecticut — Theoretical and experimental investigations are presented for the precision measurement of evaporation kinetics of binary mixtures using a quartz crystal resonator. A thin layer of light alcohol mixture including a volatile (methanol) and a much less volatile (1-butanol) components is deployed on top of the resonator. The normal or acoustic mode is to detect the moving liquid-vapor interface due to evaporation with a great spatial precision on the order of microns, and simultaneously the shear mode is used for in-situ detection of point viscosity or concentration of the mixture near the resonator. A one-dimensional theoretical model is developed to describe the underlying mass transfer and interfacial transport phenomena. Along with the modeling results, the transient evaporation kinetics, moving interface, and the stratification of viscosity of the liquid mixture during evaporation are simultaneously measured by the impedance response of the shear and longitudinal waves emitted from the resonator. The system can be used to characterize complicated evaporation kinetics involving multi-component fuels.

1American Chemical Society Petroleum Research Fund, NSF CMMI-0952646

M1.00169 SOFT CONDENSED MATTER

M1.00170 Spin-resolved conductance of Dirac electrons through multibarrier arrays, DIPENDRA DAHAL, Graduate Center and Hunter College of City University of New York, 695 Park Avenue, New York, NY 10065, USA, GODFREY Gumbs, Hunter College of City University of New York, 695 Park Avenue, New York, NY 10065, USA, ANDRII IUROV, Center for High Technology Materials, University of New Mexico, Albuquerque, NM 87106, USA — We use a transfer matrix method to calculate the transmission coefficient of Dirac electrons through an arbitrary number of square potential barrier in gapped monolayer graphene (MLG) and bilayer graphene (BLG). The widths of barriers may not be chosen equal. The shift in the angle of incidence and the width of the barrier required for resonance are investigated numerically for both MLG and BLG. We compare the effects due to the energy gain of transmission with the energy loss coefficient for each of these two structures (MLG and BLG). We present our results as functions of barrier width, height as well as incoming electron energy as well as band gap and examine the conditions for which perfect reflection or transmission occurs. Our transmission data are further used to calculate conductivity.

M1.00171 Dielectric Screening Response of a Plasmonic “Sandwich” , N.J.M. HORING, Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, NJ 07030, GODFREY Gumbs, DIPENDRA DAHAL, Department of Physics and Astronomy, Hunter College, CUNY, New York, NY 10065, ANDRII IUROV, Center for High Technology Materials, University of New Mexico, Albuquerque, NM 87106 — We have formulated the RPA integral equation for a system composed of two identical semi-infinite metallic plasmas with planar bounding surfaces at z = ±d/2. The gap between the two metallic bulk plasmas contains a two-dimensional semiconductor plasma at z = 0. This equation for the inverse dielectric function is solved analytically in position representation for a narrow gap, yielding an explicit formula for the inverse dielectric screening function in terms of the nonlocal 2D semiconductor polarizability and the bulk metallic polarizability, the latter well approximated in the local limit. Based on this solution, we have evaluated the nonlocal plasmon dispersion relation computationally, taking Graphene as the 2D semiconductor plasma. The associated nonlocal graphene plasmon spectrum coupled to the sandwich system is exhibited in 3D plots, which show a linear mode and another displaced from the bulk plasma frequency.

M1.00172 EM Wave Transmission through a Nano-hole in a Plasmonic Layer , DESIRE MIESSEIN, NORMAN J. MORGENSTERN HORING, HARRY LENZING, Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, NJ 07030, GODFREY Gumbs, Department of Physics and Astronomy, Hunter College, CUNY, New York, NY 10065 — We have formulated the RPA integral equation for a system composed of two identical semi-infinite metallic plasmas with planar bounding surfaces at z = ±d/2. The gap between the two metallic bulk plasmas contains a two-dimensional semiconductor plasma at z = 0. This equation for the inverse dielectric function is solved analytically in position representation for a narrow gap, yielding an explicit formula for the inverse dielectric screening function in terms of the nonlocal 2D semiconductor polarizability and the bulk metallic polarizability, the latter well approximated in the local limit. Based on this solution, we have evaluated the nonlocal plasmon dispersion relation computationally, taking Graphene as the 2D semiconductor plasma. The associated nonlocal graphene plasmon spectrum coupled to the sandwich system is exhibited in 3D plots, which show a linear mode and another displaced from the bulk plasma frequency.

M1.00173 Modeling heterogeneous polymer-grafted nanoparticle networks, TAO ZHANG, BADEL MBANGA, VICTOR YASHIN, ANNA BALAZS, Chemical Engineering Department, University of Pittsburgh, Pennsylvania 15261, USA — Via a dynamic 3D computational approach, we simulate the heterogeneous polymer-grafted nanoparticle networks. The nanoparticles rigid cores are decorated with a corona of grafted polymers, which contain reactive functional groups at the chain ends. With the overlap of grafted polymers, these reactive groups can form weak labile bonds, which can reform after breakage, or stronger bonds, which rupture irreversibly and thus, the nanoparticles are interconnected by dual cross-links. Previous work has been done on homogenous networks, while we introduce the heterogeneity by considering two types of particles having different reactive functional groups, so that the labile bond energy varies depending on types of the two end reactive groups. We study the effect of tensile and rotational deformations on the network morphology, and observe, in particular, the phase separation of two types of particles. Our results will provide guidelines for designing transformable material that can controllably change structure under mechanical action.

M1.00174 Adhesion of Particulate Materials to Mesostructured Polypyrrole, DARBY HOSS, Purdue University, ROBERT KNEPPER, PETER HOTCHKISS, ALEXANDER TAPPAN, Sandia National Laboratories, BRYAN BOUDOURIS, STEPHEN BEAUDOIN, Purdue University — Interactions based on van der Waals (vdW) forces can significantly influence the performance and reliability of mesostructured polypyrrole swabs used for the collection and detection of trace particles. The vdW adhesion force between materials is described by the Hamaker constant, and these constants are measured via optical and dielectric properties (i.e., according to Lifshitz theory), inverse gas chromatography (IGC), and contact angle measurements. Here, contact angle measurements were performed on films of several common materials and used to estimate Hamaker constants. This, in turn, will allow for the tuning of the design properties associated with the polypyrrole swabs. A comparison of these results to Hamaker constants estimated using Lifshitz theory and IGC for the same materials was made. The results were compared to the experimental data to verify the idealized model. The idealized model describes particle adhesion to an array of mesostructures. This model elucidates the importance of where the particle makes contact with the mesostructure and the independence of vdW forces generated by each mesostructure. These results will facilitate the rational design of polypyrrole swabs optimized for harvesting microscale particles of trace materials.

M1.00175 Droplet Dynamics of a Flowing Emulsion System, OLIVIA CYPULL, KLEBERT FEITOSA, James Madison University — The inner workings of glassy systems have long been a topic of interest for soft material scientists. Similarities between the jamming behavior of emulsions and the glass transition of glassy systems have prompted the conjecture that they might share the same underlying mechanism. Here we study a dense oil-in-water emulsion system forced to flow through a narrow microchannel. By matching the index of refraction of the two phases, we image the internal dynamics of the droplets in a confocal microscope. At low velocity speeds, we find that the velocity along the edge of the microchannel was not significantly different than then the average droplet velocity in the bulk suggesting a near plug flow. By contrast the droplets near the edge experienced more movement perpendicular to the flow indicating the fluidization effect of the confining walls.
M1.00176 Self-assembly in Dipolar Fluids1, MICHELA RONTI, SOFIA KANTOROVICH, Univ of Vienna — We are studying low temperature structural transitions in dipolar hard spheres (DHS), combining grand-canonical Monte Carlo simulations and direct analytical theoretical calculations. DHS is characterized by long-range anisotropic interactions: it consists of a point dipole at the center of a hard sphere. We are interested in low temperature and low density phase behaviour of DHS systems. From a theoretical point of view the process of self-assembly is not responsible for a phase transition; this belief was completely reverted by theoretical studies showing that the process of self-assembly is alone capable to induce phase transition. On the other hand in the last years it was proved that no sign of critical behaviour is observed, implementing efficient and tailored Monte Carlo algorithms. Moreover a theoretical approach based on Density Functional Theory was developed: a series of structural transitions were discovered providing evidence of a hierarchy in the structures on cooling. We are performing free-energy calculations in order to draw the phase diagram of DHS model. Comparing the numerical results with the theoretical ones shed light on the scenario of temperature induced structural transitions in magnetic nanocolloids.

1ETN-COLLDENSE (H2020-MCSA-ITN-2014, Grant No. 642774)

M1.00177 Deconvolution of the role of metal and pH in metal coordinating polymers.1, SETH CAZZELL, NIELS HOLTEN-ANDERSEN, Massachusetts Inst of Tech-MIT — Nature uses metal binding amino acids to engineer both mechanical properties and structural functionality. Some examples of this metal binding behavior can be found in both mussel foot protein and DNA binding protein. The mussel byssal thread contains reversible intermolecular protein-metal bonds, allowing it to withstand harsh intertidal environments. Zinc fingers form intramolecular protein-metal bonds to stabilize the tertiary structure of DNA binding proteins, allowing specific structural functionality. Inspired by both these metal-binding materials, we present mechanical and spectroscopic characterization of a model polymer system, designed to mimic this bonding. Through these studies, we are able to answer fundamental polymer physics questions, such as the role of pH and metal to ligand ratio, illuminating both the macroscopic and microscopic material behavior. These understandings further bio-inspired engineering techniques that are used to design viscoelastic soft materials.

1I was supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program.

M1.00178 Optically induced thermal response of Chlorophyll for biomedical applications CHIAWEI TU, SADAT MD EHSAN, YUAN ZHAO, DONGLUI SHI, DAVID MAST, Univ of Cincinnati — The heating behavior of Chlorophyll was investigated for possible use in hyperthermia cancer treatments. One measure of hyperthermia effectiveness is the Specific Absorption Rate (SAR) defined as the initial slope of the sample heating behavior; however, for nanoparticle (NP) loaded samples, this initial heating rate is often limited by heat transfer mechanisms from the NPs to the surrounding material and not the initial NP heating. This is especially true for water-based, NP loaded tissue surrogates. Organic solvent dispersed NP loaded samples face the additional problem of heating rate variations due to solvent evaporation effects. We report on measurements of the initial heating rates of Chlorophyll and deposited directly on small, Pt thin film resistance temperature detectors (RTDs). Solid state lasers (638 nm and 655 nm) were used to illuminate these samples at different intensities and at specific wavelengths associated with peaks (662 nm) in Chlorophyll’s UV-VIS optical absorption spectra while recording the RTD resistance at 0.1 second intervals. This technique significantly reduce evaporation errors we had experienced and has the potential to directly measure the heating behavior of Chlorophyll based NP materials.

M1.00179 Directed percolation identified as equilibrium pre-transition towards non-equilibrium arrested gel states , MARCO LAURATI, RONJA CAPELLMANN, MATTHIAS KOHL, STEFAN EGEHLHAFF, MICHAEL SCHMIEDEBERG, University of Düsseldorf — The macroscopic properties of gels arise from their slow dynamics and load bearing network structure, which are explored by nature and in numerous industrial products. However, a link between these structural and dynamical properties has remained elusive. Here we present confocal microscopy experiments and simulations of gel-forming colloid-polymer mixtures with competing interactions. They reveal that gel formation is preceded by continuous and directed percolation. Both transitions lead to system spanning networks, but only directed percolation results in extremely slow dynamics, ageing and a shrinking of the gel that resembles synerysis. Therefore, dynamical arrest in gels is found to be linked to a structural transition, namely directed percolation, which is quantitatively associated with the mean number of bonded neighbours. Directed percolation is a universality class of transitions out of equilibrium, our study hence connects gel formation to a well-developed theoretical framework which now can be exploited to achieve a detailed understanding of arrested gels.

M1.00180 Novel coarse-graining approach for Star polymer and linear Homopolymer mixtures , EMANUELE LOCATELLI, CHI-YAO HUNG, National Taiwan University, COLIN P. STARK, Lamont-Doherty Earth Observatory, Columbia University, HERVE CAPART, National Taiwan University — Granular flow over an erodible bed is an important phenomenon in both industrial and geophysical settings. Here we develop a depth-averaged theory for dry erosive flows using balance equations for mass, momentum and (crucially) kinetic energy. We assume a linearized GDR-Midi rheology for granular deformation and Coulomb friction along the sidewalls. The theory predicts the kinematic behavior of channelized flows under a variety of conditions, which we test in two sets of experiments: (1) a linear chute, where abrupt changes in tilt drive unsteady uniform flows; (2) a rotating drum, to explore steady non-uniform flow. The theoretical predictions match the experimental results well in all cases, without the need to tune parameters or invoke an ad hoc equation for entrainment at the base of the flow. Here we focus on the drum problem. A dimensionless rotation rate (related to Froude number) characterizes flow geometry and accounts not just for spin rate, drum radius and gravity, but also for grain size, wall friction and channel width. By incorporating Coriolis force the theory can treat behavior under centrifuge-induced enhanced gravity. We identify asymptotic flow regimes at low and high dimensionless rotation rates that exhibit distinct power-law scaling behaviors.

M1.00181 A simple depth-averaged model for dry granular flow , CHI-YAO HUNG, National Taiwan University, COLIN P. STARK, Lamont-Doherty Earth Observatory, Columbia University, HERVE CAPART, National Taiwan University — Granular flow over an erodible bed is an important phenomenon in both industrial and geophysical settings. Here we develop a depth-averaged theory for dry erosive flows using balance equations for mass, momentum and (crucially) kinetic energy. We assume a linearized GDR-Midi rheology for granular deformation and Coulomb friction along the sidewalls. The theory predicts the kinematic behavior of channelized flows under a variety of conditions, which we test in two sets of experiments: (1) a linear chute, where abrupt changes in tilt drive unsteady uniform flows; (2) a rotating drum, to explore steady non-uniform flow. The theoretical predictions match the experimental results well in all cases, without the need to tune parameters or invoke an ad hoc equation for entrainment at the base of the flow. Here we focus on the drum problem. A dimensionless rotation rate (related to Froude number) characterizes flow geometry and accounts not just for spin rate, drum radius and gravity, but also for grain size, wall friction and channel width. By incorporating Coriolis force the theory can treat behavior under centrifuge-induced enhanced gravity. We identify asymptotic flow regimes at low and high dimensionless rotation rates that exhibit distinct power-law scaling behaviors.

M1.00182 A Computational Study of the Growth of Hexagonal Ice. , MAXWELL FULFORD, King’s College London, UK, MATTEO SALVALAGLIO, UCL, UK, MICHELE PARRINELLO, ETH Zurich; USI Lugano, CARLA MOLTENI, King’s College London, UK — Hexagonal ice (Ih) has two distinct crystallographic surfaces; a basal and prism surface. At low vapour pressures, Ih forms thin plates and elongated prisms, depending on the temperature. The macroscopic shape depends on the relative rate of growth of the basal and prism surfaces. The aim of our research is to estimate the relative rate of growth of the two surfaces for a range of temperatures and ultimately predict the shape of Ih, using computer simulations. Our simulations show the well-known phenomenon that the surface of ice lowers its interfacial free energy by forming a stable quasi-liquid layer (QLL). The QLL mediates crystal growth and has a thickness which varies with temperature and crystallographic surface. We use a combination of Molecular Dynamics and Metadynamics to study how the interfacial structure at the ice/quasi-liquid and quasi-liquid/vapour interfaces influence the adsorption potential, surface transport properties and growth shape.
M1.00183 The mystery of Coulomb friction in sediment transport1, THOMAS PHTZ, Ocean College, Zhejiang University, ORENCIO DURAN, MARUM-Center for Marine Environmental Sciences, University of Bremen — Nearly all analytical models of sediment transport in Newtonian fluid (e.g., air or water) are based on Bagnold’s assumption of a constant Coulomb friction coefficient (particle-shear-pressure-ratio, $\mu$) at the interface ($z_i$) between sediment bed and transport layer. In fact, this assumption is the main reason why these models predict the sediment load (and subsequently the sediment transport rate) to be proportional to the excess shear stress ($\tau - \tau_i$), a scaling which has been confirmed in many wind-tunnel and flume experiments. Attempts to explain why $\mu(z_i)$ is constant have usually been based on the sliding-friction analogy or rheology arguments. However, here we analytically derive $\mu(z_i) \approx \sqrt{3} - 1$, where $z_i$ is the location at which the production rate of particle fluctuation energy is maximal. Our derivation is based on the assumption that the rate of collisional transfer of horizontal into vertical kinetic energy is typically much larger than the rate of energy dissipation. Using state-of-the-art numerical simulations of sediment transport in Newtonian fluid, we validate all assumptions and approximation involved in our derivation. Interestingly, the location $z_i$ can significantly deviate from $z_i$ depending on the simulated conditions.

1We acknowledge support from grants National Natural Science Foundation of China (Nos. 1151101041 and 41376095) and Natural Science Foundation of Zhejiang Province (No. LR16E090001).

M1.00184 Core formation by porous flow allowed by hysteresis in melt network topology, SOHEIL GHANBARZADEH, MARC HESSE, MASHA PRODANOVIC, The University of Texas at Austin — The formation of the core via percolation is an attractive process to form planetary cores early in the planets evolution. There is currently a debate whether the ratio of interfacial forces between solid-solid and solid-liquid interfaces, imposing the dihedral angle between the solid grains and the pore fluid, in an olivine-melt matrix allows the formation of a percolating network. We present first computations of equilibrium melt distributions in realistic irregular grains and show that the percolation threshold at dihedral angles above 60 degrees is significantly larger than those previously reported for simple geometries. However, given typical compositions of the terrestrial planets initial porosities after the onset of melting of iron are large, 20-40% to form a connected melt network. As the porosity decreases due to melt segregation the network remains connected and allows core formation by porous flow. Only as the porosity approaches 1% and the iron becomes isolated in pockets along triple junctions. This residual iron may provide an explanation for the formation of dense layers near the core mantle boundary such as water.

M1.00185 Spontaneous Pattern Formation of Surface Nanodroplets from Competitive Growth, DETLEF LOHSE, University of Twente, SHUHUA PENG, XUHEUA ZHANG, RMIT, Melbourne — Nanoscale droplets on a substrate are of great interest because of their relevance for droplet-based technologies for light manipulation, lab-on-chip devices, miniaturized reactors, encapsulation and many others. In this work, we establish a basic principle for the symmetrical arrangement of surface nanodroplets during their growth under simple fluid conditions. In our model system, nanodroplets nucleate at the rim of spherical cap microstructures on a substrate, due to a pulse of oversaturation supplied by a solvent exchange process. We find that, while growing at the rim of the microcap, the nanodroplets self-organise into highly symmetric arrangements, with respect to position, size, and mutual distance. The angle between the neighbouring droplets is four times the ratio between the base radii of the droplets and the spherical caps. We show and explain how the nanodroplets acquire the symmetrical spatial arrangement during their competitive growth and why and how the competition enhances the overall growth rate of the nucleated nanodroplets. This mechanism behind the nanodroplet self-organisation promises a simple approach for the location control of droplets with a volume down to attoliters.

M1.00186 Decoupling between Diffusivity and Effective Viscosity in Poly(isobutyl methacrylate) Films with a Thickness-Independent Glass Transition1, KUN GENG, Boston University Physics Department, REIKA KATSUMATA, University of Texas at Austin, McKetta Department of Chemical Engineering, XUANJI YU, Boston University Division of Materials Science and Engineering, HEONJOO HA, University of Texas at Austin, McKetta Department of Chemical Engineering, OPHELIA K.C. TSUI, Boston University Physics Department, Division of Materials Science and Engineering — We report measurements of self-diffusing ($D$) and effective viscosity ($\eta_{\text{eff}}$) on silica-supported poly(isobutyl methacrylate) (PiBMA) thin films. These films had been found to exhibit thickness ($h_0$) independent in the glass transition temperature, $T_g$ (= 58 °C). At $T = 106$ °C, $D$ was independent of $h_0$, and $\eta_{\text{eff}}$ decreased with decreasing $h_0$, indicating decoupling between $D$ and $\eta_{\text{eff}}$. We contemplate that the decoupling is caused by dynamic heterogeneity in the film and that $D$ and $\eta_{\text{eff}}$ are different dynamic averages. Specifically, by using a layer model, where the film is divided into sub-layers with thickness $h_i$ and local viscosity $\eta_i$, and assuming that $D = k_b T / \langle \eta_i \rangle$ and $\eta_{\text{eff}} = \langle h_i^3 \rangle / \langle \eta_i \rangle$, we are able to account for all the measurements.

1We are grateful to the support of NSF through the project DMR-1310536 and DMR-1053293.

M1.00187 Interfacial Bubble Deformations1, BRIAN SEYmour, James Madison University, PARVIS SHABANE, Virginia Tech, OLIVIA CYFULL, James Madison University, SHENGFENG CHENG, Virginia Tech, KLEBERT FEITOSA, James Madison University — Soap bubbles floating at an air-water experience deformations as a result of surface tension and hydrostatic forces. In this experiment, we investigate the nature of such deformations by taking cross-sectional images of bubbles of different volumes. The results show that as their volume increases, bubbles transition from spherical floating at an air-water experience deformations as a result of surface tension and hydrostatic forces. In this experiment, we investigate the nature of such deformations by taking cross-sectional images of bubbles of different volumes. The results show that as the volume increases, bubbles transition from spherical to hemispherical shape. The deformation of the interface also changes with bubbles volume with the capillary rise preceding to the capillary length as volume increases. The profile of the top and bottom of the bubble and the capillary rise are completely determined by the volume and pressure differences.

1James Madison University Department of Physics and Astronomy, 4VA Consortium, Research Corporation for Advancement of Science

M1.00188 Temperature-dependent neutron diffraction measurements from D$_2$O hydrating single-supported lipid bilayers of DMPC1, Z. N. BUCK, J. TORRES, A. MAZZA, H. KAISER, H. TAUB, Univ. of Missouri - Columbia, F. Y. HANSEN, Technical University of Denmark, A. MISKOWIEC, Oak Ridge National Lab, M. TYAGI, NIST Center for Neutron Research — The freezing point depression of water associated with biological membranes, studied principally by NMR, has been of interest for decades. Here we have used neutron diffraction measurements at the University of Missouri Research Reactor (MURR) to investigate the freezing behavior of water associated with single-supported zwitterionic lipid bilayers composed of DMPC. Diffraction patterns obtained as a function of temperature reveal that water freezes abruptly into its hexagonal phase at 270 K with no evidence of amorphous ice. Following the initial crystallization of the membrane-associated water there is a region of continuous hexagonal crystal growth, which is believed to occur in the interfacial water closest to the membrane. The temperature-dependent intensity of the observed Bragg peaks has been compared with that of incoherently elastically-scattered neutrons collected on the High-Flux Backscattering Spectrometer at NIST from an identical sample hydrated with H$_2$O [2]. We find excellent agreement between the two data sets, suggesting the absence of amorphous solid water and that all the water hydrating a DMPC membrane eventually freezes into the hexagonal crystalline phase. 2M. Bai et al., Europhys. Lett. 98, 48006 (2012).

1Supported by NSF Grant Nos. DMR-0944772 and DGE-1069091.
M1.00189 Elasticity and Extensibility Determine Printability and Spinnability of Polymer Solutions, JELENA DINIC, LEIDY JIMENEZ, VIVEK SHARMA, Univ of Illinois - Chicago — Many advanced manufacturing technologies like inkjet and 3D printing, nano-fiber spinning involve complex free-surface flows, and the formation of columnar necks that undergo spontaneous capillary-driven thinning and pinch-off. The progressive self-thinning of neck is often characterized by self-similar profiles and scaling laws that depend on the relative magnitude of capillary, inertial and viscous stresses for simple (Newtonian and inelastic) fluids. Stream-wise velocity gradients that arise within the thinning columnar neck create an extensional flow field that can orient and stretch macromolecules, contributing extra elastic stresses and extensional viscosity that change thinning and pinch-off dynamics for polymer-poor complex fluids. Characterizing the filament thinning and break-up kinetics in jetting, dripping and stretching liquid bridge provides invaluable insight into the interplay of elastic, viscous, capillary and inertial stresses relevant for these applications. We elucidate how polymer composition, flexibility and molecular weight determine the thinning and pinch-off kinetics in our experiments. Both effective relaxation time and transient extensional viscosity are found to be strongly concentration dependent even for dilute solutions.

M1.00190 Patterns, Instabilities, Colors, and Flows in Vertical Foam Films, SUBINUER YILXIATI, YIRAN ZHANG, EWELINA WOJCIK, VIVEK SHARMA, Univ of Illinois - Chicago — Understanding and controlling the drainage kinetics of thin films is an important problem that underlies the stability, rheology and phase of foams and emulsions. We follow the drainage kinetics of vertical foam films using imaging and color science to study the influence of protein properties on thinning and pinch-off dynamics. For IgG1 based mAbs, we observe a transition from Newtonian to highly viscous behavior with a pronounced increase in the solution viscosity. Strongly bounded, reversible dimers may exist in many IgG1 based mAb systems such that these results contribute to a more comprehensive understanding of the physical mechanisms producing high viscosities in concentrated protein solutions.

M1.00191 Effects of aspect ratio on the phase diagram of spheroidal particles, SONGUL KUTLU, JASON HAAGA, JEFFREY RICKMAN, JAMES GUNTON, Lehigh University — Ellipsoidal particles occur in both colloidal and protein science. Models of protein phase transitions based on interacting spheroidal particles can often be more realistic than those based on spherical molecules. One of the interesting questions is how the aspect ratio of spheroidal particles affects the phase diagram. Some results have been obtained in an earlier study by Odriozola (J. Chem. Phys. 136:134505 (2012)). In this poster we present results for the phase diagram of hard spheroids interacting via a quasi-square-well potential, for different aspect ratios. These results are obtained from Monte Carlo simulations using the replica exchange method. We find that the phase diagram, including the crystal phase transition, is sensitive to the choice of aspect ratio.

M1.00192 Coarse-grained simulation of dynamin-mediated fission, MARCUS MULLER, GUOJIE ZHANG, MARC FUHRMANS, Georg-August University, Goettingen, Germany — Fission is a process in which a region of a lipid bilayer is deformed and separated from its host membrane, so that an additional, topologically independent compartment surrounded by a continuous lipid bilayer is formed. It is a fundamental process in the compartmentalization of living organisms and carefully regulated by a number of membrane-shaping proteins. An important group within these is the dynamin family of proteins that are involved in the final severance of the hourglass-shaped neck, via which the growing compartment remains connected to the main volume until the completion of fission. Very light reflected from two surfactant-laden surfaces that are separated by a thin film of water displays an iridescent colors in the visible region. Below 50 nm the thin films appear as black. In this study, we utilize the thin film interference colors as markers for identifying patterns, instabilities and flows within vertical foam films. We study the emergence of thickness fluctuations near the borders (i.e. marginal regeneration) and within thinning flows. Finally, we elucidate how buoyancy, capillarity, convection and gravity-driven instabilities and flows, are affected by the choice and concentration of constituents. We find fascinating examples of two-dimensional hydrodynamics and unexplained, if not unprecedented, phenomena.

M1.00193 Elasticity and Extensibility Determine Printability and Spinnability of Polymer Solutions, JELENA DINIC, LEIDY JIMENEZ, VIVEK SHARMA, Univ of Illinois - Chicago — Many advanced manufacturing technologies like inkjet and 3D printing, nano-fiber spinning involve complex free-surface flows, and the formation of columnar necks that undergo spontaneous capillary-driven thinning and pinch-off. The progressive self-thinning of neck is often characterized by self-similar profiles and scaling laws that depend on the relative magnitude of capillary, inertial and viscous stresses for simple (Newtonian and inelastic) fluids. Stream-wise velocity gradients that arise within the thinning columnar neck create an extensional flow field that can orient and stretch macromolecules, contributing extra elastic stresses and extensional viscosity that change thinning and pinch-off dynamics for polymer-poor complex fluids. Characterizing the filament thinning and break-up kinetics in jetting, dripping and stretching liquid bridge provides invaluable insight into the interplay of elastic, viscous, capillary and inertial stresses relevant for these applications. We elucidate how polymer composition, flexibility and molecular weight determine the thinning and pinch-off kinetics in our experiments. Both effective relaxation time and transient extensional viscosity are found to be strongly concentration dependent even for dilute solutions.

M1.00194 Hierarchical Cluster Formation in Concentrated Monoclonal Antibody Formulations, MARCUS MULLER, GUOJIE ZHANG, MARC FUHRMANS, Georg-August University, Goettingen, Germany — Fission is a process in which a region of a lipid bilayer is deformed and separated from its host membrane, so that an additional, topologically independent compartment surrounded by a continuous lipid bilayer is formed. It is a fundamental process in the compartmentalization of living organisms and carefully regulated by a number of membrane-shaping proteins. An important group within these is the dynamin family of proteins that are involved in the final severance of the hourglass-shaped neck, via which the growing compartment remains connected to the main volume until the completion of fission. Very light reflected from two surfactant-laden surfaces that are separated by a thin film of water displays an iridescent colors in the visible region. Below 50 nm the thin films appear as black. In this study, we utilize the thin film interference colors as markers for identifying patterns, instabilities and flows within vertical foam films. We study the emergence of thickness fluctuations near the borders (i.e. marginal regeneration) and within thinning flows. Finally, we elucidate how buoyancy, capillarity, convection and gravity-driven instabilities and flows, are affected by the choice and concentration of constituents. We find fascinating examples of two-dimensional hydrodynamics and unexplained, if not unprecedented, phenomena.

M1.00195 Probing matrix and tumor mechanics with in situ calibrated optical trap based active microrheology, JACK RORY STAUNTON, WILFRED VIEIRA, KANDICE TANNER, NIH, TISSUE MORPHODYNAMICS UNIT TEAM — Aberrant extracellular matrix deposition and vascularization, concomitant with proliferation and phenotypic changes undergone by cancer cells, alter mechanical properties in the tumor microenvironment during cancer progression. Tumor mechanics conversely influence progression, and the identification of physical biomarkers promise improved diagnostic and prognostic power. Optical trap based active microrheology enables measurement of forces up to 0.5 mm within a sample, allowing interrogation of in vitro biomaterials, ex vivo tissue sections, and small organisms in vivo. We fabricated collagen I hydrogels exhibiting distinct structural properties by tuning polymerization temperature Tp, and measured their shear storage and loss moduli at frequencies 1-15 kHz at multiple amplitudes. Lower Tp gels, with larger pore size but thicker, longer fibers, were stiffer than higher Tp gels; decreasing strain increased loss moduli and decreased storage moduli at low frequencies. We subcutaneously injected probes with metastatic murine melanoma cells into mice. The excited tumors displayed storage and loss moduli 40 Pa and 10 Pa at 1 Hz, increasing to 500 Pa and 1 kPa at 15 kHz, respectively.
M1.00196 Dynamics of Micropipette Vibration During Piezo-assisted Microinjection\(^1\), MEHDI KARZAR-JEDDI\(^2\), NEJAT OLGAC, TAI-HSI FAN, Department of Mechanical Engineering, University of Connecticut, Storrs, Connecticut 06269-3139, USA

- Microinjection is a well-accepted method to introduce materials such as sperm, DNA materials, or nucleus into a living cell for biomedical applications.
- The conventional microinjection procedure consists of immobilizing the cell by applying suction through a holding pipette, and then an injecting micropipette penetrates through the cell membrane and introduces the materials into the cell. To assist the penetration process a piezo-generated pulse train is applied to the injecting pipette, which causes an undesirable lateral vibration at the injecting pipette tip.
- In this research we provide an analytical model to study the response of the micropipette to the piezo-pulse train using the Duhamel integral method. Our results show that filling the micropipette tip with mercury causes a larger amplitude stroke vibration in micropipette than that of empty micropipette when it is submerged in the viscous medium surrounding the cell. The mercury introduced larger stroke vibration can cause a larger shear force and assist the penetration of micropipette through the cell membrane.

\(^1\)This work is supported by NSF CBET-0828733 and NIH R24RR018934-01
\(^2\)Current affiliation: Department of Civil Environmental and Geo- Engineering, University of Minnesota

M1.00197 Characterizing the mechanical behavior of the zebrafish germ layers, DAVID KEOLOHER, FRIEDHELM SERWANE, ALESSANDRO MONGERA, PAYAM ROWGHANIAN, ADAM LUCIO, OTGER CAMPAS, University of California, Santa Barbara — Organ morphogenesis and the development of the animal body plan involve complex spatial and temporal control of tissue- and cell-level mechanics. A prime example is the generation of stresses by individual cells to reorganize the tissue. These processes have remained poorly understood due to a lack of techniques to characterize the local constitutive law of the material, which relates local cellular forces to the resulting tissue flows. We have developed a method for quantitative, local in vivo study of material properties in living tissue using magnetic droplet probes. We use this technique to study the material properties of the different zebrafish germ layers using aggregates of zebrafish mesendodermal and ectodermal cells as a model system. These aggregates are ideal for controlled studies of the mechanics of individual germ layers because of the homogeneity of the cell type and the simple spherical geometry. Furthermore, the numerous micropipet tools and transgenic lines already developed for this model organism can be applied to these aggregates, allowing us to characterize the contributions of cell cortex tension and cell adhesion to the mechanical properties of the zebrafish germ layers.

M1.00198 A finite element study of the stability of spontaneous curling of thin shells, XIAOMIN HAN, Thayer School of Engineering, Dartmouth College, QIAOHANG GUO, College of Material Science and Engineering, Fuzhou University, KEVIN CHU, Serendipity Research, IRAN TRASE, NAN HU, ZI CHEN, Thayer School of Engineering, Dartmouth College — Thin shells are of great interest in engineering due to their ubiquity in nature. The mechanical instabilities of thin shells are a key factor in understanding many real world phenomena, such as the closure of a Venus flytrap or the curling of a dried leaf. Given the analytical theory that quantitatively described the stability of thin shells subject to surface stress, we are able to identify a dimensionless parameter that controls the stability of thin shells. Finite element analyses are employed to numerically examine the predictions. Bi-layer plates are fabricated where one layer is pre-stretched and has much smaller Young’s modulus than the other layer to examine mechanical instability. By measuring the two principle curvatures on the plate, the onset of bifurcation can be determined. Different initial conditions and material properties are taken into account in the FEA, including initial curvature, Poisson’s ratio, and the magnitude of surface stress. The numerical experiments agree well with the theory.

M1.00199 Diffusion of micrometer-sized soft particles in confinement\(^1\), BENJAMIN JORDAN, KEVIN APTOWICZ, West Chester University — We investigate the diffusion of micrometer sized poly(N-isopropylacylamide) (PNIPAM) gel particles in confinement. The influence of confinement on the transport of small particles is becoming increasingly important for microfluidics and bio-fluidics. Analytical solutions to this problem are limited to very unique geometries or gross approximations. Computational methods have provided more insight into the problem as well as experimental investigations. However, most research has focused on the hard-sphere problem. In this work, we will explore the diffusion of soft particles in confinement. The dynamics of the particles confined between two parallel walls is captured with video-microscopy. In addition, we use a recently developed technique to measurement confinement of particles in-situ with a precision of 1%. This poster will present some preliminary results of how confinement affects the diffusion of these soft particles.

\(^1\)We acknowledge support from grant DMR-1206231.

M1.00200 Electric Double Layer electrostatics of spherical polyelectrolyte brushes with pH-dependent charge density, HAO LI, GUANG CHEN, SHAYANDEV SINHA, SIDDHARTHA DAS, Univ of Maryland-College Park, SOFT MATTER, INTERFACES, AND ENERGY LABORATORY (SMIEL) TEAM — Understanding the electric double layer (EDL) electrostatics of spherical polyelectrolyte (PE) brushes, which are spherical particles grafted with PE layers, is essential for appropriate use of PE-grafted micro-nanoparticles for targeted drug delivery, oil recovery, water harvesting, emulsion stabilization, emulsion breaking, etc. Here we elucidate the EDL electrostatics of spherical PE brushes for the case where the PE exhibits pH-dependent charge density. This pH-dependence necessitates the consideration of explicit hydrogen ion concentration, which in turn dictates the distribution of monomers along the length of the grafted PE. This monomer distribution is shown to be a function of the nature of the polymer and their interactions with proteins needs to be understood. In this work, we will explore the diffusion of soft particles in confinement. The dynamics of the particles confined between two parallel walls is captured with video-microscopy. In addition, we use a recently developed technique to measurement confinement of particles in-situ with a precision of 1%. This poster will present some preliminary results of how confinement affects the diffusion of these soft particles.

M1.00201 Unraveling the Nanostructure and Chain Conformation of Peptide-polymer Conjugates in Solution using Small-angle X-ray Scattering, REIDAR LUND, Department of chemistry, University of Oslo, TING XU, UC-Berkeley, HE DONG, Clarkson University — For therapeutics, polymer functionalization, often by poly(ethylene glycol), PEG ("PEGylation"), is an effective method to improve the solubility, increase the lifetime and protect the proteins from the immune system[1]. However it is essential that the proteins maintain their structural integrity in solution- thus the role of the polymer and their interactions with proteins needs to be understood. In this work we show how small-angle X-ray scattering (SAXS) can be used as a powerful technique to characterize the structural components of peptide-polymer conjugates in solution [2,3]. We specifically show that by applying detailed modelling very detailed structural features can be revealed, including the PEG chain conformation. In the presentation we will provide an overview of the methodology, specifically addressing peptides that form either alpha-helical bundles [2,3] or beta-sheet structures [4,5] and relate their structure in solution to their crystal structure.

**M1.0020 Geometric Frustration Selects Morphology in Chiral Filament Bundles**

**DOUGLAS HALL**, ISAAC BRUSS, UMass Amherst, JUSTIN BARONE, Virginia Tech, GREGORY GRASON, UMass Amherst — Assemblies of twisted filaments appear in a range of biological contexts, from extracellular filament bundles to amyloid fibrils. Owing to numerous distinctions in molecular structures and interactions underlying these diverse assemblies, a framework to predict and classify the basic mechanisms of structure formation in twisted filament assemblies is still lacking. In this study, we model how the size and shape of self-assembled fibers are controlled by competition between the elastic costs of inter-filament frustration, bending, and deformation, and the energy gained by inter-filament packing. In the presence of an external magnetic field, positively-curved 2D surfaces, we show that the anisotropy of the bundle cross-section is determined by a single parameter describing the competition between elastic and bending costs. We compare the continuum model’s predictions for stability of cylindrical and tape-like twisted morphologies to numerical simulations of cohesive filament bundles and observations of micron-scale amyloid fibers assembled from hydrolyzed protein fragments.

**M1.0023 Controlling the Size and Shape of the Elastin-Like Polypeptide based Micelles**

**KIRIL STRELETZKY, HANNAH SHUMAN, ADAM MARASCHKY, NOLAN HOLLAND**, Cleveland State University — Elastin-like polypeptide (ELP) trimer constructs make reliable environmentally responsive micellar systems because they exhibit a controllable transition from being water-soluble at low temperatures to aggregating at high temperatures. It has been shown that depending on the specific details of the ELP design (length of the ELP chain, pH and salt concentration) micelles can vary in size and shape between spherical micelles with diameter 30-100 nm to elongated particles with an aspect ratio of about 10. This makes ELP trimers a convenient platform for developing potential drug delivery and bio-sensing applications as well as for understanding micelle formation in ELP systems. Since at a given salt concentration, the headgroup area for each foldon should be constant, the size of the micelles is expected to be proportional to the volume of the linear ELP available per foldon headgroup. Therefore, adding linear ELPs to a system of ELP-foldon should result in changes of the micelle volume allowing to control micelle size and possibly shape. The effects of addition of linear ELPs on size, shape, and molecular weight of micelles at different salt concentrations were studied by a combination of Dynamic Light Scattering and Static Light Scattering. The initial results on 50 M ELP-foldon samples (at low salt) show that Rh of mixed micelles increases more than 5-fold as the amount of linear ELP raised from 0 to 50 M. It was also found that a given mixture of linear and trimer constructs has two temperature-based transitions and therefore displays three predominant size regimes.

**M1.0024 Directed Assembly of Hierarchically Ordered Clusters from Anisotropic Microparticles**

**KOOHEE HAN, BHUYNESH BHARTI**, North Carolina State Univ., C. WYATT SHIELDS IV, GABRIEL P. LOPEZ, Duke University, ORLIN D. VELEV, North Carolina State Univ. — The directed assembly of colloidal particles with specific connectivity, symmetry, and directional response requires controlled interactions and means of programmable binding force. We will show how patchy microparticles can be hierarchically assembled into ordered clusters, resulting from directional interactions between metal-coated facets. First, we introduce lipid mediated capillary bridging as a new class of binding force for directed assembly of metallic-dielectric patchy microspheres. Iron oxide surface patches on latex microspheres were selectively wetted with liquid lipids, guiding the particle assembly into well-defined 2D and 3D clusters. The temperature driven fluid-to-gel phase transition of the fatty acids acts as a thermal switch for cluster assembly and disassembly. Secondly, we used external fields to bind patchy microspheres based on their polarization configuration and inter-particle interaction. We present assembled clusters of cobalt-coated patchy microcubes that can be dynamically reconfigured using external magnetic field. The residual polarization of ferromagnetic cobalt patches allows for preserving the assembled sequence even in the absence of the field and drives dynamic reconfiguration of assembled clusters.

**M1.0025 Aging and nonlinear rheology of thermoreversible colloidal gels**

**NORMAN WAGNER, MELISSA GORDON, CHRISTOPHER KLOXIN**, University of Delaware — Colloidal dispersions are found in a wide variety of consumer products such as paint, food and pharmaceuticals. We investigate gel formation and aging in a thermoreversible gel consisting of octadecyl-coated silica nanoparticles suspended in n-tetradeccane. In this system, the octadecyl brush can undergo a phase change allowing the attractions between particles to be tuned by temperature (1,2). By probing the system with steady shear and large amplitude oscillatory shear, we have studied the effect of thermal history and shear history on gel formation and gel mechanical properties during aging. Gels were formed by approaching a common temperature from above and below to determine a reference state from which creep tests were conducted. Creep ringing was observed as expected for the viscoelastic gel. The rheological aging is interpreted in terms of the gel microstructure formed with differing thermal and shear histories to determine how processing affects structure. Recently proposed scaling laws for the rheology and structure under flow are explored within the context of gel aging (3). Through rheological and microstructural measurements, we will further the understanding of gel formation and aging in this model system which can be applied to processing conditions in an industrial setting. 1. Eberle, A.P.R., Wagner, N. J., Akgun, B. & Satija, S. K. Langmuir 26, 3003–3007 (2010). 2. Eberle, A.P.R., Casta˜ neda-Priego, R., Kim, J. M. & Wagner, N. J. Langmuir 28, 1866–1878 (2012). 3. Eberle, A.P.R., et al., Physical Review E, 89, 050302 (2014).

**M1.0026 Dissolution of a Colloidal Particle in an Oscillatory Fluid Medium**

**DEZHuang ye, Ji-Qin LI**, Mechanical Engineering, University of Connecticut, ROBIN BOGNER, Pharmaceutical Sciences, University of Connecticut, TAI-HSI FAN, Mechanical Engineering, University of Connecticut — Understanding dissolution kinetics of a colloidal particle in an aqueous solution is of great importance in many pharmaceutical and biochemical applications. We present theoretical analysis of low Reynolds number transient dynamics and mass transfer of a dissolving spherical particle in a unidirectional oscillatory flow. The coupling of fluid flow and passive motion of the particle are resolved analytically, and the transient mass transfer associated with the oscillation of the particle is numerically computed. The flow patterns, diffusive and convective transport phenomena, and the dissolution kinetics under various saturation concentrations and flow conditions are characterized by the frequency parameter, Schmidt number, and Peclet number. The result severs as a basic case in determining the efficiency of drug dissolution or reconstitution that depends on various shaking methods.

**M1.0027 Effective temperatures and the breakdown of the Stokes-Einstein relation for particle suspensions**

**CARLOS MENDOZA**, Materials Research Institute UNAM, IVAN SANTAMARIA-ROKE, UMDI-J Facultad de Ciencias UNAM, AGUSTIN PREZ-MADRIL, Departament de Fisica Fonamental, Universitat de Valencia — The short- and long-time breakdown of the classical Stokes-Einstein relation for colloidal suspensions at arbitrary volume fractions is explained here by examining the role that confinement and attractive interactions play in the intra- and inter-cage dynamics executed by the colloidal particles. We show that the short-time diffusion coefficient is larger than the one predicted by the classical Stokes-Einstein relation due to a non-equilibrated energy transfer between kinetic and configuration degrees of freedom. This transfer can be incorporated in an effective temperature that replaces the bath temperature in a Generalized Stokes-Einstein relation (GSER). This relation then allows to obtain the diffusion coefficient once the viscosity is known. On the other hand, the temporary cluster formation induced by confinement and attractive interactions of hydrodynamic nature, makes the long-time diffusion coefficient to be smaller than the one obtained from the classical Stokes-Einstein relation.

Additionally, we provide a simple expression based on a differential effective medium theory (DEMT) that allows to calculate the diffusion coefficient at short and long times. Comparison of our results with experiments and simulations for suspensions of hard and porous spheres shows an excellent agreement in all cases.

**M1.0028 Geometric Frustration Selects Morphology in Chiral Filament Bundles**

**UNAM DGAPA IN-110613**

Hydrodynamic interactions in colloidal systems confined to linear geometries with a singular corner.  

**M1.00209** Effect of Salts on Drainage of Foam, **SOUMYADIP SETT**, University of Illinois at Chicago, **STOYAN KARAKASHEV**, University of Sofia, Bulgaria, **STOYAN SMOKOV**, University of Cambridge, UK, **ALEXANDER YARIN**, University of Illinois at Chicago — Gravitational drainage from thin planar vertical sodium dodecyl sulfate (SDS) films in the presence of inorganic salts was experimentally studied. Strong ion-specific effects of the counter ions were found to affect the stability and the rate of drainage of the planar foam films as a function of concentration of the inorganic salts. The counter-ions can either stabilize (below the critical concentration) or destabilize the foam films. We found that the strongest foam destabilizer salt became the strongest foam destabilizer beyond its critical concentration.

**M1.00210** The role of the anchoring conditions in the electro rheological behavior of a nematic constrained by two coaxial cylinders and submitted by a pressure drop, **DANIEL MARTINEZ SNCHEZ**, Universidad Autonoma de la Ciudad de Mexico, **JUAN ADRIN REYES CERVANTES**, Universidad Nacional Autonoma de Mexico — We study a nematic liquid crystal (LC) filled in a region between two coaxial cylinders subjected to the simultaneous action of both a pressure gradient applied parallel to the axis of the cylinders and a radial low frequency electric field. For the LC 4'-n-pentyl-4-cyanobiphenyl (5CB), we consider soft anchoring boundary conditions to obtain the configuration of the director and the velocity profile and the pressure gradient for nonslip boundary conditions. Finally, we calculate the effective viscosity, the first normal stress difference, and the dragging forces on the cylinders.

**M1.00211** Colloidal particles embedded in liquid crystal droplets, **DREW MELCHERT**, **MONIROSADAT SADATI**, **YE ZHOU**, **JUAN J. DE PABLO**

Institute for Molecular Engineering, University of Chicago — In this work, we encapsulate polystyrene and silica particles in nematic liquid crystal (LC) droplets dispersed in water using microfluidic glass capillary devices. While polystyrene particles induce planar anchoring on the surface, silica particles, treated with DMOAP, create homeotropic anchoring of the LC molecules at their surface. Sodium dodecyl sulfate (SDS) is added to the aqueous phase to stabilize LC droplets and promote a radial configuration with point defect in the center of LC droplet. Our experimental and computational studies show that, when trapped inside the LC droplets, particles with both anchoring types become mostly localized at the defect point (at the center) and interact with the radial configuration. Interestingly, a twisting structure is observed for polystyrene particle with strong planar anchoring. Although localization of the particles at the droplet center is the most stable state and with the lowest free energy, off-center positions also emerge, displacing the defect point from the center to near the surface of a radial droplet.

This work was made possible by the Natural Sciences and Engineering Research Council of Canada and Compute Ontario.

**M1.00212** Coarse-Grained Molecular Monte Carlo Simulations of Liquid Crystal-Nanoparticle Mixtures

Institute for Molecular Engineering, University of Chicago — Coarse-grained intermolecular potentials have proven capable of capturing essential details of interactions between complex molecules, while substantially reducing the number of degrees of freedom of the system under study. In the domain of liquid crystals, the Gay-Berne (GB) potential has been successfully used to model the behavior of rod-like and disk-like mesogens. However, only ellipsoid-like interaction potentials can be described with GB, making it a poor fit for many real-world mesogens. In this work, the results of Monte Carlo simulations of liquid crystal domains using the Zewdie-Corner (ZC) potential are presented. The ZC potential is constructed from an orthogonal series of basis functions, allowing for potentials of essentially arbitrary shapes to be modeled. We also present simulations of mixtures of liquid crystalline mesogens with nanoparticles. Experimentally these mixtures have been observed to exhibit microphase separation and formation of long-range networks under some conditions. This highlights the need for a coarse-grained approach which can capture salient details on the molecular scale while simulating sufficiently large domains to observe these phenomena. We compare the phase behavior of our simulations with that of a recently presented continuum theory.

This research was supported by the National Sciences and Engineering Research Council of Canada and Compute Ontario.

**M1.00213** ABSTRACT WITHDRAWN

**M1.00214** Magnetic domains and defects in ferromagnetic liquid crystal colloids realized with optical patterning

University of Colorado Boulder — A promising approach in designing composite materials with unusual physical behavior combines solid nanostructures and orientationally ordered soft matter at the mesoscale. Such composites not only inherit properties of their constituents but also can exhibit emergent behavior, such as ferromagnetic ordering of colloidal metal nanoparticles forming mesoscopic magnetization domains when dispersed in a nematic liquid crystal. Here we demonstrate the optical patterning of domain structures and topological defects in such ferromagnetic liquid crystal colloids which allows for altering their response to magnetic fields. Our findings reveal the nature of the defects in this soft matter system which is different as compared to non-polar nematic and ferromagnetic systems alike.

**M1.00215** Conformation of charged vesicles: the Debye Huckel and the low curvature limit

Indian Inst of Tech-Bombay — The shape as well as tension and pressure inside an uncharged vesicle are determined by the reduced volume. These parameters are important for a vesicle or a biological cell, since it can affect bio-physical processes such as osmosis and permeation, interaction with external agents such as bio-macromolecules and thermal fluctuations of the bilayer membrane of a vesicle. Charged membranes are ubiquitous in nature, most biological cell bio-membranes are charged, and therefore the knowledge of shape, tension and pressure of charged vesicles is critical. Additionally, the distribution of charges in the inner and outer leaflets is also important as it can affect the spatial interaction of a bilayer membrane with proteins. This work addresses these issues in the low charge and curvature limit. Our analysis indicates that despite a very strong two-way coupling between the charge and the curvature, the shapes of charged vesicles remain similar to that of uncharged vesicles at comparable reduced volumes, even for reasonable values of total charge. However, the tension and pressure values are higher, and are accurately estimated. Similarly the charge distribution on the outer and inner leaflet is strongly affected by the curvature. The value of spontaneous curvature due to charge redistribution is estimated. The insensitivity of the shape to charges persists even when only the outer leaflet is charged instead of charged inner and outer leaflets.

This research was supported by the NSF grant DMR-1420736.
M1.00216 Emergence of DNA-encapsulating liposomes from a DNA-lipid blend film1. SHUNSUKE SHIMOBAYASHI, Department of Physics, Kyoto University, MAFUMI HISHIDA, Department of Chemistry, Tsukuba University, TOMO KURIMURA, MASATOSHI ICHIKAWA, Department of Physics, Kyoto University — A Micro-scale giant unilamellar vesicle (GUV) densely encapsulating molecular systems is one of the simplest life-mimicking model systems. The dehydration-rehydration process proposed by Deamer et al. more than 30 years ago generates vesicles to satisfy the constraints of micro-scale size, unilamellarity and densely polymer-encapsulation [1]. Nevertheless, the physico-chemical mechanism of a set of dehydration-rehydration process has been poorly understood. The present study reveals crucial factors on the process through fluorescent microscopic observation [2] and Small-angle x-ray scattering. From the results, we propose a plausible physical mechanism for the process, making it possible to optimize the encapsulation of any agent. [1] D. W. Deamer, G. L. Barchfield, J. Mol. Evol, 18, 203-206 (1982). [2] S. Shimobayashi and M. Ichikawa, J. Phys. Chem. B 118, 10658-10694 (2014).

1This work was supported by Grant-in-Aid for JSPS Fellows Grant (No. 25-1270) and by KAKENHI (Nos. 26707020, 25103012, and 26115709).

M1.00217 Lipid transfer energetics between free-standing and solid supported membranes: reconciling discrepancies. BENNY WAH, JOSEPH ADAMS, JEFFREY BREIDIGAN, LI GE, PIOTR HORBAL, Univ of Illinois - Chicago, LIONEL PORCAR, University of Delaware, SUMIT GARG, URSULA PEREZ-SALAS, Univ of Illinois - Chicago — The membranes of animal cells have significant variation in the lipid and protein composition. If it weren’t for the active work of proteins that maintain most of these variations, membranes would ultimately homogenize throughout by mixing. It has been long been recognized that the study of the passive movement of lipids between and within membranes can provide insight into this energetic toll. Using small angle neutron scattering, a non-invasive in situ technique, we recently demonstrated that tags or small structure changes in the lipids can have a huge effect on their transport characteristics. In the present study we compare lipid transfer and energetics between supported free standing membranes. We find that exchange and flipping process are comparable while the presence of the surface slightly increases inter and intra-membrane transport rates. The activation energies for exchange appear to be nearly unaffected by the presence of the surface while for flip-flop it slightly increases. The increase in the rates due to the presence of the surface may possibly explain the apparent contradicting behavior previously reported on supported flat membrane systems and in free-standing membranes.

M1.00218 Photo-Regeneration of Severed Gel Using Photo-Controlled Radical Polymerization, AWANEESH SINGH, Univ of Pittsburgh, OLGA KUKSENOK, Clemson University, JEREMIAH A. JOHNSON, Massachusetts Institute of Technology, ANNA C. BALAS, Univ of Pittsburgh — Using the framework of dissipative particle dynamics (DPD) simulation, we developed a novel computational model that enables photo-regeneration of the gel matrix when a significant portion of the material is severed. We considered photo-controlled radical polymerization (photo-CRP) within polymer networks with embedded initiators (initiators for the photo-CRP reaction). These initiators turn on the polymerization process in the presence of light with monomers and cross-linkers in the solution. This "photo-growth" allow us to effectively regenerate severed gels under the application of light. The growth process can be turned off once the polymerization is near completion, which forms a new cross-linked gel that resembles the uncut material. The polymerization rate can be modulated by altering the light intensity.

M1.00219 Frictional Properties of UV illuminated ZnO Thin Films Grown by Pulsed Laser Deposition1, HSiang-ChHi Chiu, HUAN-Pu Chang, FANG-Yu LQ, YU-TING YEH, Department of Physics, National Taiwan Normal University, DEPARTMENT OF PHYSICS, NATIONAL TAIWAN NORMAL UNIVERSITY COLLABORATION — Zinc Oxide (ZnO) nanostructures have potential applications in nano-electro-mechanical systems (NEMS) due to their unique physical properties. ZnO is also an excellent lubricant and hence a promising candidate for protective coatings in NEMS. By means of atomic force microscopy (AFM), we have investigated the frictional properties of ZnO thin films prepared by pulsed laser deposition technique. In addition, UV illumination is used to convert the surface wettability of ZnO thin films from being more hydrophobic to superhydrophilic via the photo-catalyst effect. We found that the frictional properties of the UV illuminated, superhydrophilic ZnO surface are strongly dependent on the surface roughness, environmental humidity and the presence of nanoscale capillary condensation forming between surface asperities at the tip-ZnO contact. Our results might find applications in future ZnO related NEMS.

1Frictional Properties of UV illuminated ZnO Thin Films Grown by Pulsed Laser Deposition

M1.00220 Fracture of molecular glasses under tension and fracture-induced crystallization. YINSHAN CHEN, TRAVIS POWELL, LIAN YU, University of Wisconsin-Madison — Molecular glasses are formed and fractured by cooling a liquid on a less thermally expansive substrate. In-plane tension is created by the mismatch of thermal expansion coefficients and accumulates to cause catastrophic network fracture. This simple experiment allowed the measurement of fracture toughness and the heat of fracture of molecular glasses for the first time. For the systems studied (α-terphenyl, indomethacin, and sucrose benzoate), the fracture condition is well described by recent theories and a material-specific energy release rate (fracture toughness) approximately 1 J/m². The heat of fracture was found to be anomalously high relative to the value expected for the energy release rate and the surface area created. The large release of heat is caused by the reduction of heat capacity for a glass film constrained on a rigid substrate. Rapid crystal growth was observed along fracture surfaces. (Ref.: Powell, C. T.; Chen, Y.; Yu, L. J. Non-Crystalline Solids 2015, 429, 122-128)

M1.00221 Supramolecular Hydrogels from Self-Assembly of di-Fmoc-L-lysine. SEYED MEYSAM HASHEMNEJAD, KINSEY NAAS, SANTANU KUNDU, Mississippi State University — Mechanical properties and nanostructure of a supramolecular hydrogel formed by self-assembly of di-Fluorenylmethoxy carbonyl-L-lysine (di-Fmoc-L-lysine) are reported here. Hydrogels were prepared by solvent switch technique in which water was added to a solution of di-Fmoc-L-lysine in dimethyl sulfoxide (DMSO). Mechanical properties of the gels were investigated using shear and cationization rheology. The gels display strain-softening behavior at moderate strain values. Morphological investigations of the samples were conducted using FTIR and CD spectroscopy, electron microscopy, and atomic force microscopy (AFM). Self-assembled fibers with lateral dimensions ranging from 10 to 50 nm were captured in microscopy studies. FTIR results indicate β-sheet-like conformation of the peptides in the hydrogel.

M1.00222 Predicting out-of-Equilibrium Phase Behavior in the Dynamic Self-Assembly of Colloidal Crystals. JAMES SWAN, ZACHARY SHERMAN, Massachusetts Inst of Tech-MIT — Crystals self-assembled from colloidal particles are useful in an array of well demonstrated applications. During fabrication however, gelation and glassification often leave these materials arrested in defective or disordered metastable states. We show how time-dependent, pulsed interparticle interactions can avoid kinetic barriers and yield well-ordered crystalline domains for a suspension of hard, spherical colloidal particles interacting through short-range attractions. This dynamic self-assembly process is analogous to the flashing Brownian ratchet. Although this is an inherently unsteady, out-of-equilibrium process, we can predict its outcome using appropriate time averages of equilibrium equations of state. The predicted phase behavior is tested and validated by examining the fluid/crystal coexistence of such dynamically self-assembly dispersions in Brownian dynamics simulations of sedimentation equilibrium and homogeneous nucleation. We also show that our dynamic self-assembly scheme offers control and tunability over the crystal growth kinetics and can even stabilize nonequilibrium structures.
Achieving synchronization with active hybrid materials: Coupling self-oscillating gels and piezoelectric films. VICTOR V. YASHIN, Department of Chemical Engineering, University of Pittsburgh, STEVEN P. LEVITAN, Department of Electrical Engineering, University of Pittsburgh, ANNA C. BALAZS, Department of Chemical Engineering, University of Pittsburgh — Our goal is to develop materials that compute by using non-linear oscillating chemical reactions to perform spatio-temporal recognition tasks. The material of choice is a polymer gel undergoing the oscillatory Belousov-Zhabotinsky reaction. The novelty of our approach is in employing hybrid gel-piezoelectric micro-electro-mechanical systems (MEMS) to couple local chemo-mechanical oscillations over long distances by electrical connection. Our modeling revealed that (1) interaction between the MEMS units is sufficiently strong for synchronization, (2) the mode of synchronization depends on the number of units, type of circuit connection (serial or parallel), and polarity of the units; (3) each mode has a distinctive pattern in phase of oscillations and generated voltage. The results indicate feasibility of using the hybrid gel-piezoelectric MEMS for oscillator based unconventional computing.

Rheological Characterization of Bioinspired Mineralization in Hydrogels. ABIGAIL RE-GITSKY, NIELS HOLTEN-ANDERSEN, Massachusetts Institute of Technology — With increasing amounts of CO$_2$ in the atmosphere linked to potentially catastrophic climate change, it is critical that we find methods to permanently sequester and store CO$_2$. Inspired by the natural mineralization of calcium carbonate (CaCO$_3$), one future goal of this project is to understand the mechanisms of CaCO$_3$ mineralization in order to ultimately optimize a bioinspired hydrogel system, which produces high value industrial powders that consume CO$_2$ as a feedstock. Along the way, we are developing a rheological technique to study mineral nucleation and growth events by measuring the modulations in mechanical properties of a hydrogel system during mineralization. Our initial system consists of a gelatin hydrogel matrix, which is preloaded with calcium ions, and an aqueous solution of carbonate ions, which are allowed to diffuse through the gel to initiate the mineralization process. In order to monitor how the growth of minerals affects the mechanical properties of the gel network, we measure the storage (G) and loss (G*) moduli of the system in situ. Future work will focus on modifying the properties of the minerals formed by changing the polymer used in the hydrogel network and adding other organic molecules into the system.

Hardening and yielding in colloidal gels. EMANUELA DEL GADO, JADER COLOMBO, MEHDI BOUZID, Georgetown University — Attractive colloidal gel networks are disordered elastic solids that can form even in extremely dilute particle suspensions. With interaction strengths comparable to the thermal energy, their stress-bearing network can locally restructure via breaking and reforming inter-particle bonds. We use molecular dynamics simulations of a model system to investigate the strain hardening and the yielding process. During shear start up protocol, the system exhibits strong localization of tensile stresses that may be released through the breaking and formation of new bonds. In this regime, the small amplitude oscillatory shear analysis shows that the storage and the loss modulus follow a power law behavior that are closely reminiscent of experimental observations. At large accumulated strains, the strain-induced reorganization of the gel may trigger flow heterogeneities and eventually lead to the yielding of the gel via a quasi brittle damage of its structure.

Agglomerate Breakdown in Shear Thickening Fluids by Large Amplitude Oscillatory Shear (LAOS). RAN TAO, KIRK D. RICE, GALE A. HOLMES, NIST — Amorphous fumed silica and polypropylene glycol (PPG) suspensions were investigated using both steady shear and oscillatory shear rheology. As-mixed and sonicated silica/PPG suspensions show different shear thickening behavior with different critical shear rates as analyzed by the MITLAOS framework as well as the Fourier Transform approach. The as-mixed suspensions show a pronounced decrease in viscosity or modulus over the course of measurement, which is ascribed to an irreversible breakdown of silica-PPG agglomerates induced by shear. We also extend research to study colloidal silica/PPG dispersions under the same LAOS framework. In particular, we seek to understand the impact of the nanoparticle's structure, i.e., fractal vs. non-fractal, on the oscillatory STF response.

**STATISTICAL AND NONLINEAR PHYSICS**

Three Dimensional Observations of Quantum Vortex Dynamics in Superfluid Helium. PETER MEGSON, PETER MEGSON, University of Maryland, College Park — Liquid helium, when cooled below 2.17 K, becomes a superfluid with exotic physical properties such as flow without friction. Superfluid flow is irrotational except about line-like topological phase defects with quantized circulation, known as quantum vortices. The dynamics of these vortices include events such as reconnection, wherein vortices meet and exchange tails, and Kelvin wave propagation, a possible mechanism for energy dissipation. We observe the dynamics of fluorescent nanoparticles trapped on the vortices using a newly developed 3D stereographic system. This talk will present new observations of reconnection events and analysis comparing vortex reconnection behavior in three dimensions to previous work that observed such events in two-dimensional projection. In particular, we discuss the power law scaling of vortex separation as a function of time and the effect of the initial angle of separation between the vortex filaments.

Tension-induced tunable corrugation in bio-inspired two-phase soft composite materials: mechanisms and implications. AHMED ELBANNA, QIANLI CHEN, University of Illinois Urbana Champaign — We numerically investigate the elastic deformation response of a two-phase bio-inspired soft composite material under externally applied concentric tension using the finite element method. We show that by carefully designing the inclusion pattern it is possible to induce corrugations normal to the direction of stretch. By stacking 1D composite fibers to form 2D membranes, these corrugations collectively lead to the formation of membrane channels with shapes and sizes that are tunable by the level of stretch. Furthermore, we show that by using specific inclusion patterns in laminated plates, it is possible to create pop-ups and troughs enabling the development of complex 3D geometries from planar construction. We have found that the corrugation amplitude increases with the stiffness of inclusion and its eccentricity from the tension axis. We discuss the mechanisms leading to the development of corrugations as well as its different implications. We discuss applications for this design in a variety of fields including tunable band gap formation, surface roughness controllability, auxetic materials and toughness enhancement via programmable evolving geometrical effects.

Phase correlation in the eigenfunctions of a class of quantum chaotic systems. JIAOZI WANG, WENGE WANG, Unv of Sci & Tech of China — The random matrix theory predicts vanishing correlation function for eigenfunctions. In this work, we study an important class of quantum chaotic systems, whose Hamiltonians have a sparse structure in unperturbed bases. It is shown that, contrary to the prediction of the random matrix theory, components of the eigenfunctions in such systems have interesting phase correlations, giving non-vanishing correlation functions. Explicit expressions for some of the correlation functions are derived and checked by numerical simulations. As an application, a relation between a type of transition probability and a survival probability amplitude is derived.

Harnessing geometric and magnetic nonlinearities in phononic meta-plates. OSAMA BILAL, ANDRE FOEHR, CHIARA DARAIO, Department of Mechanical and Process Engineering, ETH-Zurich — Owing to their physical realization, locally resonant metamaterials retain narrow subwavelength band gaps. Moreover, the fixed geometry and dimensions of the unit cell set a hardbound on the central frequency of these band gaps, which can be particularly small compared to the unit cell width. Real-time tunable metamaterials extend the range of applications and further enable the realization of new sensors, filters, and switches. Our work harnesses the interaction between geometric nonlinearity and nonlinear magnetic potentials to engineer frequency- agile subwavelength band gaps. The concept is general and applicable to various metamaterials systems. Both numerical simulations and experimental realization of the proposed concept will be presented.
M1.00232 Propagation of mechanical waves through a stochastic medium with spherical symmetry. CARLOS AVENDANO, Universidad Autonoma de la Ciudad de Mexico, ADRIAN REYES, Universidad Nacional Autonoma de Mexico — We analyze the propagation of mechanical waves through an anisotropic and inhomogeneous medium with spherical symmetry. We assume that both its elastic and density properties are random functions of spatial coordinates with specific statistical properties, which allow us to represent media whose properties are not completely determined. We compute the expected value of this system.

M1.00233 A network model of human aging: Limits, errors, and information. SPENCER FARRELL, ARNOLD MITNITSKI, KENNETH ROCKWOOD, ANDREW RUTENBERG, Dalhousie University — The Frailty Index (FI) quantifies human aging using the fraction of accumulated age-related deficits. The FI correlates strongly with mortality and accumulates non-linearly and stochastically with age. Clinical data shows a nearly universal limit of FI ≤ (1.7). We computationally model an aging population using a network model of interacting deficits. Deficits damage and repair at rates that depend upon the average damage of connected nodes. The model is parametrized to fit clinical data. We find that attribution errors, especially false negative, allow the model to recover the frailty limit. Mutual information allows us to assess how well the FI can predict mortality. Mutual information provides a non-parametric measure of how the FI predicts mortality. We find that attribution errors have a small effect on the mutual information when many deficits are included in the model. The mutual information of our model and of the clinical data are comparable.

M1.00234 Changes in the Distribution of Avalanches on a Conical Bead Pile with Cohesion. JUSTINE WALKER, SUSAN LEHMAN, College of Wooster, KARIN DAHMEN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, JONATHAN UHL, Retired — The probability distributions for avalanches of varying size are experimentally determined for a slowly driven, conical bead pile. The pile is composed of roughly 20,000 steel spheres, 3 mm in diameter, atop a circular base; it is driven by adding one bead at a time to the apex of the pile. We investigate the dynamic response of the pile by recording avalanches off the pile over the course of tens of thousands of bead drops. The avalanching behavior is studied at different drop heights and different amounts of cohesion between the beads. The level of cohesion is tuned through use of an applied uniform magnetic field. Smaller, local avalanches are distinguished from larger, non-local avalanches and the moments of the avalanche distribution are calculated separately for these different populations. The resulting moments scale with cohesion differently, and the results are compared to the scaling predictions from an analytic mean-field model and corresponding simulation of slip avalanches in a shear system [Dahmen, Nat Phys 7, 554 (2011)].

M1.00235 Improving detection of avalanches on a conical bead pile. AVI VAJPEYI, SUSAN LEHMAN, College of Wooster, KARIN DAHMEN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, JONATHAN UHL, Retired — A conical bead pile subject to slow driving and an external magnetic field is used as a simple system to investigate the variations in the avalanche size probability distribution function. Steel beads are dropped onto the pile from different heights and at different strengths of applied magnetic field. Avalanches are recorded by the change in mass as beads fall off the pile. Experimentally we observe an increasing deviation from power law behavior as the field and thus cohesion between the beads increases. We compare our experimental results to the probability distribution function of the results of an analytic theory from a mean-field model of slip avalanches [Dahmen, Nat Phys 7, 554 (2011)]. The model also makes predictions for avalanche duration, which is not measurable with the existing system. To more fully characterize the avalanching behavior of the pile over time, a high-speed camera has been added to the system to record the largest avalanches and allow more detailed analysis. The conical pile geometry presents a challenge for observation and particle tracking over the full pile. Our implementation scheme and preliminary results from the video analysis are presented.

M1.00236 Effects of sudden density changes in disordered superconductors and semiconductors. HIBA ASSI, HARSHWARDHAN CHATURVEDI, MICHEL PLEMLING, UWE TÄUBER, Department of Physics, Virginia Tech — Vortices in type-II superconductors in the presence of extended, linear defects display the strongly pinned Bose glass phase at low temperatures. This disorder-dominated thermodynamic state is characterized by suppressed lateral flux line fluctuations and very slow structural relaxation kinetics: The vortices migrate between different columnar pinning centers to minimize the mutual repulsive interactions and eventually optimize the system’s pinning configuration. To monitor the flux lines’ late-time structural relaxations, we employ a mapping between an effectively two-dimensional Bose glass system and a modified Coulomb glass model, originally developed to describe disordered semiconductors at low temperatures. By means of Monte Carlo simulations, we investigate the effects of the introduction of random bare site energies and sudden changes in the vortex or charge carrier density on the soft Coulomb gap that appears in the density of states due to the emerging spatial anticorrelations. The non-equilibrium relaxation properties of the Bose and Coulomb glass states and the ensuing aging kinetics are studied through the two-time density autocorrelation function and its various scaling forms.

M1.00237 Autonomous Brownian motors driven by nonadiabatic variation of internal parameters. ALEX PLYUKHIN, Saint Anselm College — We study a family of autonomous motors based on a Brownian particle driven from thermal equilibrium by periodic in time variation of the internal potential through which the particle interacts with molecules of the surrounding thermal bath. We demonstrate for such motors the absence of a linear response regime: The average driving force and drift velocity are shown to be quadratic in both the frequency and amplitude of the variation. The adiabatic approximation (of an infinitely slow variation) and the leading correction to it (linear in the variation’s frequency) lead to zero drift and are insufficient to describe the motor’s operation.

M1.00238 Modeling the Earth: Climate on an Icosphere. STEPHANIE FOUTS, Washington and Lee University, L. JONATHAN COOK, Roanoke College — The totally asymmetric simple exclusion process with Langmuir kinetics is a one-dimensional transport model used to study the motion of particles through a lattice. Its applications include systems in the fields of biology, climatology, mathematics, civil engineering, and physics. In our research, we examine the temporal dynamics through the power spectra, as well as the time-averaged particle distribution on the lattice via Monte Carlo simulations. We have applied our particle transport model to an icosahedron in an attempt to model Earth’s changing climate. In our research, we examine the temporal dynamics of the particle distribution on the lattice, as they correspond to seasonal heat fluctuations in the polar and equatorial regions of the globe. Using Monte Carlo simulations, we alter the input parameters of the system to explore the resultant actions of the Earth-system model. Our findings include seasonal oscillations consistent with those seen in reality. We also built a mathematical framework for our model which, when solved numerically, matches the oscillations seen in our physical system.
Directed Nanopatterning with Nonlinear Laser Lithography. ONUR TOKEL, OZGUN YAVUZ, EMRE ERGECEK, IHOR PAIVLOV, GHAITH MAKEY, FATIH OMER ILDAY. Bilkent University — In spite of the successes of maskless optical nanopatterning methods, it remains extremely challenging to create any isotropic, periodic nanopattern. Further, available optical techniques lack the long-range coverage and high periodicity demanded by photonics and photovoltaics applications. Here, we provide a novel solution with Nonlinear Laser Lithography (NLL) approach [1]. Notably, we demonstrate that self-organized nanopatterns can be produced in all possible Bravais lattice types. Further, we show that carefully chosen defects or structured noise can direct NLL symmetry. Exploitation of directed self-organization to select or guide to predetermined symmetries is a new capability. Predictive capabilities for such far-from-equilibrium, dissipative systems is very limited due to a lack of experimental systems with predictive models. Here we also present a completely predictive model, and experimentally confirm that the emergence of motifs can be regulated by engineering defects, while the polarization of the ultrafast laser preserves lattice symmetry, which in turn reinforces translational invariance. Thus, NLL enables a novel, maskless nanofabrication approach, where laser-induced nanopatterns can be rapidly created in any lattice symmetry. [1] Nature Photonics, 7, 897(2013)

M1.00240 purohit@seas.upenn.edu , XIAOJUN LIANG, PRASHANT PوروHIT, University of Pennsylvania — The thermal fluctuations of lipid bilayer membranes are key to their interaction with cellular components as well as the measurement of their mechanical properties. Typically, membrane fluctuations are analyzed by decomposing into normal modes or by numerical simulations. Here we propose a new approach to calculate the partition function of a membrane. We view the membrane as a fluctuating von Karman plate and discretize it into triangular elements. We express its energy as a function of nodal displacements, and then compute the partition function and covariance matrix using Gaussian integrals. We recover well-known results for the dependence of the projected area of the membrane on the applied tension and recent simulation results on the dependence of membrane free energy on geometry, spontaneous curvature and tension. As new applications we compute the fluctuations of the membrane of a malaria infected cell and analyze the effects of boundary conditions on fluctuations. We also compare our calculation with some simulation method to show our time efficiency as well as accuracy.

Back-and-forth micromotion of aqueous droplets in a dc electric field. TOMO KURIMURA, MASATOSHI ICHIKAWA, Kyoto University, MASAIRO TAKINOUKE, Tokyo Institute of Technology, KENICHI YOSHIKAWA, Doshisha University — Recently, it was reported that an aqueous droplet in an oil phase exhibited rhythmic back-and-forth motion under stationary dc voltage on the order of 100 V. Here, we demonstrate that the threshold voltage for inducing such oscillation is successfully decreased to the order of 10 V through downsizing of the experimental system [1]. Notably, the threshold electric field tends to decrease with a nonlinear scaling relationship accompanied by the downsizing. We derive a simple theoretical model to interpret the system size dependence of the threshold voltage. This model equation suggests the unique effect of additional noise, which is qualitatively characterized as the coherent resonant enhancement in large droplets as a kind of coherent resonance. Our results will provide insight into the construction of micrometer-sized self-commutating motors and actuators in microfluidic and micromechanical devices. [1] TK, MI, MT and KY, Phys.Rev.E 88, 042918 (2013).

M1.00242 Phase Transitions in a Model of Y-Molecules Abstract , DANIELLE HOLZ, DONOVAN RUTH, Lehigh University, RAUL TORAL, Institute for Cross-Disciplinary Physics and Complex Systems, JAMES GUNTON, Lehigh University — Immunoglobulin is a Y-shaped molecule that functions as an antibody to neutralize pathogens. In special cases where there is a high concentration of immunoglobulin molecules, self-aggregation can occur and the molecules undergo phase transitions. This prevents the molecules from completing their function. We used a simplified model of 2-Dimensional Y-molecules with three identical arms on a triangular lattice with 2-dimensional Grand Canonical Ensemble. The molecules were permitted to be placed, removed, rotated or moved on the lattice. Once phase coexistence was found, we used histogram reweighting and multicanonical sampling to calculate our phase diagram.

M1.00243 ABSTRACT WITHDRAWN —

M1.00244 Social Network Influence and Personal Financial Status. SHAOJUN LUO, FLAVIANO MORONE, City College of CUNY, CARLOS SARRAUTE, Grandata, Buenos Aires, Argentina, HERMAN MAKSE, City College of CUNY — Networks of social ties emerging from individual economic needs display a highly structured architecture. In response to socio-economic demands, people reshape their circle of contacts for maximizing their social status, and ipso facto, the pattern of their interconnections is strongly correlates with their personal financial situation. In this work we transform this qualitative and verbal statement into an operative definition, which allows us to quantify the economic well-being of individuals trough a measure of their collective influence. We consider the network of mobile phone calls made by the Mexican population during three months, in order to study the correlation of person’s economic situation with her network location. Notably, we find that rich people tend to be also the most influential nodes, i.e., they self-organize to optimally position themselves in the network. This finding may be also raised at the level of a principle, a fact that would explain the emergence of the phenomenon of collective influence itself as the result of the local optimization of socio-economic interactions. Our method represents a powerful and efficient indicator of socio-economic robustness, which may be applied to maximize the effect of large scale economic intervention and stimulus policies

M1.00245 Statistical Mechanics of Japanese Labor Markets. HE CHEN1. Hokkaido University — We introduce a probabilistic model to analyze job-matching processes of recent Japanese labor markets, in particular, for university graduates by means of statistical physics. To make a model of the market efficiently, we take into account several hypotheses. Namely, each company fixes the (business year independent) number of opening positions for newcomers. The ability of gathering newcomers depends on the result of job matching process in past business years. This fact means that the ability of the company is weakening if the company did not make their quota or the company gathered applicants too much over the quota. All university graduates who are looking for their jobs can access the public information about the ranking of companies. By assuming the above essential key points, we construct the local energy function of each company and describe the probability that an arbitrary company gets students at each business year by a Boltzmann-Gibbs distribution. We evaluate the relevant physical quantities such as the employment rate and Gini index. We discuss social inequalities in labor markets, and provide some ways to improve these situations, such as the informal job offer rate, the job-worker mismatch between students and companies.

1Graduate School of Information Science and Technology

Agitated granular rod monolayers: Tetric or uniaxial nematic?1 . THOMAS MUELLER, Experimentalphysik V, University of Bayreuth, DANIEL DE LAS HERAS, Theoreticalphysik II, University of Bayreuth, INGO REHBERG, KAI HUANG, Experimentalphysik V, University of Bayreuth — The ordering of granular rod monolayers under vertical agitations against gravity is investigated experimentally and compared quantitatively with equilibrium Monte Carlo simulations and density functional theory. At sufficiently high number density, short rods form a tetratic state and long rods form a uniaxial nematic state. The ordering transitions are found to be independent of the agitation frequency and strength, suggesting that despite of driven far from thermodynamic equilibrium, agitated granular systems may share similar features with corresponding equilibrium systems. Finally, we summarize the universal and non-universal aspects between nonequilibrium granular rod and equilibrium liquid crystal systems in a state diagram.

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M1.00247 Buckling of Patterned Top Films, DOKYEONG KWON, Seoul Natl Univ, HYO SEON SUH, University of Chicago, KOOKHEON CHAR, Seoul Natl Univ — 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 on the top. Recently, many studies on the microstructure created by the buckling with flat top films have been reported and physics behind them has almost been well received. However, only a few work has been done for the buckling structure with micro- or nano-patterned top films and buckling mechanics for patterned top film-PDMS bilayers has not yet been established in full. Here, we present the buckling and the phase diagram on top of elastomeric PDMS substrates. Geometrical patterns were prepared by unconventional lithography techniques such as thermal imprinting of polystyrene (PS) films. Buckling instability was induced by applying mechanical stress to the patterned top surface-PDMS bilayers. Resulting buckled structures showed different mechanical structures as shape and structural parameters of the top thin films were varied. The structural changes were analyzed by introducing a beam theory or a plate theory for the simple modeling of the top surfaces, giving insights on the buckling mechanics of top films with complicated patterns placed on PDMS substrates.

M1.00248 Triggered Snap-Through of Bistable Shells, YIJIE CAI, Wuhan University of Technology, SHICHENG HUANG, JAN TRASE, NAM HU, ZI CHEN, Dartmouth College — Elastic bistable shells are common structures in nature and engineering, such as the lobes of the Venus flytrap or the snapping shrimp. Despite their ubiquity, the parameters that control the bistability of such structures are not well understood. In this study, we explore how the geometrical features of radially symmetric elastic shells affect the shape and potential energy of a shell’s stable states, and how to tune certain parameters in order to generate a snap-through transition from a convex semi-stable state to a concave stable state. We fabricated a series of elastic shells with varying geometric parameters out of silicone rubber and measured the resulting potential energy in the semi-stable state. Finite element simulations were also conducted in order to determine the deformation and stress in the shells during snap-through. It was found that the energy of the semi-stable state is controlled by only two geometrical parameters and a dimensionless ratio. We also noted two distinct transitions during snap-through; one between monostability and semi-bistability (the state a popper toy is in before it snaps-through and jumps), and a second transition between semi-bistability and true bistability. This work shows that it is possible to use a set of simple parameters to tailor the energy landscape of an elastic shell in order to generate complex trigger motions for their potential use in smart applications.


M1.00250 Thermodynamics and Phase Transitions of Ising Model on Inhomogeneous Stochastic Recursive Lattice, RAN HUANG, Shanghai Jiao Tong Univ — As one of the few exactly solvable thermodynamic models, the Ising model on recursive lattice is featured by its impressive advantages and successful applications in various thermodynamic and statistical researches. However this model was considered that, since the recursive calculation demands homogeneous structure, it can only describe the bulk and even systems with narrow utilization. In this work we figured out a practical methodology to extend the conventional homogeneous structure of single-unit Husimi lattice to be random inhomogeneous lattices with variable units and structures, while keeping the feature of exact calculation. Three designs of inhomogeneous recursive lattices: the random-angled rhombus lattice, the Husimi lattice of variable units, and the randomly multi-branched Husimi square lattice; and the corresponding exact recursive calculations based on the partial partition function algorithm, which is derived from the Bethe cavity method, have been investigated and developed.

With the "total-symmetry assumption" and the "iterative-recipe trick" we were able to exactly solve the classical ferromagnetic spin-1 Ising models on these lattices, to describe the complex systems that can only be solved by approximations or simulations on regular lattices. Our work may enhance the application of the exact calculation on recursive lattices in various fields of materials science and applied physics, especially it may serve as a powerful tool to explore the cross-dimensional thermodynamics and phase transitions.

M1.00251 Nonlinear dynamics of Bohmian trajectories in a double-well potential, O. F. DE ALCANTARA BONFIM, Univ of Portland, JOAO FLORENCIO, Universidade Federal Fluminense, RJ-Brazil — We investigate the dynamics of a quantum particle in a one-dimensional double-well potential within the framework of Bohm’s quantum mechanics. We find that the behavior of the trajectories is linked to the degree of complexity of the initial wave packet. By increasing the complexity of the wave packet we obtain trajectories that are either periodic, quasiperiodic, or chaoticlike.

M1.00252 Nematic-columnar phase transition in oriented hard rectangles, TRISHA NATH, The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India, DEEPAK DHAR, Department of Theoretical Physics, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai, 400005, India, R. RAJESH, The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India — We consider an assembly of monodispersed hard rectangles of size $d \times d$ on a square lattice with only hard core interactions amongst them. The long axes of the rectangles can be oriented along the horizontal or vertical directions. For large enough aspect ratios, it is known that this system undergoes three phase transitions as the density ($\rho$) of rectangles is increased: first an isotropic-nematic transition (at $\rho_c^1$), second a nematic-columnar transition (at $\rho_c^2$), and third a columnar-sublattice transition (at $\rho_c^3$). In the nematic phase, only the orientational symmetry is broken. The columnar and sublattice phases correspond to additional broken translational symmetries along one (perpendicular to the nematic orientation) and both directions respectively. Interestingly, the critical value $\rho_c^3$ remains finite, approximately 0.73, even as $d \to \infty$. We develop a systematic high density expansion for the surface tension between two differently-ordered columnar phases. Keeping only the first order perturbative correction term and setting this surface tension to zero, we get an estimate of $\rho_c^3$ in excellent agreement with estimates from Monte Carlo simulations, for all $d \geq 2$.

M1.00253 BIOLOGICAL PHYSICS —
M1.00254 Single-molecule studies of collagen mechanics

G. Shi, T. Wüst, Y. W. Li and D. P. Landau
The University of Georgia, Thomas Wüst, ID Scientific IT Services, ETH Zürich, Switzerland, Simon Fraser University — Collagen is the fundamental structural protein in vertebrates. Its triple helical structure at the molecular level is believed to be strongly related to its mechanical role in connective tissues. However, the mechanics of collagen at the single-molecule level remain contentious. Estimates of its persistence length span an order of magnitude, from 15-180 nm for this biopolymer of 300 nm contour length. How collagen responds to applied force is also controversial, with different single-molecule studies suggesting one of three different responses: extending entropically, overwinding, or unwinding, all at forces below 10 pN. Using atomic force microscopy to image collagen derivatives from solution, we find that their flexibility depends strongly on ionic strength and pH. To study force-dependent structural changes, we are performing high-throughput enzymatic cleavage assays of triple-helical collagen from our new compact centrifuge force microscope. Because proteolytic cleavage requires a locally unwound triple helix, these experiments are revealing how local collagen structure changes in response to applied force. Our results can help resolve long-standing debates about collagen mechanics and structure at the molecular level.

M1.00255 Population Dynamics of Viral Inactivation

K. Freeman, D. Li, Carnegie Mellon University, M. Behrens, Lund University, K. Streletzky, Cleveland State University, U. Olsson, Lund University, A. Evilevitch, Carnegie Mellon University — We investigated the population dynamics of viral inactivation in vitro using time-resolved cryo electron microscopy combined with light and X-ray scattering techniques. This is the first time-varying experiment to look at fluctuations within the protein at equilibrium. We simulate apoBirA, liganded BirA, as well as two mutants, M211A and V219A. In agreement with simulations, we find that the triggering process is directly dependent on the conformational state of the encapsidated DNA. The results of this work provide insight into how the in vivo kinetics of the spread of viral infection is influenced by intra- and extracellular environmental conditions.

M1.00256 Theory of sequence-dependent scaling and confinement of viral RNA molecules

J. Kelly, Univ of California - Los Angeles — We present a general theory for the fractal dimensions of the genomic viral RNA molecules of small RNA viruses and apply the theory as well to RNA encapsidation competition experiments.

M1.00257 Convex Lens-induced Confinement to Visualize Biopolymers and Interaction Parameters

F. Stabile, D. Berard, G. Henkin, M. Shyeghan, F. Michaud, S. Leslie, McGill University — We used the combination of the neutron spin-echo (NSE) and the small angle neutron scattering (SANS) techniques to study the inter-domain motions of the inorganic pyrophosphate (IPPase) enzyme derived from thermostable microorganisms Thermococcus thioreducens. Our results provide a better picture of the local flexibility and conformational substates unique to these types of proteins, which will help us better understand the relation between protein dynamics and their biological activities.

M1.00258 Slow Domain Motions of an Oligomeric Protein from Deep-Sea Hyperthermophile probed by Neutron Spin Echo

In this poster, we present a versatile CLiC (Convex Lens-induced Confinement) microscopy system to access a broad range of biopolymer visualization and interaction parameters. In the CLiC technique, the curved surface of a convex lens is used to deform a flexible coverslip above a glass substrate, creating a nanoscale gap that can be tuned during an experiment to load and confine molecules into nanoscale features, both linear and circular, embedded in the bottom substrate. We demonstrate and characterize massively parallel DNA nanochannel-based stretching, building on prior work. Further, we demonstrate controlled insertion of reagent molecules within the CLiC imaging chamber. We visualize real-time reaction dynamics of nanoconfined species, including dye/DNA intercalation and DNA/DNA ligation reactions, demonstrating the versatility of this nanoscale microscopy platform.

M1.00259 Replica-exchange Wang-Landau simulations of the HOP lattice protein model

G. Shi, T. Wüst, Y. W. Li and D. P. Landau
The University of Georgia, Thomas Wüst, ID Scientific IT Services, ETH Zürich, Switzerland, Ying Wai Li, National Center for Computational Sciences, Oak Ridge National Laboratory, David P. Landau, Center for Computational Physics, The University of Georgia — The hydrophobic-polar (HP) lattice protein model has been the subject of intensive investigation in an effort to aid our understanding of protein folding. However, the high ground state degeneracies caused by its simplification stands in contrast to the generally unique native states of natural proteins. Here we proposed a simple modification, by introducing a new type of “neutral” monomer, 0, i.e. neither hydrophobic nor polar, thus rendering the model more realistic without increasing its difficulties of sampling significantly. With the replica-exchange Wang-Landau (REWL) scheme, we investigated several widely studied HP proteins and their HP counterparts. Dramatic differences in both ground state and thermodynamic properties have been found. For example, the HOP version of Crambin shows more clear two-step folding and 3 order of magnitudes less ground state degeneracy than its HP counterpart.

M1.00260 Identifying paths of allostERIC communication in the protein BirA through simulations

G. Custer, D. Beckett, S. Matysiak, University of Maryland — Biotin ligase/repressor (BirA) is a bifunctional enzyme which adenylates biotin and transfers the product, biotinyl-5-AMP (bio-5-AMP) to biotin carboxyl carrier protein (BCCP). In the absence of BCCP, bio-5-AMP promotes the dimerization of BirA. In dimer form, the BirAbio-5-AMP complex is able to bind to the biotin operator and prevents further synthesis of biotin. The bio-5-AMP binds away from the dimer interface, so it is acting as an allosteric activator. We perform all-atom molecular dynamics simulations with BirA to look at fluctuations within the protein at equilibrium. We simulate apoBirA, liganded BirA, as well as two mutants, M211A and V219A. In agreement with experimental observations, several loops of the protein become stabilized for the liganded BirA when compared to the apo protein. In addition, changes in the dimer interface are observed for the M211A and V219A mutations, which are located in the ligand binding region. Using inter-residue correlation coefficients and pair energies a communication network through the protein is constructed. With this network we have identified paths which have the potential to be important in allostERIC activation of BirA. These paths and the methods we use to identify them will be presented.
α particles represent a fluctuating dipole, thus introducing structural polarization into the coarse-grained model. With this model, we were able to achieve significant folding mechanisms using all-atom molecular dynamics simulations is a challenge due to time and length scale issues. We recently developed a low resolution model that captures the essential mechanics of protein unfolding. This model allows us to study the folding and unfolding of proteins in a more computationally feasible manner.

Peptides are important biomolecules that play a crucial role in various biological processes. They are involved in a wide range of functions, including signal transduction, immune response, and protein-protein interactions. In this context, we investigate the mechanical unfolding process of ubiquitin with (or really outside) an idealized proteasome pore, and compare such processes for degradation. While the proteasome nanomachine has been extensively studied, the mechanism for unfolding proteins with the proteasome pore is still poorly understood. Here, we focus on the functional roles of proteasomes in the degradation process. We observe that the proteasome can unfold proteins through a process that involves the coordinated movement of its subunits.

The mechanical unfolding of proteins is a complex process that involves multiple steps, including the denaturation of the protein, the unfolding of its structure, and the release of the unfolded protein from the proteasome. Understanding this process is crucial for understanding the role of the proteasome in protein degradation. In this study, we focus on the mechanical unfolding of ubiquitin, a small protein that is often used as a model system for studying protein unfolding.

The structural properties of human CaMKII Ca2+/Calmodulin-Dependent Protein Kinase II (CaMKII) are important for understanding its function and regulation. In this study, we use X-ray crystallography to investigate the structural properties of CaMKII. We observe that CaMKII exists in two conformations, denoted as ΔT and ΔM, with distinct structural and functional properties.

The mechanical properties of biomolecular motors, such as kinesin and myosin, are critical for understanding their function in transport processes within cells. In this study, we investigate the mechanical properties of myosin VI, a molecular motor that moves along actin filaments to transport cargo within a cell. We use a combination of experimental and theoretical approaches to study the mechanical properties of myosin VI. We observe that myosin VI is capable of moving against a load, and we use this capability to study the mechanical properties of the motor.

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M1.00267 Molecular Dynamics Simulation and Statistics Analysis Reveals the Defense Response Mechanism in Plants, ZHICHAO LIU, YUNJIE ZHAO, CHEN ZENG, Department of Physics, The George Washington University, COMPUTATIONAL BIOPHYSICS LAB TEAM — As the main protein of the bacterial flagella, flagellin plays an important role in perception and defense response. The newly discovered locus, FLS2, is ubiquitously expressed. FLS2 encodes a putative receptor kinase and shares many homologies with some plant resistance genes and even with some components of immune system of mammals and insects. In Arabidopsis, FLS2 perception is achieved by the recognition of epiteptide flg22, which induces FLS2 heteromerization with BAK1 and finally the plant immunity. Here we use both analytical methods such as Direct Coupling Analysis (DCA) and Molecular Dynamics (MD) Simulations to get a better understanding of the defense mechanism of FLS2. This may facilitate a redesign of flg22 or de-novo design for desired specificity and potency to extend the immune properties of FLS2 to other important crops and vegetables.

M1.00268 Multiscale modeling of three-dimensional genome, BIN ZHANG, PETER WOLYNES, Rice University — The genome, the blueprint of life, contains nearly all the information needed to build and maintain an entire organism. A comprehensive understanding of the genome is of paramount interest to human health and will advance progress in many areas, including life sciences, medicine, and biotechnology. The overarching goal of my research is to understand the structure-dynamics-function relationships of the human genome. In this talk, I will be presenting our efforts in moving towards that goal, with a particular emphasis on studying the three-dimensional organization, the structure of the genome with multi-scale approaches. Specifically, I will discuss the reconstruction of genome structures at both interphase and metaphase by making use of data from chromosome conformation capture experiments. Computationally modeling of chromatin fiber at atomic level from first principles will also be presented as our effort for studying the genome structure from bottom up.

M1.00269 Quantifying the DNA binding characteristics of ruthenium based threading intercalator $\Lambda\Lambda-P$ with optical tweezers, NICHOLAS BRYDEN, Bridgewater State University, MA, MICAH McCALLEY, Northeastern University, MA, FREDRIK WESTERLUND, PER LINCOLN, Chalmers University of Technology, Sweden, IOULIA ROUZINA, Ohio State University, OH, MARK WILLIAMS, Northeastern University, MA, THAYAPARAN PARAMANATHAN, Bridgewater State University, MA — Utilizing optical tweezers, biophysicists have been able to study drug-DNA interactions on the single molecule level. Binuclear ruthenium complexes are a particular type of drug molecule that have been found to have potential cancer-fighting qualities, due to their high binding affinity and low dissociation rates. These complexes are threading intercalators, meaning that they must thread their bulky side chains through DNA base pairs to allow the central planar moiety to intercalate between the bases. In this study, we explored the binding properties of the binuclear ruthenium complex, $\Lambda\Lambda-P\left(\Lambda\Lambda-\text{[bidppz(phen)Ru}_{2}]^{4+}\right)$. A single DNA molecule is held at a constant force and the $\Lambda\Lambda-P$ solution introduced to the system in varying concentrations until equilibrium is reached. DNA extension data at various concentrations of $\Lambda\Lambda-P$ recorded as a function of time provide the DNA binding kinetics and equilibrium binding affinity. Preliminary data analysis suggests that $\Lambda\Lambda-P$ exhibits fast binding kinetics compared to the very similar $\Delta\Delta-P$. These complexes have the same chemical structure and only differ in their chirality, which suggests that the left handed ($\Lambda\Lambda$) threading moieties require less DNA structural distortion for threading compared with the right handed ($\Delta\Delta$) threading moieties.

M1.00270 Temperature Dependent Rotational Correlation in Lipids1, CHRISTINA OTHON, NEDA DADASHVAND, EDUARDO VEGA LOZADA, Wesleyan University — The lateral heterogeneity of lipid dynamics is explored in free standing lipid monolayers. As the temperature is lowered the lipids exhibit increasingly broad and heterogeneous rotational correlation. This increase in heterogeneity appears to exhibit a critical onset, similar to those observed for glassy fluids. We explore this heterogeneous relaxation by measuring the rotational diffusion of a fluorescent probe (NBD-PC) using time-resolved fluorescence anisotropy microscopy, in single constituent lipid monolayer of DMPC. The observed relaxation exhibits a narrow, liquid-like distribution at high temperatures ($T >2.4$ ns), consistent with previous experimental measures by different methods. However, as the temperature is quenched, the distribution broadens, and we observe the appearance of a long relaxation population ($16.5$ ns). This demonstrates that the nanoscale diffusion and reorganization in lipid structures can be significantly complex, even in the simplest unstructured architectures. This result can have a significant impact on the organization, permeability and energetics of natural membrane structures.

1 Temperature Dependent Rotational Correlation in Lipids

M1.00271 A study of the eigenvectors of low frequency vibrational modes in crystalline cytidine via high pressure infrared absorption and molecular dynamics simulations, CARL STARKEY, University of Toledo, KRISTINA WOODS, Carnegie-Mellon University, SCOTT LEE, University of Toledo — High-pressure infrared absorption experiments and molecular dynamics simulations have been used to study the eigenvectors and eigenvalues of the vibrational modes of crystalline cytidine at 295 K by evaluating the logarithmic derivative of the vibrational frequency with respect to pressure: $\frac{d\omega}{dP}$. Crystalline samples of molecular materials such as cytidine have vibrational modes that are localized within a molecular unit (“internal” modes) as well as modes in which the molecular units vibrate against each other (“external” modes). The value of the logarithmic derivative is a diagnostic probe of the nature of the eigenvector of the vibrational modes, making high pressure experiments a very useful probe for such studies. Internal stretching modes have low logarithmic derivatives while external as well as internal torsional and bending modes have higher logarithmic derivatives. Modes at about 503, 757, 795, 3093 and 3351 cm$^{-1}$ are found to have negative logarithmic pressure derivatives, indicating a weakening of the effective force constants associated with those modes. The two modes above 3000 cm$^{-1}$ are hydrogen-bond-stretching modes. The identity of all of these modes will be determined via molecular dynamical simulations.

M1.00272 Computational Study of Pseudo-phosphorylation of the Microtubule associated Protein Tau, DMITRIY PROKOPOVICH, LUCA LARIINI, Rutgers University-Camden — This computational study focuses on the effect of pseudo-phosphorylation on the aggregation of the microtubule associated protein tau. In the axon of the neuron, tau regulates the assembly of microtubules in the cytoskeleton. This is important for both stabilization of and transport across the microtubules. One of the hallmarks of the Alzheimer’s disease is that tau is hyper-phosphorylated and aggregates into neurofibrillary tangles that lay waste to the neurons. It is not known if hyper-phosphorylation directly causes the aggregation of tau into tangles. Experimentally, pseudo-phosphorylation mimics the effects of phosphorylation by mutating certain residues of the protein chain into charged residues. In this study, we will consider the fragment called PHF43 that belongs to the microtubule binding region and has been shown to readily aggregate.
M1.00273 Quantum Computational Calculations of the Ionization Energies of Acidic and Basic Amino Acids: Aspartate, Glutamate, Arginine, Lysine, and Histidine.\textsuperscript{1} C. P. DE GUZMAN, M. ANDRIANARIA-JONA, Y. S. LEE, V. ANDRIANARIA-JONA, Department of Physics, Pacific Union College, Angwin, CA, 94508 — An extensive knowledge of the ionization energies of amino acids can provide vital information on protein sequencing, structure, and function. Acidic and basic amino acids are unique because they have three ionizable groups: the C-terminus, the N-terminus, and the side chain. The effects of multiple ionizable groups can be seen in how Aspartate’s ionizable side chain heavily influences its preferred conformation (J Phys Chem A. 2011 April 7; 115(13): 2900–2912). Theoretical and experimental data on the ionization energies of many of these molecules is sparse. Considering each atom of the acidic amino as a potential departing site for the electron gives insight on how the three ionizable groups affect the ionization process of the molecule and the dynamic coupling between the vibrational modes. In the following study, we optimized the structure of each acidic and basic amino acid then exported the three dimensional coordinates of the amino acids. We used ORCA to calculate single point energies for a region near the optimized coordinates and systematically went through the x, y, and z coordinates of each atom in the neutral and ionized forms of the amino acid. With the calculations, we were able to graph energy potential curves to better understand the quantum dynamic properties of the amino acids.

\textsuperscript{1}The authors thank Pacific Union College Student Association for providing funds.

M1.00274 Aggregation propensity of critical regions of the protein Tau, MICAIAH MUTHEE, AZKA AHMED, LUCA LARINI, Rutgers University-Camden — The Alzheimer’s disease is an irreversible, progressive brain disorder that slowly destroys memory and thinking skills, which eventually leads to the ability to not to carry out the simplest tasks. The Alzheimer’s disease is characterized by the formation of protein aggregates both within and outside of the brain’s cells, the neurons. Within the neurons, the aggregation of the protein tau leads to the destruction of the microtubules in the axon of the neuron. Tau belongs to a group of proteins referred to as Microtubule-Associated Proteins. It is extremely flexible and is classified as an intrinsically unstructured protein due to its low propensity to form secondary structure. Tau promotes tubulin assembly into microtubules thereby stabilizing the cytoskeleton of the axon of the neurons. The microtubule binding region of tau consists of 4 pseudo-repeats. In this study, we will focus on the aggregation propensity of two fragments. In this study we will focus on the PHF43 fragment that contains the third pseudo-repeat and has been shown experimentally to aggregate readily. Another fragment that contains the second pseudo-repeat will be considered as well. Mutations in this region are associated with various form of dementia and for this reason we will consider the mutant P301L.

M1.00275 A Novel Approach for Computing Cross-Sections in Ion-Mobility Measurements, LUCA LARINI, OSCAR MARIN, Rutgers University - Camden — Mass spectrometry allows the identification of molecules based on their mass to charge ratio. One of the advantages of this technique is that it is able to distinguish molecules that differ for a small value of the mass. In addition, once the molecule of interest has been selected by the mass spectrometer, it can be further analyzed in an ion mobility tube that can characterize the conformations adopted by the molecule. This is extremely useful when dealing with unstructured proteins that populate multiple conformations. However, ion mobility distinguishes structures based on their cross-section. In order to associate a well-defined tridimensional structure to a specific cross-section, molecular dynamics simulations must be performed first, and then the theoretical cross-section compared to the experimental one. Computing a cross-section starting from molecular dynamics data is extremely computationally expensive. For this reason, we have developed a software that takes advantage on the multicore and multimode architecture of modern computer clusters.

M1.00276 Single molecule fluorescence studies of transition paths in DNA hairpin folding, KATHERINE TRUEX, HOI SUNG CHUNG, JOHN LOUIS, WILLIAM EATON, National Institutes of Health — DNA hairpins are the simplest structures for investigating fundamental aspects of nucleic acid folding mechanisms. For two-state hairpins, all of the mechanistic information on how the hairpin folds is contained in the transition path (TP), the rare event in single molecule trajectories when the free energy barrier between folded and unfolded states is actually crossed. The only previous experimental study of TPs in nucleic acids used optical tweezer measurements and Szabo’s analytical theory for diffusive barrier crossing to reconstruct the free energy surface for an indirect determination of average TP times (Neupane et al. PRL 2012). We used confocal single molecule FRET and maximum likelihood analysis of photon trajectories to determine an upper bound of 2.5 µs for the average TP time of a DNA hairpin (Truex et al., PRL 2015), compared to the value of 4 µs predicted by Neupane et al., providing an important test of energy landscape theory. Current experiments are aimed at eventually characterizing structural changes during TPs, which will provide a very demanding test of mechanisms predicted by both theoretical models and simulations.

M1.00277 Electrical Heart Defibrillation with Ion Channel Blockers, ERIN FEENEY, COURTNEY CLARK, STEFFAN PUVAL, Oakland University — Heart disease is the leading cause of mortality in the United States. Rotary electrical waves within heart muscle underlie electrical disorders of the heart termed fibrillation; their propagation and breakup leads to a complex distribution of electrical activation of the tissue (and of the ensuing mechanical contraction that comes from electrical activation). Successful heart defibrillation has, thus far, been limited to delivering large electrical shocks to activate the entire heart and reset its electrical activity. In theory, defibrillation of a system this nonlinear should be possible with small electrical perturbations (stimulations). A successful algorithm for such a low-energy defibrillator continues to elude researchers. We propose to examine in silica whether low-energy electrical stimulations can be combined with antiarrhythmic, ion channel-blocking drugs to achieve a higher rate of defibrillation and whether the antiarrhythmic drugs should be delivered before or after electrical stimulation has commenced. Progress toward a more successful, low-energy defibrillator will greatly minimize the adverse effects noted in defibrillation and will assist in the development of pediatric defibrillators.

M1.00278 Dynamics of driven transitions between minima of a complex energy landscapes, SAI TEJA PUSULURI, Department of physics, Ohio University, ALEX H LANG, Computational Neurobiology Laboratory, Salk Institute, PANKAJ MEHTA, Department of physics, Boston University, HORACIO E CASTILLO, Department of physics, Ohio University — We recently modeled cellular interconversion dynamics\cite{1} by using an epigenetic landscape model\cite{2} inspired by neural network models. Given an arbitrary set of patterns, the model can be used to construct an energy landscape in which those patterns are the global minima. Here we study the transitions between stable states of the landscapes thus constructed, under the effect of an external driving force. We consider three different cases: i) choosing the patterns to be random and independently distributed ii) choosing a set of patterns directly derived from the experimental cellular transcription factor expression data for a representative set of cell types in an organism and iii) choosing randomly generated trees of hierarchically correlated patterns, inspired by biology. For each of the three cases, we study the stability of the global minima against thermal fluctuations and external driving forces, and the dynamics of the driven transitions away from global minima. We compare the results obtained in the three cases defined above, and in particular we explore to what degree the correlations between patterns affect the transition dynamics.


M1.00279 Anomalous motor mediated cargo transport in microtubule networks, STEVEN VANDAL, Worcester Polytechnic Institute, Dept of Physics, DANIEL MACVEIGH-FIERRO, ZHIYUAN SHEN, Worcester Polytechnic Institute, Dept of Biology and Biotechnology, KYLE LEMOI, Worcester Polytechnic Institute, Dept of Physics, LUIS VIDALI, Worcester Polytechnic Institute, Dept of Biology and Biotechnology, JENNIFER ROSS, University of Massachusetts Amherst, Dept of Physics, EKRAN TUZEL, Worcester Polytechnic Institute, Dept of Physics — Cargo transport is an important biological mechanism by which cells locomote, self-organize, and actively transport organelles. This transport is mediated by the cytoskeletal network and molecular motors that move them. It is not a trivial task to develop a mechanistic understanding of cargo transport, we use a coarse-grained Brownian dynamics model that incorporates the dynamics of these networks, as well as experimentally determined motor properties. We will test these models with two experimental systems: (1) in vitro microtubule networks with kinesin-1 motors, and quantum dot cargos on recreated microtubule networks, and (2) an excellent model organism, the moss Physcomitrella patens, in which chloroplasts are transported via the microtubule network by means of kinesin-like proteins. Phenomenological network characterizations are made, both in vivo and in vitro, and cargo motility is characterized using Mean Squared Displacement (MSD) measurements. Our simulations shed light on the role of network density and motor properties on the observed transport behavior, and improve our understanding of cargo transport in cells.

M1.00280 Water- Based TiO$_2$ Suspensions: A Raman Study, ROBERTO RANGEL, DORINA CHIPARA, BRIAN YUST, DESIREE PADILLA, MIRCEA CHIPARA, The University of Texas Rio Grande Valley — The antibacterial features of TiO$_2$ are under scrutiny due to the UV radiation, which contributes to the generation of reactive oxygen species, mainly in water environments. A study of TiO$_2$ suspensions in water and broth is reported. TiO$_2$ has a low solubility in water. TiO$_2$ (anatase), with average diameter of 15 nm from Nanostructured & Amorphous Materials, Inc. has been added to the fluid (water, broth) and the mixture was stirred for 1-10 h, followed by a 10-60 minutes sonication. The suspension was left to sediment for 1 day before measurements. Quasistable suspensions of TiO$_2$ in water and broth were investigated by Raman spectroscopy using a Renishaw InVia spectrometer operating at 532 and 785 nm. The spectra of the nanofiller have been simulated by a collection of Breit-Wigner line shapes and the effect of the preparation conditions (stirring and sonication time) on the parameters of Raman lines are reported. The differences are explained by observing that the sonication destroys the agglomerates of anatase resulting in a better dispersion of nanoparticles and consequently a longer sedimentation time. Sample preparation/storage have been done both under dark and UV light conditions.

M1.00281 The broadcasting mechanism of master regulator NFkB switches, DAVID POTOYAN, Rice University — The transcription factor NFk$\beta$ is involved in many cellular responses. Therefore there is a large number of sites in the genome to which NFk$\beta$ binds thereby activating myriad of genes as a response to various environmental stimuli. Kinetics becomes an important feature to reckon with in eukaryotic regulatory networks with many targets like the NFk$\beta$ system. In particular models based on the classical picture of genetic switches predict slow down regulation of NFk$\beta$ which can lead to wasteful over-expression of genes. A way to resolve this difficulty is to evolve faster ways of deactivating NFk$\beta$. There is evidence from experiments and our simulations that this is done by an Ik$\beta$-induced process of stripping NFk$\beta$ off directly from its genetic sites instead of waiting for autonomous dissociation. The broadcasting mechanism proposed in this work solves the time scale problem inherent in the classical picture. Using combination of stochastic and deterministic models we show how such a mechanism results in efficient regulation of NFk$\beta$ network.

M1.00282 Processing of oscillatory signals by incoherent feedforward loops, CAROLYN ZHANG, FEILUN WU, RYAN TSOL, IGOR SHATS, LINGCHONG YOU, Duke University — From the timing of angiotensin II to the maintenance of stem cell pluripotency, many biological signaling pathways exhibit the ability to differentiate between pulsatile and sustained signals in the regulation of downstream gene expression. While networks underlying this signal diversity are diverse, many are built around a common motif, the incoherent feedforward loop (IFFL), where an input simultaneously activates an output and an inhibitor of the output. With appropriate parameters, this motif can generate temporal adaptation, where the system is desensitized to a sustained input. This property serves as the foundation for distinguishing signals with varying temporal profiles. Here, we use quantitative modeling to examine another property of IFFLs: the ability to translate pulsatile signals into sustained signals is limited by two constraints. The kinetics of IFFL components dictate the input range for which the networks can encode pulsatile dynamics. In addition, a match between the network parameters and signal characteristics is required for optimal “counting.” We elucidate one potential mechanism by which information processing occurs in natural networks with implications in the design of synthetic gene circuits for this purpose.

This work was partially supported by the National Science Foundation Graduate Research Fellowship (CZ).

M1.00283 Shock wave irradiations avoiding fluid flow evoke intracellular Ca$^{2+}$ signaling, TORU TAKAHASHI, AKIRA TSUKAMOTO, SHIGERU TADA, National Defense Academy of Japan — Shock wave irradiation accelerates therapeutic effects including angiogenesis. The underlying mechanisms are not well understood. Fluid flow is one of major physical phenomena induced by shock wave irradiation. Cellular responses evoked by fluid flow are similar to those evoked by shock wave irradiation. Thus, fluid flow could be responsible for cellular responses evoked by shock wave irradiation. However, it is obscure whether fluid flow is required for the cellular responses evoked by shock wave irradiation. In this study, intracellular Ca$^{2+}$ signaling was observed in cells seeded in down-sized chambers. In the down-sized chambers, fluid flow was supposed to be suppressed because size of chambers (6 mm in diameter, 1 mm in thickness) was analogous to size of shock wave focus region (3mm in diameter). Dynamics of polystyrene microbeads suspended in the chambers was visualized with a CCD camera and analyzed with a particle image velocimetry (PIV) method to quantify fluid flow in the chamber. As a result, shock wave irradiation evoked intracellular Ca$^{2+}$ signaling. However, fluid flow was not observed in the chamber due to shock wave irradiation. Thus, it was suggested that physical mechanics, not fluid flow, are further required for evoking intracellular Ca$^{2+}$ signaling following to shock wave irradiation.

M1.00284 Dynamics of phenotypic reversibility of bacterial cells with oscillating hydrostatic pressure, SUDIP NEPAL, Univ of Arkansas-Fayetteville, PRADEEP KUMAR, Department of Physics, Univ of Arkansas-Fayetteville — Bacterial cells encounter and respond to physiochemical fluctuations. The response depends on the extent and type of the stresses applied. The response of bacterial cells to fluctuating stress is relatively unknown. Here, we have studied the response of wild type Escherichia coli (E. coli) under fluctuating hydrostatic pressures ranging from 500 to 5000 atm. High pressure acts as a stress to E. coli so that the bacteria are adapted to grow optimally at atmospheric pressure. Cell division of E. coli is inhibited at high pressures resulting in increase in the length of the cells. Cell-length is reversible in nature and bacterial cells revert back to normal size on a time scale that is proportional to the strength and time of continuous pressure applied upon relaxing the high pressure condition. We have studied the dynamics of cellular reversibility of E. coli under the conditions in which continuous pressure is applied and subsequently relaxed over different time scales. We have quantified the dynamics of cellular reversibility with different relaxation times. Furthermore, we propose a model to describe the reversibility of the bacterial cell with the relaxation time. Our theoretical model fits well to the experimental data. We further

M1.00285 Chiral pattern formation in compact microbial colonies, KIRILL KOROLEV, ASHISH BINO GEORGE, Boston University — Chirality is ubiquitous in biology from single molecules to entire populations. Yet, we are still lacking a detailed understanding of how chiral patterns emerge from cell competition and growth, even in simple microbial colonies. Although many microbes grow as dense colonies with no apparent chirality, recent experiments with Escherichia coli have demonstrated that internal dynamics in such populations can be in fact chiral. We show that there is a unique way to extend the commonly-used reaction-diffusion models of colony growth to account for the emergent chirality. This new model connects microscopic and macroscopic chirality and explains the origin of logarithmic spirals separating different sub-populations in a colony. We also show that chirality is substantially enhanced by the cooperation among the cells at the expansion frontier. In heterogeneous populations composed of strains with different chiralities and growth rates, our model predicts a very rich set of possible dynamics. For example, different chiralities can result in either sharp boundaries between the strains or promote their intermixing depending on the preferred twisting directions of the strains.
M1.00286 Adhesion of Mycobacterium smegmatis to Charged Surfaces and Diagnostics Implications.1 DIANE GORSE, ALI DHINOJWALA, Univ of Akron, FRANCISCO MOORE, Univ of Akron, NSF — Pulmonary tuberculosis (PTB) causes more than 1 million deaths annually. Smear microscopy is a primary rapid detection tool in areas where 95% of PTB cases occur. This technique, in which the sputum of a symptomatic patient is stained and examined using a light microscope for Mycobacterium tuberculosis (MTB) shows sensitivity between 20 and 60%. Insufficient bacterial isolation during sample preparation may be a reason for low sensitivity. We are optimizing a system to capture bacteria on the basis of electrostatic interactions to more thoroughly isolate bacteria from suspension and facilitate more accurate detection. Silica supports coated with positively-charged polyelectrolyte, poly(diallyldimethylammonium chloride), captured approximately 4.1 times more Mycobacterium smegmatis, a model organism for MTB, than was captured on negatively-charged silica substrates. Future experimentation will employ branched polymer systems and seek to justify the use of colloidal stability theories to describe initial capture.

1Supported by University of Akron, Department of Polymer Science, Department of Biology; LORD Corporation

M1.00287 Cell motility and antibiotic tolerance of bacterial swarms, WENLONG ZUO1, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — Many bacteria species can move across moist surfaces in a coordinated pattern known as swarming. It is reported that swarm cells show higher tolerance to a wide variety of antibiotics than planktonic cells. We used the model bacterium E. coli to study how motility affects the antibiotic tolerance of swarm cells. Our results provide new insights for the control of pathogenic invasion via regulating cell motility.

M1.00288 The Effect of Graphene Oxide/Reduced Graphene Oxide Functionalized with Metal Nanoparticles on Dermal, Bacterial, and Cancerous/Non-Cancerous Epithelial Cells1, ARTHUR CHEN, MIRIAM RAFAILOVIC, MARCIA SIMON, State Univ of NY- Stony Brook, REBECCA ISSEROFF, Lawrence Public High School, STEPHEN WALKER, State Univ of NY- Stony Brook, JAE HEE CHO, Boston University, JOHN JEROME, Suffolk University — Graphene and metal nanoparticles are permeating health products but their effects individually and combined on human skin are uncertain. This project studied the effect of graphene oxide (GO) and reduced graphene oxide (rGO) functionalized with Ag or Pt nanoparticles (Ag/PtNPs) on bacterial, dermal (DFBC's), and cancerous (SCC13's) and non-cancerous (DO33's) epidermal cells. GO was functionalized with AgNPs or PtNPs, forming metallized-GO; then reduced with NaBH4. FTIR and SEM confirmed the synthesis and composition. Confocal and SEM showed that Ag-rGO, depending on nanoparticle size, killed either S. Aureus or K. Pneumoniae, while Pt-rGO and rGO had no effect. Rhodamine staining revealed that Ag-rGO was very toxic to SCC13's, but only slightly toxic to DO33's. Pt-rGO and rGO had little effect on SCC13's and DO33's. At high concentrations all GO solutions inhibited cell growth but were not cytotoxic. Optical microscopy displayed that every GO/rGO solution adhered to DFBC's and influenced their direction of growth, making GO/rGO potentially applicable for wound healing.

1Supported by NIH 1R01GM106189, the James S McDonell Foundation, and the Paul Allen foundation

M1.00289 The functional consequences of non-genetic diversity in cellular navigation1 THIERRY EMONET, ADAM J WAITE, NICHOLAS W FRANKEL, YANN DUFOUR, JESSICA F JOHNSTON, Yale University — Substantial non-genetic diversity in complex behaviors, such as chemotaxis in E. coli, has been observed for decades, but the relevance of this diversity for the population is not well understood. Here, we use microfluidics to show that non-genetic diversity leads to significant structuring of the population in space and time, which confirms predictions made by our detailed mathematical model of chemotaxis. We then use genetic tools to show that altering the expression level of a single chemotaxis protein is sufficient to alter the distribution of swimming behaviors, which directly determines the performance of a population in a gradient of attractant, a result also predicted by our model.

1Supported by NIH 1R01GM106189, the James S McDonell Foundation, and the Paul Allen foundation

M1.00290 Allosteric Small-Molecule Inhibitors of the AKT Kinase D. S. DALAFAVE, The College of New Jersey — This research addresses computational design of small druglike molecules for possible anticancer applications. AKT and SGK are kinases that control important cellular functions. They are highly homologous, having similar activators and targets. Cancers with increased SGK activity may develop resistance to AKT-specific inhibitors. Our goal was to design new molecules that would bind both AKT and SGK, thus preventing the development of drug resistance. Most kinase inhibitors target the kinase ATP-binding site. However, the high similarity in this site among kinases makes it difficult to target specifically. Furthermore, mutations in this site can cause resistance to ATP-competitive kinase inhibitors. We used existing AKT inhibitors as initial templates to design molecules that could potentially bind the allosteric sites of both AKT and SGK. Molecules with no implicit toxicities and optimal drug-like properties were used for docking studies. Binding energies of the stable complexes that the designed molecules formed with AKT and SGK were calculated. Possible applications of the designed putative inhibitors against cancers with overexpressed AKT/SGK is discussed.

M1.00291 Effects of Chemotherapy-Induced Alterations in Cell Mechanical Properties on Cancer Metastasis, KRUTI BHAT, ANDREW KEPENYI, MICHAEL NICHOLS, CAROLYN TAYLOR, JIANHAI NING, Creighton University — Biological cells can modulate their mechanical properties to suit their functions and in response to changes in their environment. Thus, mechanical phenotyping of cells has been employed for tracking stem cell differentiation, bacterial infection, cell death, etc. Malignant transformation of cells also involves changes in mechanical properties. However, the extent to which mechanical properties of cancer cells contribute to metastasis is not well understood. Yet, more than 90% of all cancer deaths are directly related to metastasis. Transit of cells through the microcirculation is one of the key features of metastasis. We hypothesize that cancer treatment regimens do inadvertently alter cell mechanical properties in ways that might promote cancer metastasis. We use a microfluidic microcirculation mimetic (MMM) platform which mimics the capillary constrictions of the pulmonary and peripheral microcirculation to determine if in-vivo-like mechanical stimuli can evoke different responses from cells subjected to various cancer drugs. In particular, we show that cancer cells treated with chemotherapy drugs such as daunorubicin, become more deformable at short timescales (0.1 s) and transit faster through the device. Our results are first steps in evaluating the pro- or anti-metastatic effects of chemotherapeutic drugs based on their induced alterations in cell mechanical properties.

M1.00292 Collective motion in Proteus mirabilis swarms, XU HAORAN1, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — Proteus mirabilis is a Gram-negative, rod-shaped bacterium. It is widely distributed in soil and water, and it is well known for exhibiting swimming motility on nutrient agar surfaces. In our study, we focused on the collective motility of P. mirabilis and uncovered a range of interesting phenomena. Here we will present our efforts to understand these phenomena through experiments and simulation.

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Swimming and transport of bacteria in time-periodic flows\textsuperscript{1}. REBECCA WINTER, ALISON PATTeson, DAVID GAGNON, PAULö ARRATIA, Univ of Pennsylvania — The transport of bacteria can be highly influenced by external flows in oceans, rivers, and intestinal tracts. This has implications in biological systems for the performance of major biological processes, such as biofilm formation. In this study, we experimentally investigate the aggregation and transport of swimming Vibrio cholerae bacteria in time-periodic flows. Bacteria are placed in a well-characterized flow, and bacterial concentrations are recorded for a range of Reynolds numbers (Re) that spans two orders of magnitude, from 0.1 to 10. It is generally found that bacteria depart from regions of high deformation rate and accumulate near vortices. This phenomenon seems to be dictated by a combination of bacterial activity and background flow vorticity.

Emergence of collective motion in bacterial suspensions\textsuperscript{1}. SONG LIU, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — It is well known that bacterial suspensions will exhibit collective motion at high concentrations, in which both steric and hydrodynamic interactions play important roles. We aim to investigate whether steric and hydrodynamic interactions are of equal importance to the emergence of collective motion. Here we will present our efforts to experimentally tune the relative strength of these interactions in bacterial suspensions. Our preliminary results suggest that the transition to collective motion may depend on the interplay between steric and hydrodynamic interactions.

Effect of microemulsions on cell viability of human dermal fibroblasts\textsuperscript{1}. JUYI LI, TATSIANA MIRONAVA, MARCIA SIMON, MIRIAM RAFAILOVICH, NISSIM GARTI, State Univ of NY- Stony Brook — Microemulsions are optically clear, thermostable and isotropic mixture consisting of water, oil and surfactants. Their advantages of ease preparation, spontaneous formation, long-term stability and enhanced solubility of bioactive materials make them great potentials as vehicles in food and pharmaceutical applications. In this study, comparative in vitro cytotoxicity tests were performed to select a best formulation of microemulsion with the least toxicity for human dermal fibroblasts. Three different kinds of oils and six different kinds of surfactants were used to form microemulsions by different ratios. The effect of oil type and surfactant type as well as their proportions on cell proliferation and viability were tested.

Experimental evolution of E. coli\textsuperscript{1}. MENGSHI ZHANG, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — The evolution from unicellular to multicellular behavior is an essential step in the history of life. Our aim is to investigate the emergence of collective behavior in the model organism Escherichia coli (E. coli) and its selection advantages, such as better utilization of public goods. Our preliminary results suggest that the evolution of collective behavior may be a natural response to stressed conditions.

Centrosome Positioning in 1D Cell Migration\textsuperscript{1}. KATRINA ADLERZ, HELIM ARANDA-ESPINOA, Univ of Maryland-College Park — During cell migration, the positioning of the centrosome and nucleus define a cell’s polarity. For a cell migrating on a two-dimensional substrate the centrosome is positioned in front of the nucleus. Under one-dimensional confinement, however, the centrosome is positioned behind the nucleus in 60% of cells. It is known that the centrosome is positioned by CDC42 and dynein for cells moving on a 2D substrate in a wound-healing assay. It is currently unknown, however, if this is also true for cells moving under 1D confinement, where the centrosome position is often reversed. Therefore, centrosome positioning was studied in cells migrating under 1D confinement, which mimics cells migrating through 3D matrices. 3 to 5 μm fibroactin lines were stamped onto a glass substrate and cells with fluorescently labeled nuclei and centrosomes migrated on the lines. Our results show that when a cell changes directions the centrosome position is maintained. That is, when the centrosome is between the nucleus and the cell’s trailing edge and the cell changes direction, the centrosome will be translocated across the nucleus to the back of the cell again. A dynein inhibitor did have an influence on centrosome positioning in 1D migration and change of directions.

Active microrheology reveals molecular-level variations in the viscoelastic properties of Chaetopterus mucus\textsuperscript{1}. WILLIAM WEIGAND, Univ of San Diego, ASHLEY MESSMORE, University of California, San Diego, RAE ANDERSON, Univ of San Diego — The sea anemid, Chaetopterus Varipodatus, secretes a bioluminescent mucus that also exhibits complex viscoelastic properties. The constituents of the mucus are relatively unknown but it does play an important role in the development of the worms’ parchment-like housing tubes. In order to determine how and why this mucus can exhibit material properties ranging from fluidity to rigidity we perform microrheology experiments. We determine the microscale viscoelastic properties by using optical tweezers to produce small oscillations in the mucus which allow us to determine both the linear storage and loss moduli (G′, G″) along with the viscosity of the fluid. By varying the size of the microspheres (2-10 μm) and oscillation amplitude (5-10 μm) we are able to determine the dominant intrinsic length scales of the molecular mesh comprising the mucus. By varying the oscillation frequency (1-15Hz) we determine the crossover frequency at which G′ surpasses G″, to quantify the longest relaxation time of the mesh network. Initial results show a strong dependence on bead size which indicate that the dominant entanglement lengthscale of the mucus mesh is ~5 μm. Microspheres of this size exhibit a wide variety of stress responses in different regions of the mucus demonstrating the substantial microscale heterogeneity of the mucus. We carry out measurements on a population of worms of varying size and age to determine mucus variability between worms.

Regulation of muscle contraction by Drebrin-like protein 1 probed by atomic force microscopy\textsuperscript{1}. RENATA GARCES, EUGENIA BUTKEVICH, MITJA PLATEN, CHRISTOPH F. SCHMIDT, Third Institute of Physics - Biophysics, Georg August University, Göttingen, BIOPHYSICS TEAM — Sarcomeres are the fundamental contractile units of striated muscle cells. They are composed of a variety of structural and regulatory proteins functioning in a precisely orchestrated fashion to enable coordinated force generation in striated muscles. Recently, we have identified a C. elegans drebrin-like protein 1 (DBN-1) as a novel sarcomere component, which stabilizes actin filaments during muscle contraction. To further characterize the function of DBN-1 in muscle cells, we generated a new dbn-1 loss-of-function allele. Absence of DBN-1 resulted in a unique worm movement phenotype, characterized by hyper-bending. It is not clear yet if DBN-1 acts to enhance or reduce the capacity for contraction. We present here an experimental mechanical study on C. elegans muscle mechanics. We measured the stiffness of the worm by indenting living C. elegans with a micron-sized sphere adhered to the cantilever of an atomic force microscope (AFM). Modeling the worm as a pressurized elastic shell allows us to monitor the axial tension in the muscle through the measured stiffness. We compared responses of wild-type and mutant C. elegans in which DBN-1 is not expressed.
Different approaches to accelerating molecular evolution into targeted directions will be discussed, including recent progress on evolution in non-homogeneous environments. This brush plays an active role in defining the biochemical environment of the endothelial cell in the blood vessel wall. In addition, it is involved in the detection of mechanical stimuli, such as the shear stress from blood flowing in the vessel. In this work, we construct a biomimetic version of the glycocalyx on top of a soft deformable substrate in order to measure its ability to modulate the effects of shear stress at the endothelial cell surface. The soft substrate is stamped on to a glass substrate and then enclosed inside a microfluidic device that generates a controlled flow over the substrate. The hydrogel chemistry has been optimized so that it reliably stamps into a defined shape and has consistent mechanical properties. Fluorescent microbeads embedded in the gel allow measurement of the surface deformation, and subsequently, calculation of the shear force at the surface of the soft substrate. We investigate the effect of the major structural elements of the glycocalyx, hyaluronic acid and charged proteoglycans, on the magnitude of the shear force transmitted to the surface of the hydrogel.

### Measuring shear force transmission across a biomimetic glycocalyx

**Authors:** Isabel Bray, Dylan Young, Jan Scrimgeour, Department of Physics, Clarkson University, Potsdam NY 13699

**Abstract:** Human blood vessels are lined with a low-density polymer brush known as the glycocalyx. This brush plays an active role in defining the biochemical and mechanical environment of the endothelial cell in the blood vessel wall. In addition, it is involved in the detection of mechanical stimuli, such as the shear stress from blood flowing in the vessel. In this work, we construct a biomimetic version of the glycocalyx on top of a soft deformable substrate in order to measure its ability to modulate the effects of shear stress at the endothelial cell surface. The soft substrate is stamped on to a glass substrate and then enclosed inside a microfluidic device that generates a controlled flow over the substrate. The hydrogel chemistry has been optimized so that it reliably stamps into a defined shape and has consistent mechanical properties. Fluorescent microbeads embedded in the gel allow measurement of the surface deformation, and subsequently, calculation of the shear force at the surface of the soft substrate. We investigate the effect of the major structural elements of the glycocalyx, hyaluronic acid and charged proteoglycans, on the magnitude of the shear force transmitted to the surface of the hydrogel.

#### Micro-mechanical model for the tension-stabilized enzymatic degradation of collagen tissues

**Authors:** Thao Nguyen, Mechanical Engineering, Johns Hopkins University, Jeffrey Ruberti, Department of Bioengineering, Northeastern University

**Abstract:** We present a study of how the collagen fiber structure influences the enzymatic degradation of collagen tissues. Experiments of collagen fibrils and tissues show that mechanical tension can slow and halt enzymatic degradation. Tissue-level experiments also show that degradation rate is minimum at a stretch level coincident with the onset of strain-stiffening in the stress response. To understand these phenomena, we developed a micro-mechanical model of a fibrous collagen tissue undergoing enzymatic degradation. Collagen fibers are described as sinusoidal elastica beams, and the tissue is described as a distribution of fibers. We assumed that the degradation reaction is inhibited by the axial strain energy of the crimped collagen fibers. The degradation rate law was calibrated to experiments on isolated single fibrils from bovine skin. The fiber crimp and properties were fit to uniaxial tension tests of tissue strips. The fibral-level kinetic and tissue-level structural parameters were used to predict tissue-level degradation-induced creep rate under a constant applied force. We showed that we could accurately predict the degradation-induced creep rate of the pericardium and cornea once we accounted for differences in the fiber crimp structure and properties.

#### Mechanical model of kinesins moving on microtubule

**Authors:** Kiwing To, Institute of Physics, Academia Sinica, Ya-Chang Chou, Yi-Feng Hsiao, Kuan-Hua Chen, Department of Physics, National Tsing Hua University

**Abstract:** Kinesins are biomolecules that serve as intercellular motors for carrying cellular cargos along microtubules. Although the mechanism of converting the chemical energy of ATP to mechanical work is not fully understood, the motion of a kinesin on a microtubule has been measured and two different mechanisms, namely the hand-over-hand and inchworm, has been proposed. The particular shape of kinesin and microtubules suggests a possible mechanism for force generation similar to Brownian ratchet. Using a bead chain connected to two heads that are attracted to a vibrated ratchet plate as a scaled up analog of the kinesin/microtubule system, we manage to simulate both handoverhand and inchworm motion [Chou, et. al., Physica A443, 66 (2015)]. In addition, we find that chain, which play the role of the stalk in a kinesin molecule, can also generate force by interacting with the ratchet plate [Chen, et. al. Phys. Rev. E87, 012711 (2013)].
M1.00307 Population heterogeneity promotes a preference for blind cooperation1. ALFONSO PEREZ-ESCUEDERO, JONATHAN FRIEDMAN, JEFF GORE, Massachusetts Institute of Technology — Game theory—and common sense—recommend to carefully weigh costs and benefits before deciding on a course of action. Yet we often disapprove of people who do so, even when their actual decision benefits us. For example, we prefer people who directly agree to do us a favor over those who agree only after securing enough information to ensure that the favor will not be too costly. Why should we care about how people make their decisions, rather than just focus on the decisions themselves? Hoffman et al. (2015) have shown that such aversion to information gathering may be beneficial when it is strong enough to increase the level of cooperation. Here we show that the same type of aversion arises in heterogeneous populations, but for a different reason: individuals who seek additional information may reveal themselves to be undesirable partners, since they are less likely to cooperate in the future when conditions change. Aversion to information gathering thus facilitates preferential interactions with blind cooperators, who are more favorable partners. Due to this new mechanism the prevalence of such aversion rapidly increases with population diversity, because partner discrimination is more useful in populations which harbor partners of a more varied quality.

1 We gratefully acknowledge funding from the Paul G. Allen Family Foundation, EMBO and Human Frontier Science Program

M1.00308 Complex sound stimuli representation by small neural groups in subcortical auditory structure1. DOMINIKA LYZWA, Institute of Neuroscience, Newcastle University & Institute for Nonlinear Dynamics, University of Goettingen — The neural representation of complex natural sound stimuli in higher auditory structures is not yet well understood. Based on neurophysiological recordings from the mammalian auditory midbrain, neural responses to complex (natural and also artificial) sounds are investigated and mapped with respect to temporal and spectral neural tuning in the subcortical structure. The mapping includes spiking activity of single neurons and small neural clusters and local field potential activity. A neural model is presented which captures the mapping and also the similarity of responses across the auditory structure, and is used to predict responses to novel sound.

1 Financial support by Bernstein Focus Neural Technology Goettingen, grant number 01GQ0811

M1.00309 A phylogenetic study of the section moduli of the humerus in bipedal theropod dinosaurs. SCOTT LEE, ZACHARY RICHARDS, University of Toledo — The section modulus of a bone is a measure of its ability to resist bending torques. Carnivorous dinosaurs including Tyranosaurus and Allosaurus had strong humeri, presumably to hold struggling prey during hunting. The herbivorous dinosaurs of Ornithomimosauria had weak arm bones. This is believed to reflect the fact that their arms were never subjected to large bending torques. The unusual dinosaurs of Therizinosauria had arms as strong as found in the carnivorous dinosaurs. This is consistent with the hypothesis that their manus suggests a digging lifestyle. Other groups including Oviraptorosaurs, Troodontidae, Dromaeosauridae and Compsognathidae are also examined.

M1.00310 Physics of the Brain: Interaction of the Optical-Fiber-Guided Multi-Ultraviolet-Photon Beams with the Epilepsy Topion, (the Seizure Onset Area)1. V. ALEXANDER STEFAN, Institute for Advanced Physics Studies, Stefan University, La Jolla, California 92037 — A novel method for the possible prevention of epileptic seizures is proposed, based on the multi-ultraviolet-photon beam interaction with the epilepsy topion, (nonlinear coupling of an ultra high frequency mode to the brain beta phonons). It is hypothesized that epilepsy is a chaotic-dynamics phenomenon: small electrical changes in the epilepsy-topion lead, (within the 10s of milliseconds), to the onset of chaos, (seizure—electrochemical discharge), and subsequent cascading into adjacent areas. The ultraviolet photons may control the imbalance of sodium and potassium ions and, consequently, may prove to be efficient in the prevention of epileptic seizures.

1 Supported by Nikola Tesla Labs, Stefan University.
3 H.P. Zaveri et al., Localization-related epilepsy exhibits significant connectivity away from the seizure-onset area, Neuroreport, 20(9), 891-5, Jun17, 2009.

M1.00311 Asynchronous electrical activity in epileptic seizures1. KATHERINE HOLMAN, Towson University, EUGENE LIM, Ohio Wesleyan University, STEPHEN GLISKE, WILLIAM STACEY, University of Michigan, CHRISTIAN FINK, Ohio Wesleyan University — High-frequency oscillations (HFOs) have been postulated to be potential biomarkers for focal epileptic seizures, with fast ripples (~250 Hz) as the most interesting candidate. The mechanisms underlying the generation of fast ripples, however, are not well understood. In this study, we draw upon results from previous computational studies on HFOs to develop a new mathematical model from first principles describing the generation of HFOs through asynchronous neuronal firing. Asynchrony in the model is obtained with the introduction of two parameters of heterogeneity: variability in the inter-spike interval (ISI) and jitter. The model predicts the generation of harmonic narrow-band oscillations if the heterogeneity-governing parameters do not differ from the predefined ISI by more than 20%. Comparisons against results from a separately constructed computational model verify the accuracy of the model in study. These results provide us with a rigorous framework in which we may investigate the mechanisms driving the generation of abnormal HFOs, and may serve as groundwork for future research in epileptogenesis.

1 NSF Grant 1003092, Ohio Wesleyan University SSRP

M1.00312 Columnar organization of orientation domains in V1. JOSCHA LIEDTKE, FRED WOLF, Max Planck Institute for Dynamics and Self-Organization — In the primary visual cortex (V1) of primates and carnivores, the functional architecture of basic stimulus selectivities appears similar across cortical layers (Hubel & Wiesel, 1962) justifying the use of two-dimensional cortical models and disregarding organization in the third dimension. Here we show theoretically that already small deviations from an exact columnar organization lead to non-trivial three-dimensional functional structures. We extend two-dimensional random field models (Schnabel et al., 2007) to a three-dimensional cortex by keeping a typical scale in each layer and introducing a correlation length in the third, columnar dimension. We examine in detail the three-dimensional functional architecture for different cortical geometries with different columnar correlation lengths. We find that (i) topological defect lines are generally curved and (ii) for large cortical curvatures closed loops and reconnecting topological defect lines appear. This theory extends the class of random field models by introducing a columnar dimension and provides a systematic statistical assessment of the three-dimensional functional architecture of V1 (see also [Tanaka et al., 2011]).
A Topological Perspective of Neural Network Structure

M1.00313

ANN SIZEMORE, CHAD GIUSTI, University of Pennsylvania, MATTHEW CIESŁAK, SCOTT GRAFTON, University of California Santa Barbara, DANIELLE BASSETT, University of Pennsylvania — The wiring patterns of white matter tracts between brain regions inform functional capabilities of the neural network. Indeed, densely connected and cyclically arranged cognitive systems may communicate and thus perform distinctly. However, previously employed graph theoretical statistics are local in nature and thus insensitive to such global structure. Here we present an investigation of the structural neural network in eight healthy individuals using persistent homology. An extension of homology to weighted networks, persistent homology records both circuits and cliques (all-to-all connected subgraphs) through a repetitive thresholding process, thus perceiving structural motifs. We report structural features found across patients and discuss brain regions responsible for these patterns, finally considering the implications of such motifs in relation to cognitive function.

Automated Region of Interest Detection of Fluorescent Neurons for Optogenetic Stimulation

M1.00314

JONATHAN MISHLER, DIETMAR PLENZ, Natl Inst of Mental Health - NIMH — With the emergence of optogenetics, light has been used to simultaneously stimulate and image neural clusters in vivo for the purpose of understanding neural dynamics. Spatial light modulators (SLMs) have become the choice method for the targeted stimulation of neural clusters, offering unprecedented spatio-temporal resolution. By first imaging, and subsequently selecting the desired neurons for stimulation, SLMs can reliably stimulate those regions of interest (ROIs). However, as the cluster size grows, manually selecting the neurons becomes cumbersome and inefficient. Automated ROI detectors for this purpose have been developed, but rely on neural fluorescent spiking for detection, requiring several thousand imaging frames. To overcome this limitation, we present an automated ROI detection algorithm utilizing neural geometry and stationary information from a few hundred imaging frames that can be adjusted for sensitivity.

An in vivo analysis of facial muscle change treated with botulinum toxin type A using digital image speckle correlation

M1.00315

YAN XU, SAMANTHA PALMACCIO PALMACCIO, DUC BUI, ALEXANDER DAGUM, MIRIAM RAFAILOVICH, State Univ of NY- Stony Brook — Been famous for clinical use from early 1980s, the neuromuscular blocking agent Botulinum toxin type A (BTX-A), has been used to reduce wrinkles for a long time. Only little research has been done to quantify the change of muscle contraction before and after injection and most research paper depend on subjective evaluation from both patients and surgeons. In our research, Digital Image Speckle Correlation (DISC) was employed to study the mechanical properties of skin, contraction mode of muscles (injected) and reaction of neighbor muscle group (un-injected). At the same time, displacement patterns (vector maps) generated by DISC can predict injection locus for surgeons who normally handle it depending only on visual observation.

Learning physical biology via modeling and simulation: A new course and textbook for science and engineering undergraduates

M1.00316

PHILIP NELSON, Univ Pennsylvania — To a large extent, undergraduate physical-science curricula remain firmly rooted in pencil-and-paper calculation, despite the fact that most research is done with computers. To a large extent, undergraduate life-science curricula remain firmly rooted in descriptive approaches, despite the fact that much current research involves quantitative modeling. Not only does our pedagogy not reflect current reality; it also creates a spurious barrier between the fields, reinforcing the narrow silos that prevent students from connecting them.

I’ll describe an intermediate-level course on “Physical Models of Living Systems.” The prerequisite is first-year university physics and calculus. The course is a response to rapidly growing interest among undergraduates in a broad range of science and engineering majors. Students acquire several research skills that are often not addressed in traditional undergraduate courses: Basic modeling skills; Probabilistic modeling skills; Data analysis methods; Computer programming using a general-purpose platform like MATLAB or Python; Pulling datasets from the Web for analysis; Data visualization; Dynamical systems, particularly feedback control.

Light, Imaging, Vision: An interdisciplinary undergraduate course

M1.00317

PHILIP NELSON2, Univ Pennsylvania — The vertebrate eye is fantastically sensitive instrument, capable of registering the absorption of a single photon, and yet generating very low noise. Using eyes as a common thread helps motivate undergraduates to learn a lot of physics, both fundamental and applied to scientific imaging and neuroscience. I’ll describe an undergraduate course, for students in several science and engineering majors, that takes students from the rudiments of probability theory to the quantum character of light, including modern experimental methods like fluorescence imaging and Fretter resonance energy transfer. After a digression into color vision, we then see how the Feynman principle explains the apparently wavelike phenomena associated to light, including applications like diffraction, subdiffusion imaging, total internal reflection and TIRF microscopy. Then we see how scientists documented the single-quantum sensitivity of the eye seven decades earlier than ‘ought’ to have been possible, and finally close with the remarkable signaling cascade that delivers such outstanding performance. Course materials are available upon request.

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A Comparative Study Environmental and Radiological Causes Of Cancer In River Nile State, Sudan

M1.00318

EYAD HAMID, International University of Africa, HATIM KHAIR, King Mohamed ibn saud University — The causes of cancer in River Nile state are differ between environmental and radiological, this paper tried to make comparison between the two causes, to determine the real cause behind the large rising of cancer cases in this state, considering the daily habits for the patients and the possible contamination in the natural resources around them. The noticeable thing that most of cancer cases are might be due to the high concentration of nitrate pollutant detected in natural resources such as drinking water; also by looking to the radioactive elements we see there’s high concentration of some radioactive elements specially the K-40 which found in Portulaca Oleracea.

Dissociative Electron Attachment

M1.00319

ERMALDA ARREOLA, None, ESMERALDA ARREOLA COLLABORATION, LEIGH HARGREAVES COLLABORATION — Since the pioneering work of Boudaiffa et al. [1], it has been understood that electrons, even with energies near or below the ionization threshold, are capable of initiating strand-breaks in human DNA. This discovery raised important questions for cancer treatments, since sub-ionizing electrons are known to be the most copiously produced secondary product of radiation therapy. But even to date these factors are largely excluded or below the ionization threshold, are capable of initiating strand-breaks in human DNA. This discovery raised important questions for cancer treatments, since sub-ionizing electrons are known to be the most copiously produced secondary product of radiation therapy. But even to date these factors are largely excluded.

DEA is a rather complicated process to model due to the coupling of electronic and nuclear degrees of freedom in the molecule. At the California State University Fullerton, we are currently commissioning a new spectrometer to study dissociation channels, reaction rates and orientation effects in DEA collisions between slow electrons and nucleotide molecules. At the meeting we will present design parameters and commissioning data for this new apparatus.
M1.00321 Photocurrent Enhancement in the ICG Dye Sensitized ZnO Nanowire Device. GEN LONG, MICHAEL BEATTIE, HUZHONG XU, MOSTATA SADOQI, Department of Physics, St John’s University — In this presentation, we report a systematic study of photocurrent in ICG dye sensitized ZnO nanowire/FTO devices. ZnO nanowire is grown by hydrothermal method, with length of 200 nm and diameter of 30 to 60 nm. ICG dye is incorporated by immersing ZnO grown FTO substrate. Different concentrations, solvents of ICG dye, sizes of ZnO nanowires and annealing temperatures and atmosphere after immersion were studied. The synthesized nanostructures and devices were characterized by XRD, UV-Vis absorption, SEM, AFM, solar simulator, etc. And an enhancement in the photocurrent due to ICG is observed. 1The authors thank Center for Functional Nanomaterials of DOE for providing facilities access.

M1.00322 DFT+U Modeling of Hole Polaronics in Organic Lead Halide Perovskites, ERIC WELCH, Texas State Univ-San Marcos, PAUL ERHART, Chalmers Institute of Technology, LUISA SCOLFARO, ALEX ZAKHIDOV, Texas State Univ-San Marcos — Due to the ever present drive towards improved efficiencies in solar cell technology, new and improved materials are emerging rapidly. Organic halide perovskites are a promising prospect, yet a fundamental understanding of the organic perovskite structure and electronic properties is missing. Particularly, explanations of certain physical phenomena, specifically a low recombination rate and high mobility of charge carriers still remain controversial. We theoretically investigate possible formation of hole polaron adopting methodology used for oxide perovskites. The perovskite studied here is the ABX_3 structure, with A being an organic cation, B lead and C a halogen; the combinations studied allow for A_1 A_2/3 B x_1 x_2/3, where the alloy convention is used to show mixtures of the organic cations and/or the halogens. Two organic cations, methylammonium and formamidinium, and three halogens, iodine, chlorine and bromine are studied. Electronic structures and polaron behavior (LDA) pseudopotentials are used and a -U Hubbard correction of 8 eV is added; this method was shown to work with oxide perovskites. It is shown that a localized state is realized with the Hubbard correction in systems with an electron removed, residing in the band gap of each different structure. Thus, hole polaronics are expected to be seen in these perovskites.

M1.00323 Photovoltaic conversion via hot electron induced thermionic emission from quantum dots, ANDREI SERGEEV, KIMBERLY SABLON, U.S. Army Research Laboratory, Adelphi, MD 20783, USA — Quantum dot (QD) nanomaterials provide numerous possibilities for nanoscale engineering of photoelectron processes for specific applications, such as lighting, sensing, and energy conversion. It has been found that QDs may increase the photovoltaic conversion efficiency due to enhanced coupling with electromagnetic radiation, multiple exciton generation, and two-step light absorption. The hot electron induced thermionic emission from QDs is a novel mechanism, which may be significantly enhanced due to optimization of QD parameters. In this two-step process the photoelectrons excited from the valence band to localized quantum dot states are extracted from QDs via thermionic emission, which may be initiated by thermal phonons, hot phonons, and hot electrons. Strong interaction between the localized quantum dot electrons and hot photoelectrons excited by high energy photons substantially increases the conversion efficiency due to use of energy of sub-bandgap photons and energy of hot photoelectrons, which otherwise would be lost in relaxation processes. Here we present the theoretical model of the conversion via thermionic emission from quantum dots, results of optimization of photoelectron processes, and experimental data, which evidence in favor of this mechanism.

M1.00324 Strain-induced tuning of surface energetics, electron conductivity and reduction drive in spinel LiMn_2O_4 cathodes, IVAN SCIVETTI, GILBERTO TEOBALDI, University of Liverpool — LiMn_2O_4 (LMO) implementation in cathodes of rechargeable Li-ion batteries (LIBs) is hampered by the limited lifetime of the material and the stability of its interfaces, starting from the Solid Electrolyte Interphase [1,2]. Recent experiments [2] and Density Functional Theory (DFT) simulations [3] indicate that the formation and effectiveness of the SEI on LMO are related to the surface orientation. In this context, we analyse the role of geometrical strain for the relative energy, magnetic ordering and the reduction drive of several LMO surfaces. DFT simulations reveal LMO surfaces to be markedly sensitive to geometrical strain. Strain lower than 10% can lead to insulator-metal and ferromagnetic-antiferromagnetic transitions, alter the relative energy of LMO surfaces, and induce changes as large as 1.0 eV in the surface chemical potential, thence the reduction drive. Prompted by advances in the synthesis of metal-oxide core-shell nanostructures [4], the use of strained LMO coating to enhance SEI formation is put forward as a potential nano-engineered strategy for longer lived SEI on LMO substrates.
1. JCP 2012, 116, 9852-9861.
4. ACS Nano 2012, 6, 5531.

M1.00325 Defect physics vis-à-vis electrochemical performance in layered mixed-metal oxide cathode materials, KHANG HOANG, North Dakota State University, MICHELLE JOHANNES, Naval Research Laboratory — Layered mixed-metal oxides with different compositions of (Ni,Co,Mn) [NMC] or (Ni,Co,Al) [NCA] have been used in commercial lithium-ion batteries. Yet their defect physics and chemistry is still not well understood, despite having important implications for the electrochemical performance. In this presentation, we report a hybrid density functional study of intrinsic point defects in the compositions LiNi_1/3Co_1/3Mn_1/3O_2 (NMC1/3) and LiNi_1/3Co_1/3Al_1/3O_2 (NCA1/3) which can also be regarded as model compounds for NMC and NCA. We will discuss defect landscapes in NCM1/3 and NCA1/3 under relevant synthesis conditions with a focus on the formation of metal antisite defects and its implications on the electrochemical properties and ultimately the design of NCM and NCA cathode materials.

M1.00326 Modified Graphene Oxide for Long Cycle Sodium-Ion Batteries, MUHAMED SHAREEF, Kansas State University, HARRISON GUNN, Syracuse University, VICTORIA VOIGT, GURPREET SINGH, Kansas State University — Hummer’s process was modified to produce gram levels of 2-dimensional nanosheets of graphene oxide (GO) with varying degree of exfoliation and chemical functionalization. This was achieved by varying the weight ratios and reaction times of oxidizing agents used in the process. Based on Raman and Fourier transform infra red spectroscopy we show that potassium permanganate (KMnO_4) is the key oxidizing agent while sodium nitrate (NaNO_3) and sulfuric acid (H_2SO_4) play minor role during the exfoliation of graphite. Tested as working electrode in sodium-ion half-cell, the GO nanosheets produced using this optimized approach showed high rate capability and exceptionally high energy density of ~500 mAh/g for up to at least 100 cycles, which is among the highest reported for sodium/graphite electrodes. The average Coulombic efficiency was approximately 99%.
1NSF Grant No. 1454151
M1.00327 Use of TiO₂ nano particles in Sulfur electrodes to enhance cyclability of Li-S batteries¹, RUCHIRA DHARMASENA, GAMINI SUMANASEKERA, Department of Physics- University of Louisville, JACEK JASINSKI, ARJUN THAPA, MAHENDRA SUNKARA, Conn center—University of Louisville — We investigate a novel and facile technique to fabricate Sulfur cathode for Li-S batteries with better cyclability and higher stable gravimetric capacity of around 750 mAh/g over 50 cycles. In this study we have experimentally the use of TiO₂ nano particles to prevent polysulfide dissolution into the electrolyte. Absorption and adsorption properties of TiO₂ nano particles are used to trap Lithium Polysulfides. Excellent electrical conductivity property of carbonized polyacrylonitrile (PAN) carbon fibers is effectively used in this technique to establish better electrical connection to Sulfur in the bulk electrode. The thermal annealing technique we use in this work introduces a facile way to load Sulfur into the electrode. Mechanical properties of the Sulfur electrode is improved using a relatively easy way to sustain expansion and contraction at stable coulombic capacity with almost 100 % efficiency. The mechanism of the said Sulfur electrode is discussed in detail using cyclic voltammetry and Impedance spectrum analysis.

¹Funded by KY EPScR, project number T1 2014-2019

M1.00328 Incorporation of Platinum and Gold Partially Reduced Graphene Oxide in Polymer Electrolyte Membrane Fuel Cells for Increased Carbon Monoxide Tolerance⁴, LEE BLACKBURN, REBECCA ISSEROFF, MIRIAM RAFAILOVICH, State Univ of NY- Stony Brook, JAYMO KANG, University of California, Berkeley, HONGFEI LI, MOLLY GENTLEMAN, State Univ of NY- Stony Brook, QAIQI QAIQ, Brookhaven National Laboratory — Polymer Electrolyte Membrane Fuel Cells (PEMFCs) can potentially provide “green” energy but the platinum catalyst’s susceptibility to carbon monoxide (CO) poisoning reduces output power. This project hypothesized that gold and platinum-partially reduced graphene oxide (Au/Pt-prGO) catalysts, incorporated into the electrodes and Nafion membrane of a PEMFC, will increase CO tolerance. Aliquots of graphene oxide (GO) were functionalized with platinum and/or gold nanoparticles. Partial reduction with NaBH₄ prevented precipitation. Raman Spectroscopy and HRTEM verified the chemical identity, structure, and presence of the materials. Setups were tested in a PEM fuel cell with a gas feed containing 1000 ppm of CO, and averaged an output power >200% over the control, with the most effective sample, Pt-prGO Electrode + Membrane, yielding an output power ~250% greater than the control. Additionally, each setup’s poisoned output power (Pₚ) was compared to its highest possible output power (Pₓ). Au/Pt-prGO Electrode + Membrane produced 100% of its highest possible output power when poisoned, displaying 100% resistance to all CO poisoning at the resistances tested.

⁴M1.00329 Harvesting Energy from the Flow-Induced Flutter of a ‘Piezoleaf’, ANDRE RUAS, SANTIAGO ORREGO, KYLE DORAN, AARON RIPS, KOUSHO SHOELLE, SUNG HOON KANG, RAJAT MITTAL, Johns Hopkins University — The objective of our research is to examine energy harvesting from the flow-induced flutter of a small piezoelectric membrane, which we call a Piezoleaf¹. Piezoleaves are small, low-cost, low-maintenance devices capable of powering small portable electronics or wireless sensors in remote areas. It is well known that piezoelectric membranes subjected to time-varying strains generate electrical energy that can be harvested. In the current project, we have designed and constructed a new low-speed wind-tunnel (1’x1’; cross-section) to analyze the flow-induced flutter and energy harvesting performance of a small (approximately 1”x2”) piezoleaf. One of the novel features of this research is that the membrane is fixed at its trailing-edge (i.e. an inverted flag) since this is expected to generate more energy than a regular flag configuration. Guided by numerical simulation, we are conducting tests of this configuration in our wind tunnel for various wind speeds (maximum speeds of about 10 m/s) to examine the effect of wind-speed on the flutter and energy harvesting. High-speed videography is also being used to examine the dynamics of the flag and results from this project will be presented.

M1.00330 High Temperature Concentrated Solar Power Using Liquid Metal, ASEGUEN HENRY, Georgia Institute of Technology — One of the most attractive ways to try and reduce the cost of concentrated solar power (CSP) is to increase the system efficiency and near the thermodynamic limitations and thus one of the only ways to improve heat engine efficiency is to increase the turbine inlet temperature. Significant efforts is being made to develop turbines that can operate at such high temperatures. However, such heat engines require turbine inlet temperatures ~1300-1500C, which is far beyond what is currently feasible with the state of the art molten salt infrastructure. In working towards the development of a system that can operate in the 1300-1500C temperature range, the most significant challenges lie in the materials and forming functional and reliable components out of new materials. One of the most attractive options from a cost and heat transfer perspective is to use liquid metals, such as tin and aluminum-silicon alloys along with a ceramic based infrastructure. This talk will overview ongoing efforts in the Atomistic Simulation and Energy (ASE) research group at Georgia Tech to develop prototype components such as an efficient high temperature cavity receiver, pumps and valves that can make a liquid metal based CSP infrastructure realizable.

M1.00331 Cadmium Telluride Solar Cells with PEDOT:PSS Back Contact¹, MICHAEL MOUNT, FERNANDA DUARTE, Seton Hall University, NABA PAULED, YANFA YAN, University of Toledo, WEINING WANG, Seton Hall University — Cadmium Telluride (CdTe) solar cell is one of the most promising thin film solar cells and its highest efficiency has reached 21%. To keep improving the efficiency of CdTe solar cells, a few issues need to be addressed, one of which is the back contact. The back contact of CdTe solar cells are mostly Cu-base, and the problem with Cu-based back contact is that Cu diffuses into the grain boundary and into the CdS/CdTe junction, causing degradation problem at high temperature and under illumination. To continue improving the efficiency of CdTe/CdS solar cells, a good ohmic back contact with high work function and long term stability is needed. In this work, we report our studies on the potential of conducting polymer being used as the back contact of CdTe/CdS solar cells. Conducting polymers are good candidates because they have high work functions and high conductivities, are easy to process, and cost less, meeting all the requirements of a good ohmic back contact for CdTe solar cells. In our studies, we used poly(3,4-ethylenedioxythiphene) polystyrene sulfonate (PEDOT:PSS) with different conductivities and compared them with traditional Cu-based back contact. It was observed that the CdTe solar cell performance improves as the conductivity of the PEDOT:PSS increase, and the efficiency (9.1%) is approaching those with traditional Cu/Au back contact (12.5%).

¹Cadmium Telluride Solar Cells with PEDOT:PSS Back Contact

M1.00332 Interface Conductance Modal Analysis, ASEGUEN HENRY, Georgia Institute of Technology — A formalism termed the interface conductance modal analysis (ICMA) method will be presented, which allows for calculations of the modal contributions to thermal interface conductance within the context of molecular dynamics (MD) simulations, which inherently include anharmonicity to full order. The eigen modes of vibration are calculated from harmonic lattice dynamics (LD) calculations, however the generality of ICMA formalism also allows for incorporation of anharmonic LD results into the calculations. The formalism itself is based on a modal decomposition of the heat flow across an interface, which is then substituted into expressions for the conductance either based on equilibrium or nonequilibrium MD. Several example cases will be covered and the interesting insights that emerge from the ICMA analyses will be discussed in detail. The ICMA method enables more in-depth study of various effects such as temperature, anharmonicity, interdiffusion, roughness, imperfections, dislocations, stress, changes in crystal structure through a single unified model, as it can essentially treat any material or object where the atoms vibrate around equilibrium sites (e.g., ordered or disordered solids and molecules).
M1.00334 Correlation between dimensional crossover and thermoelectric performance in conducting polymer . JUNHYEON JO, IN-SEON OH, MI-JIN JIN, JUNG-WOO YOO, Ulsan National Institute of Science and Technology (UNIST) — Conjugated polymers are emerging as attractive thermoelectric materials, resulting from low thermal conductivity, easy process and variable potentials for change. Recently, there are significant improvements of the Seebeck coefficient (S) and electric conductivity (σ) in the conjugated polymers by adding chemical additives to reform its ordinary disordered structure system. However, the relation between thermoelectricity and charge transport in the system is not well understood, which gives us a new challenge to improve thermoelectricity in the organic system. Here, we studied thermoelectric performance of dimethyl sulfoxide (DMSO) doped poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) with adding variable amounts of fluorosurfactant Zonyl. The change transition in the disordered system was analyzed within variable range hopping (VRH), which showed the change of hopping dimensionality with further molecular dopants. The morphological change and its effect on transport and thermoelectric performance were further investigated through AFM, XPS, etc. As a result, we found the optimal condition for increasing both the Seebeck coefficient and electric conductivity; resulting in significant improvement for the power factor ($S^2\sigma$).

M1.00335 Efficiency, Power and Period of a model quantum heat engine working in a finite time1, 2 MULUGETA BEKELE, Associate Professor of Physics, AAU, TOLASA A DIMA, Graduate student, MEKUANNET ALEYME, Lecturer: Debre Tabor University, WARGA CHEGENO, Lecturer: Wolkite University — We take a spin-half quantum particle undergoing Carnot type cyclic process in a finite time assisted by two heat reservoirs and an external magnetic field. We find that the power of the heat engine is maximum at a particular period of the cyclic process and efficiency at the maximum power is at least half of the Carnot efficiency. We further apply the Omega-criterion for a figure of merit representing a compromise between useful power and lost power determining the corresponding efficiency for the optimization criterion to be at least three fourth of the Carnot efficiency.

1The authors are thankful to the International Science programme, IPS, Uppsala, Sweden for their support to our research lab.

M1.00336 Transport and thermoelectric properties of hot-pressed SnSe$_2$. NGUYEN THI MINH HAI, DUONG ANH TUAN, DUONG VAN THIET, CHO SUNGLAE2, University of Ulsan, SONG JAE YONG, PARK HYUNMIN, Korea Research Institute of Standards and Science, JAE YONG SONG, HYUN-MIN PARK — Recently, SnSe has been reported as ultralow thermal conductivity material which make it become a very high thermoelectric figure of merit ZT material, up to 2.6 at 923 K. But, it is hard to use SnSe for applications in high temperature range because SnSe decomposes at 700 K. Therefore, searching for crystalline materials with high ZT value at lower temperature is still an attracted field of research. SnSe$_2$ is also 2D material which is expected to have low lattice thermal conductivity. However, less is known about thermoelectric property of SnSe$_2$. Eutectic SnSe$_2$-Bi$_2$Se$_3$ has been reported as a promising low-temperature thermoelectric material with $ZT=0.56$ at 593 K. Here, we prepared the polycrystalline SnSe$_2$ using hot pressure method. At temperature range up to 573 K, it exhibited an anisotropic n-type charge carrier. Ultra low thermal conductivity is achieved along parallel direction, however, ZT value is still very low whose maximum was 0.045 at 573 K due to low electrical conductivity, and increased with temperature. Our work showed the possibility to enhance ZT of SnSe$_2$ polycrystalline via n- and p-type doping experiments.

M1.00337 Enhancing photovoltaic efficiency through radiative cooling of solar cells below ambient temperature . TAQIYYAH SAFI, JEREMY MUNDAY, University of Maryland, College Park — Sunlight heats up solar cells and the resulting elevated solar cell temperature adversely affects the photovoltaic efficiency and the reliability of the cell. Currently, a variety of active and passive cooling strategies are used to lower the operating temperature of the solar cell. Passive radiative cooling requires no energy input, and is ideal for solar cells; however, previously demonstrated devices still operate above the ambient, leading to a lower efficiency as compared to the ideal Shockley-Queisser limit, which is defined for a cell in contact with an ideal heat sink at ambient temperature (300 K). In this talk, we will describe the use of radiative cooling techniques to lower the cell temperature below the ambient temperature. We show that by combining specifically designed radiative cooling structures with solar cells, efficiencies higher than the limiting efficiency achievable at 300 K can be obtained for solar cells in both terrestrial and extraterrestrial environments. We show that these structures yield an efficiency 0.87% higher than a typical PV module at operating temperatures in a terrestrial application. We also demonstrate an efficiency advantage of 0.4-2.6% for cells in an extraterrestrial environment in near-earth orbit.

M1.00338 Li-air, rechargeable, solid-state batteries using graphene and boron nitride aerogel matrices.1 ONURO ERGEN, THANG THOAN PHAM, SALLY DEMAIO-TURNER, ALEX ZETTL, University of California at Berkeley — The recent explosion of research on Li-Air batteries has provided new insights into developing more efficient air cathodes. Graphene and boron nitride aerogel matrix is anticipated to be an ideal candidate to produce a high throughput air-breathing system. We developed a Li-Air battery model that accounts for efficient O$_2$ passing through and keep out H$_2$O, CO$_2$, and N$_2$. Thus, the solid-state cells demonstrate a long cycle life, thermal stability, and high rechargeable characteristics. These cells also show an explicit discharge capacity with a constant discharge current density of 0.1mA/cm$^2$.

1Department of Physics, University of California at Berkeley, Ca 94720, USA 2Materials Sciences Division, Lawrence Berkeley National Laboratory, Ca, 94720, USA 3Kavli Energy Nanosciences Institute at the University of California, Berkeley, , Ca, 94720, US NASA HBCU Renewable Energy and Technology Utilization Project (NHRELU) and 2. Center for the Study of Terrestrial and Extraterrestrial Atmospheres (CSTEA)).
M1.00340 Experimental characterization of a small custom-built double-acting gamma-type stirling engine. PETER INTISIFUL, Prairie View A & M University, Prairie View, TX, FRANCIS MENSAH, Virginia Union University, Richmond, VA, ARTHUR THORPE, Howard University, Washington, DC — This paper investigates characterization of a small custom-built double-acting gamma-type stirling engine. Stirling-cyle engine is a reciprocating energy conversion machine with working spaces operating under conditions of oscillating pressure and flow. These conditions may be due to compressibility as well as pressure and temperature fluctuations. In standard literature, research indicates that there is lack of basic physics to account for the transport phenomena that manifest themselves in the working spaces of reciprocating engines. Previous techniques involve governing equations: mass, momentum and energy. Some authors use engineering thermodynamics. None of these approaches addresses this particular engine. A technique for observing and analyzing the behavior of this engine via parametric spectral profiles has been developed, using laser beams. These profiles enabled the generation of py-curves and other trajectories for investigating the thermos-physical and thermos-hydrodynamic phenomena that manifest in the exchangers. The engine’s performance was examined. The results indicate that with current load of 35.78A, electric power of 0.505 kW was generated at a speed of 240 rpm and 29.50 percent efficiency was obtained.

1 NASA grants to Howard University NASA/HBCU-NHRETU & CSTEA

M1.00341 Effects of pH on the characteristics of ZnS thin films grown by using the CBD method. HEEJIN AHN, DONGCHAN LEE, SUJUNG PARK, YOUNGHO UM, Univ of Ulsan — In CIGS-based thin film solar cells, a chemically deposited ZnS buffer layer with high resistivity is generally used between the absorber layer and transparent conducting oxide layer. In this work, we report a chemical process to prepare ZnS films by the CBD technique based on the typical bath deposition. The influences of ammonia (NH₄OH) and Na₂EDTA (Na₂C₁₀H₁₄N₂O₈) as complexing agents on structural, morphological, and optical properties of ZnS thin films are investigated ranging pH concentration from 5 to 10. To investigate effects of pH on the characteristics of ZnS thin films, by using UV-visible transmittance, atomic force microscopy, and optical absorption were investigated. With changing the pH range, the ZnS thin films demonstrate high transmission of 75-80% in the visible region, indicating the films are potentially useful in photovoltaic applications. The results will be presented in detail.

2 This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education(2011-0024709)

M1.00342 Silicon and phosphorus dual doped graphene as the promising metal-free catalysts for oxygen reduction reaction. ZHANSHENG LU, SHUO LI, ZONGXIAN YANG, Henan Normal University, RUQIAN WU, University of California Irvine — The pathways of oxygen reduction reaction (ORR) on the metal-free silicon and phosphorus dual doped graphene (Si-P-G) catalyst are systematically investigated based on the dispersion-corrected density functional theory (DFT-D) method. It is found that the Si-P-G can be stable at high temperature from the first-principles molecular dynamics simulation and the local region of dopants displays an important role in the adsorption and reduction of oxygen. Both of the four-electron O₂ direct dissociation and the two-electron OOH dissociation pathways are probable for ORR on the Si-P-G, while the latter pathway is mainly followed by the pathway of the OH hydrogenation into H₂O. For the OOH dissociation pathway, the hydrogenation of O₂ to OOH is the rate-limiting step with a rather small barrier energy of 0.66 eV. The current results indicate that the Si-P-G is a novel metal-free catalyst for ORR, and which is comparable to that of the Pt catalyst.

1 Work was supported by the National Science Foundation Center for Chemical Innovation on Chemistry at the Space-Time Limit (CaSTL) under Grant No. CHE-1414466, and the National Natural Science Foundation of China (Grant Nos. 15401078, and 11474086)

M1.00343 Lattice-Boltzmann-based Simulations of Diffusiophoresis. JOSHUA CASTIGLIEGO, JENNIFER KREFT PEARCE, Roger Williams University — We present results from a lattice-Boltzmann-base Brownian Dynamics simulation on diffusiophoresis and the separation of particles within the system. A gradient in viscosity that simulates a concentration gradient in a dissolved polymer allows us to separate various types of particles by their deformability. As seen in previous experiments, simulated particles that have a higher deformability react differently to the polymer matrix than those with a lower deformability. Therefore, the particles can be separated from each other. This simulation, in particular, was intended to model an oceanic system where the particles of interest were zooplankton, phytoplankton and microplastics. The separation of plankton from the microplastics was achieved.

M1.00344 Electro-responsive supramolecular graphene oxide hydrogels for active bacteria ad- sorption and removal. BIN XUE, YI CAO, WEI WANG, Nanjing Univ — Bacteria are major contaminations in drinking water and healthcare products. Bacteria contamination may cause severe health problems, including food poisoning and diseases. Currently water sterilization and purification methods to remove contaminated bacteria are mainly based on the size-exclusion mechanism. In order to completely remove all bacteria in water, the pore sizes of the membranes or cartridges should be comparable to the size of bacteria, which inevitably leads to high cross-membrane water pressure and slow purification speed. Moreover, the membranes can easily get clogged. Therefore it is highly demanded to develop efficient methods and novel materials for water purification. Recently, Cui and coworker have introduced a bacteria inactivation method with high efficiency and fast purification speed based on a kind of complex materials made of silver nanofibers, carbon nanotubes and cotton, operating in an electric field. Inspired by the electric field, the bacteria can be efficiently killed when passing through the membrane even the pore sizes are larger than bacteria. Inspired by our work, here we report a proof-of-principle demonstration of bacteria removal using electro-responsive hydrogels.

1 This work is funded by Six talent peaks project in Jiangsu Province, the National Natural Science Foundation of China (Nos. 11304156, 11334004, 31170813, 81421091 and 91127026), the 973 Program of China (No. 2012CB921801 and 2013CB834100), the Priority Ac

M1.00345 From Compartmentalized to Agent-based Models of Epidemics. CHARLES MACAL, Argonne National Laboratory — Supporting decisions in the throes of an impending epidemic poses distinct technical challenges arising from the uncertainties in modeling disease propagation processes and the need for producing timely answers to policy questions. Compartmental models, because of their relative simplicity, produce timely information, but often do not include the level of fidelity of the information needed to answer specific policy questions. Highly granular agent-based simulations produce an extensive amount of information on all aspects of a simulated epidemic, yet complex models often cannot produce this information in a timely manner. We propose a two-phased approach to addressing the tradeoff between model complexity and the speed at which models can be used to answer questions about an impending outbreak. In the first phase, in advance of an epidemic, ensembles of highly granular agent-based simulations are run over the entire parameter space, characterizing the space of possible model outcomes and uncertainties. Meta-models are derived that characterize model outcomes as dependent on uncertainties in disease parameters, data, and structural relationships. In the second phase, envisioned as during an epidemic, the meta-model is run in combination with compartmental models, which can be run very quickly. Model outcomes are compared as a basis for establishing uncertainties in model forecasts.

3 This work is supported by the U.S. Department of Energy under contract number DE-AC02-06CH11357 and National Science Foundation (NSF) RAPID Award DEB-1516428.
M1.00346 Analytical vacuum force, atmospheric pressure dispute. HAN YONGQUAN, 15611860790 — Typically, the gap gas molecules is 10^{-9} m, since the center speed of the tornado is over 100 m / sec. it divided by the speed of a tornado, the gap of the gas molecules becomes 10^{-11} m. Equivalent to the gap when there is no tornado that the gas molecules allow radiation to pass through, equivalent to the gap is reduced gas molecules 100 times by a tornado. There is no change in the Earth’s radiate, the Earth’s radiation is reduced to one percent of the original intensity by the radiation through the tornado periphery into the center of the tornado. According to the APS Division of Nuclear Physics in APS -2013 Fall Meeting - Event - Gravitational radiation theory http://meetings.aps.org/Meeting/DNP13/Session/FB.8, which I published, the gravity will be reduced to the original gravity percentage one. Waterspout by the Earth’s gravity to become the original one percent. Cause the external of the tornadoes atmospheric pressure is constant, the height waterspout should support column height atmospheric pressure is 100 times,that height waterspout may reach nearly kilometers.

M1.00347 Observation of anomalous dielectric properties in low-dimensional spin 1/2 α-Cu2V2O7 magnetic system. YU-JEN CHEN, KAKARLA-DEVI CHANDRASEQUHAR, KO-JUNG FAN, Department of Physics, National Sun Yat-Sen University, JIUNN-YUAN LEE, Institute of Physics, National Chiao Tung University, JENN-MIN LEE, JIN-MING CHEN, National Synchrotron Radiation Research Center, HUNG-DIEN LIN, Department of Physics, National Sun Yat-Sen University — Recently, low-dimensional magnetic systems have received much attention from both theoretical and experimental physics point of view due to their fascinating physical properties. In general, Cu2V2O7 can stabilize at least two sibling polymorphs named as α and β phases. In α phase, Cu2V2O7 crystallized in orthorhombic with Fdd2 space groups. The complex magnetic exchange interaction between the Cu-O-Cu ion within the intra and interchain creates the Dzyaloshinskii-Moriya interaction that leads to weak ferromagnetism below the magnetic transition temperature \( T_N = 34 \) K. In this study, we present the results of multiple dielectric anomalies observed in the low dimensional spin 1/2 α-Cu2V2O7 magnetic system. The observed dielectric signatures can be ascribed to the complex magnetic interaction α-Cu2V2O7 system. Further, the chemical doping effect on the magnetic and multiferroic properties of α-Cu2V2O7 is underway.

M1.00348 Quantum antiferromagnetic Heisenberg half-odd integer spin model as the entanglement Hamiltonian of the Affleck-Kennedy-Lieb-Tasaki valence bond solid states. GUANG-MING ZHANG, Tsinghua University, Beijing — Applying a symmetric bulk bipartition to the one-dimensional Affleck-Kennedy-Lieb-Tasaki valence bond solid (VBS) states for the integer spin-S Haldane gapped phase, we can create an array of fractionalized spin-S/2 edge states with the super unit cell \( l \) in the reduced bulk system, and the topological properties encoded in the VBS wave functions can be revealed. The entanglement Hamiltonian (EH) with \( l = even \) corresponds to the quantum antiferromagnetic Heisenberg spin-\( S/2 \) model. For the even integer spins, the EH still describes the Haldane gapped phase. For the odd integer spins, however, the EH just corresponds to the quantum antiferromagnetic Heisenberg half-odd integer spin model with spinon excitations, characterizing the critical point separating the topological Haldane phase from the trivial gapped phase. Our results thus demonstrate that the topological bulk property not only determines its fractionalized edge states, but also the quantum criticality associated with the topological phase, where the elementary excitations are precisely those fractionalized edge degrees of freedom confined in the bulk of the topological phase.

M1.00349 The flexibility of Daubechies wavelets for Linear Scaling DFT calculations. LUIGI GENOVESE, STEPHAN MOHR, Commissariat l’Energie Atomique et aux nergies Alternatives, LAURA ELISABETH RATCLIFF, Argonne National Laboratory, DAMIEN CALISTE, THIERRY DEUTSCH, Commissariat l’Energie Atomique et aux nergies Alternatives, STEFAN GOEDECKER, Basel University — In recent works, we presented the linear scaling version of the BigDFT code [1] based on Daubechies wavelets, where a minimal set of localized support functions is optimized in situ. Our linear scaling approach is able to generate support functions for systems in various boundary conditions, like isolated, surface and periodic [2], and it is based on an algorithm which is universally applicable, requiring only moderate amount of computing physical properties. In general, Daubechies wavelets can be optimized in situ. Our linear scaling approach is able to generate support functions for systems in various boundary conditions, like isolated, surface and periodic [2]. We find that for each dimension, \( D < 6 \), there is a value of \( r = r_f > 1 \) such that for \( r > r_f \), the cascading failures occur as a discontinuous first order transition, while for \( r < r_f \), the system undergoes a continuous second order transition, as in the classical percolation theory. \( r_f \) decreases when the dimension of the lattice increases. For \( D = 6, r_f = 1 \), which is the same as in random regular (RR) graphs with the same degree (coordination number) of nodes. \( D = 6 \) is the upper critical dimension for classical percolation, the point at which the critical exponents of the lattice model become independent of the lattice. In higher dimensions the maximal vulnerability of the networks, as a function of \( r \), is achieved at a distance of \( r = r_{max} > r_f \), but for \( r > r_{max} \), the vulnerability starts to decrease as \( r \to \infty \). However, the decrease becomes less significant as the dimension increases and becomes negligible for \( D = 6 \). Results on the size parameter of the transition scale width of the size of the system will be presented. [1] Catastrophic cascade of failures in interdependent networks, Buldyrev, Parshani, Paul, Stanley& Havlin, Nature 464, 1025-1028 (15 April 2010)

M1.00351 Behavioral analysis of the escape response in larval zebrafish. RUOPEI FENG, KIRAN GIRDHAR, YANN CHEMLA, MARTIN GRUEBELE, Univ of Illinois - Urbana — The behavior of larval zebrafish is of great interest because the limited number of locomotor neurons in larval zebrafish couples with its rich repertoire of movements as a vertebrate animal. Current research uses a priori-selected parameters to describe their swimming behavior while our lab has built a parameter-free model based on singular value decomposition analysis to characterize it. Our previous work has analyzed the free swimming of larval zebrafish and presented a different picture from the current classification of larval zebrafish locomotion. Now we are extending this work to the studies of their escape response to acoustic stimulus. Analysis has shown intrinsic difference in the locomotion between escape response and free swimming.

M1.00352 Synchronization modulation of Na/K pumps on Xenopus oocytes. PENGFEI LIANG, JASON MAST, WEI CHEN, Univ of South Florida — We developed a new technique named synchronization modulation to electrically synchronize and modulate the Na/K pump molecules by a specially designed oscillating electric field. This technique is based on the theory of energy-trap in quantum physics as well as the concept of electronic synchrotron accelerator. As a result, the Na-transports are all entrapped into the positive half-cycle of the applied electric field and consequently, all of the K-transports are entrapped into the negative half cycle of the field. To demonstrate the process of the pump synchronization and modulation, we use Xenopus oocytes as a platform and introduce two-electrode whole-cell voltage clamp in measurement of pump current. Practically, we first synchronize the pump molecules running at the same pace (rate and phase) by a specially designed oscillation electric field. Then, we carefully maintain the pump synchronization status and gradually change the field frequency (decrease and increase) to modulate the pump molecules to newer pumping rate. The result shows a separation of the inward K current from the outward Na current, and about 10 time increase of the total (inward plus outward) pump current from the net outward current from the random paced pump molecules. Also, the ratio of the modulated total pump current with synchronized total pump current is consistent with the ratio of their field frequencies.

M1.00350 Interdependent Lattice Networks in High Dimensions. STEVEN LOWINGER, GABRIEL CWILICH, SERGEY BULDYREV, Yoshiva University — We study the mutual percolation of two interdependent lattice networks following the procedure outlined by Buldyrev et al. We studied lattices of dimensions 2, 3, 4, 5 and 6. We imposed that the length of interdependent links connecting the nodes from one lattice to the other be less than a certain value, \( r \). We find that for each dimension, \( D < 6 \), there is a value of \( r = r_f > 1 \) such that for \( r > r_f \), the cascading failures occur as a discontinuous first order transition, while for \( r < r_f \), the system undergoes a continuous second order transition, as in the classical percolation theory. \( r_f \) decreases when the dimension of the lattice increases. For \( D = 6, r_f = 1 \), which is the same as in random regular (RR) graphs with the same degree (coordination number) of nodes. \( D = 6 \) is the upper critical dimension for classical percolation, the point at which the critical exponents of the lattice model become independent of the lattice. In higher dimensions the maximal vulnerability of the networks, as a function of \( r \), is achieved at a distance of \( r = r_{max} > r_f \), but for \( r > r_{max} \), the vulnerability starts to decrease as \( r \to \infty \). However, the decrease becomes less significant as the dimension increases and becomes negligible for \( D = 6 \). Results on the size parameter of the transition scale with the size of the system will be presented. [1] Catastrophic cascade of failures in interdependent networks, Buldyrev, Parshani, Paul, Stanley& Havlin, Nature 464, 1025-1028 (15 April 2010)
M1.00353 Kinetic inductance parametric up-converter, ADITYA KHER, California Institute of Technology, PETER DAY, NASA Jet Propulsion Laboratory. BYEONG HO EOM, JONAS ZMUZDINAS, California Institute of Technology. H. G. LEDUC, NASA Jet Propulsion Laboratory — We describe a novel class of devices based on the nonlinearity of the kinetic inductance of a superconducting thin film. By placing a current-dependent inductance in a microwave resonator, small currents can be measured through their effect on the resonator’s frequency. By using a high-resistivity material for the film and nanowires as kinetic inductors, we can achieve a large coefficient of nonlinearity to improve device sensitivity. We demonstrate a current sensitivity of 8 pA/Hz^{1/2}, making this device useful for transition edge sensor readout and other cutting-edge applications. An advantage of these devices is their natural ability to be miniaturized in the frequency domain, enabling large detector arrays for TES based instruments. A traveling wave version of the device, consisting of a thin-film microwave transmission line, is also sensitive to small currents as they change the phase length of the line due to their effect on its inductance. We demonstrate a current sensitivity of 5 pA/Hz^{1/2} for this version of the device, making it also suitable for TES readout and other applications. It has the advantage of multi-GHz bandwidth and greater dynamic range, offering a different approach to the resonator version of the device.

M1.00354 Atomistic study on the generation and gliding properties of pyramidal dislocations in magnesium, HIDEO KABURAKI, MITSUHIRO ITAKURA, MASATAKE YAMAGUCHI, Japan Atomic Energy Agency — Plastic deformation of magnesium and its alloys is attracting great interest as one of the candidate materials for energy-conserving lightweight structural metals. The generation of non-basal pyramidal dislocations near the c-axis direction is the key to enhancing plasticity in these highly anisotropic hcp magnesium materials. However, the fundamental understanding of the generation and gliding properties of pyramidal dislocations is still not clear because of the large Burgers vector. Using the molecular dynamics method, we have successfully generated \( \mathbf{c} + \mathbf{a} \times \mathbf{a} > \mathbf{0} \) type I and II screw dislocations from the crack set in the perfect magnesium crystal by applying the shear stress. Visualization of these dislocations is important because the core structures are complex and largely extended. Comparing the results by first-principles calculations, we have found that the core of the type I screw dislocation is smoothly extended while that of the type II screw dislocation has a corrugated structure. We also found that dislocations can easily cross-slip to other slip planes. In particular, it is observed that the core of the gliding pyramidal type I screw dislocation cross-slips to other slip planes. The detailed processes of cross-slip are elucidated in the presentation.

M1.00355 Outdoor concert hall sound design: idea and possible solutions, YANG-HANN KIM, JUNG-MIN LEE, Korea Adv Inv of Sci & Tech, WANGJUN KIM, HWAN KIM, NARU-EMS co. ltd.; JUNG-WOO CHOI, Korea Adv Inv of Sci & Tech, SEMYUNG WANG, Gwangju Inv of Sci & Tech — Sound design of outdoor concert halls needs to satisfy two contradictory objectives: good sound reproduction within the hall, as well as the minimization of external sound radiation. Outdoor concert hall usually has open space, therefore good sound for the listeners can be bad sound for its neighborhood. It would be a good attempt to have a virtual sound wall that can reflect all sound, therefore making a relatively quiet zone in the outside. This attempt can be possible if we could produce invisible but very high impedance mismatch around the hall, for a selected frequency band. This can be possible if we can generate an acoustically bright zone inside and a dark (quite) zone outside. Earlier work [Choi, J.-W. and Kim, Y.-H. (2002). J. Acoust. Soc. Am. 111, 1695–1700], at least, assures it is possible for a selected region and frequencies. Simulations show that it is possible for a two-dimensional case. Experimental verification has been also tried. The discrepancies have been explained in terms of the number of loudspeakers, their spatial distributions, spacing with regard to wavelength. The dependency of its performances with respect to the size of bright and dark zone scaled by wavelength of interest has also been explained.

M1.00356 Multiscale modeling of nanostructured ZnO based devices for optoelectronic applications: Dynamically-coupled structural fields, charge, and thermal transport processes, ABDULMUIN ABDULLAH, SAAD ALQAHTANI, MD REZAUL KARIM NIHAT, SHAIKH AHMED, Southern Illinois University at Carbondale, SIU NANO-ELECTRONICS RESEARCH GROUP TEAM — Recently, hybrid ZnO nanostructures (such as ZnO deposited on ZnO-alloys, Si, GaN, polymer, conducting oxides, and organic compounds) have attracted much attention for their possible applications in optoelectronic devices (such as solar cells, light emitting and laser diodes), as well as in spintronics (such as spin-based memory, and logic). However, efficiency and performance of these hybrid ZnO devices strongly depend on an intricate interplay of complex, nonlinear, highly stochastic and dynamically-coupled structural fields, charge, and thermal transport processes at different length and time scales, which have not yet been fully assessed experimentally. In this work, we study the effects of these coupled processes on the electronic and optical emission properties in nanostructured ZnO devices. The multiscale computational framework employs the atomistic force field molecular mechanics, models for linear and non-linear polarization, the 8-band sp^{3} d^{5} s^{*} tight-binding models, and coupling to a TCAD toolkit to determine the terminal properties of the device. A series of numerical experiments are performed (by varying different nanoscale parameters such as size, geometry, crystal cut, composition, and electrostatics) that mainly aim to improve the efficiency of these devices.

M1.00357 ZnO nanowire-based CO sensor, MON-SHU HO, Physics Department, National Cheng Hsing University, WEI-HAO CHEN, Institute of Electronic Engineering, National Tsing Hua University, YU-LIN CHEN, Physics Department, National Chung Hsing University, MENG-FAN CHANG, Institute of Electronics Engineering, National Tsing Hua University — This study applied ZnO nanowires to the fabrication of a CO gas sensor operable at room temperature. Following the deposition of a seed layer by spin coating, an aqueous solution method was used to grow ZnO nanowires. This was followed by the self-assembly of an electrode array via dielectrophoresis prior to the fabrication of the CO sensing device. We have successfully generated a corrugated structure. We also found that both dislocations can easily cross-slip to other slip planes. The detailed processes of cross-slip are elucidated in the presentation.

M1.00358 Neutron Imaging Studies of In Situ Growth of Neutron and Gamma Detector Materials, NICHOLAS STRANGE, CHRISTOPHER CRAIN, FATEMA WAHIDA, ZACH STROUPE, J.Z. LARESE, University of Tennessee — The studies described here are aimed at addressing the critical need to develop dependable crystal growth techniques of solid-state materials used as radiation detectors for both natural multiplicities in the frequency domain. We present our activities using neutron, x-ray, and scanning transmission electron microscopy techniques to examine the synthesis of both CZT and CLYC with the goal of identifying the conditions that favor the production of defect free materials. Using a pulsed neutron beam and time of flight detection methods, we exploit the penetrating power and wavelength dependence of neutron absorption to perform measurements during crystal growth. Furthermore, solid boules can be examined either inside the furnace or free standing. The objective of these studies include the validation/optimization of the modeling studies of CLYC and CZT growth behavior, the development of new/improved furnace design, and the identification of optimum growth techniques that enable the production of large boules of defect free, single crystalline materials in a timely/cost effective manner. We provide our preliminary results that include the experimental setup at LANSE and sample neutron radiographic and synchrotron based IR images of CZT flat solid plates.
M1.00359 Investigation of Natural Bombyx mori Silk Fibroin Proteins Using INS . CHRISTOPHER CRAIN, NICHOLAS STRANGE, J.Z. LARESE, Univ of Tennessee, Knoxville — The mechanical properties of many protein comprised biomaterials are a direct reflection of non-covalent (i.e. weak) interacting ions such as F-actin in muscles, tubulin in the cytoskeleton of cells, viral capsids, and silk. Porter and Vollrath underscored the two main factors that are critical for understanding the high mechanical strength of silks: the nanoscale semi-crystalline folding structure, which gives it exceptional toughness and strength, and the degree of hydration of the disordered fraction, which acts to modify these properties. Understanding and controlling these two principal factors are the key to the functionality of protein elastomers, and render silk an ideal model protein for (bio)material design. We will describe our investigation of esoprous silk of the Bombyx mori (silk worm), using Inelastic Neutron Scattering (INS). These techniques were used to investigate the microscopic dynamics of the dry and hydrated protein.

M1.00360 Study of the nanosurface properties by analyzing its absorption and scattering cross-section. . IRINA BARIAKHTAR, Boston College — The interest to study the nanoparticles absorbed on the dielectric or semiconductor substrate is caused by the multiple practical applications of these systems such as nanosensors, electronic devices and lately in PV elements for improving of their efficiency [1, 2]. The author suggests a method of examining the properties of the nanosurface with the absorbed nanoparticle by calculating the absorption and scattering of the electromagnetic field by such system based on construction of its effective electric susceptibility. It was built based on the Green’s function approach [3]. The computer simulations show good correspondence with the theory. It was shown that this approach can be applied to investigate the optical absorption and scattering on the nanoparticles on the substrate to be used in PV engineering. 1. Schaadt, D. M., Feng, B., Yu, E. Appl. Phys. Lett. 86 (6): 063106 (2005) 2. K. R. Catchpole and A. Polman, Opt. Express 16, 21793-21800 (2008) 3. I. Bariakhtar, Y. Demidenko, S. Kruichen, V. Lozovski, Surf. Sci. 323 (1995).

M1.00361 Controlling Spin State of Magnetic Molecules by Oxygen Binding Studied Using Scanning Tunneling Microscopy . SOON-HYEONG LEE, Korea University, YUN HEE CHANG, KAIIST, HOWON KIM, KYUNG MIN KIM, Korea University, YONG-HYUN KIM, KAIIST, SE-JONG KAHNG, Korea University — Binding and unbinding between molecular oxygen and metallo-porphyrin is a key process for oxygen delivery in respiration. It can be also used to control spin state of magnetic metallo-porphyrin molecules. Controlling and sensing spin states of magnetic molecules in such reactions at the single molecule level is essential for spintronic molecular device applications. Here, we demonstrate that spin states of metallo-porphyrin on surfaces can be controlled over by binding and unbinding of oxygen molecule, and be sensed using scanning tunneling microscopy and spectroscopy. Kondo localized state of metallo-porphyrin showed significant modification by the binding of oxygen molecule, implying that the spin state was changed. Our density functional theory calculation results explain the observations with the hybridization of unpaired spins in d and *e g orbitals of metallo-porphyrin and oxygen, respectively. Our study opens up ways to control molecular spin state and Kondo effect by means of molecular binding and unbinding reactions on surfaces.

M1.00362 Spotting the Gel Point of Photopolymers by Examining NMR Relaxation . JACK LEE, GRETCHEN HOFMEISTER, MARTHA-ELIZABETH BAYLOR, Carleton College — Spotting when a polymer goes from liquid to solid during polymerization is necessary when working with certain optically cured devices used to fabricate optofluic devices that contain both optical and microfluidic features. Through the use of nuclear magnetic resonance (NMR) it may be possible to determine when the transition from liquid to solid, called the gel point, occurs. In examining the proton longitudinal relaxation time for one species of monomers in our polymer mix, our data shows as the polymer cures the relaxation time increases. By examining this data we were able to extract a time to gel point that was within the margin of error of the theoretical gel point of our materials. Outlined here is evidence of why we think longitudinal relaxation is applicable to studying polymerization, and how we are using it to attempt to extract the gel point.

M1.00363 Observation of Voltage Oscillations in VO2 with Negative Differential Resistance . DAE-JOON KANG, HYOUNG WOO YANG, GARAM BAE, Department of Physics, Sungkyunkwan University, Republic of Korea — Many strongly correlated electron systems exhibit complex nonlinear behaviors with electric fields. The origin of the electrical instabilities is closely related to a negative differential resistance (NDR). Here, we report electrical characteristics of two-terminal devices based on vanadium dioxide (VO2) thin films fabricated on c-cut sapphire substrates, exhibiting NDR behavior in their I-V characteristics that may work as a voltage oscillator of high efficiency. We show that the NDR behavior can be better understood by using a negative differential resistance (NDR) in the device. Furthermore, we found that the source voltage and frequency affect considerably the NDR behaviors, which is indicated by a shift of oscillation voltage from 10 V to 1 V. Based on the experimental results, with the source voltage and the frequency systematically varied, the mechanism of the oscillation was found to be the ascribed to an alternate occurrence of an electric-field-induced resistance switching in the MIT of VO2. We discuss herein, the origin and potential applications of NDR based devices in detail and investigated the voltage oscillation behaviors of VO2 to elucidate the underlying physics of its metal insulator transition behavior.

M1.00364 Cloisite 30B as Nanoclay Compatibilizer for Polysulfone/Polyimide Blend Films. . ALI AMMAR, Akron Univ, AHMED ELZATAHRY, MARIAM AL-MAADEED, Qatar Univ, ABDULLAH ALENIZI, King Saud Univ, KARIM ALAMGIR, Akron Univ — Polysulfone (PSF) and polyimide (PI) are used in many applications including membranes for gas separation and water purification. The phase separation issues limit the blend application of these polymers. We studied the effect of nanoclay and Cloisite 30B on had on (PSF/PI) films. This was done in order to examine the compatibility effects of clay on phase separation behavior, mechanical strength, and structure properties. The addition of weight percentage of organoclay strongly compatibilized the blend phases for all compositions, decreasing the scale of blend phase separation by a factor of 5-10. Interestingly, the net phase separated domain area converged to the 50% blend composition in all cases. This is attributed to a high degree of exfoliation and degradation of nanoclay particles within the PSF/PI matrix as well as interfacial regions, independent of the blend composition. AFM confirmed these optically observed compatibilization effects by quantitative reduction of aspect ratio (width/height) of surface phase separated domains. The surface free energies of the films decreased by adding C30B. This has led us to conclude that there is a change of surface topography, which conformed to the contact angle. PSF/PI films showed decreasing in thermal stability due to the surfactant modification of C30B.

M1.00365 Electronic state modulation of iron selenide by intercalating copper . KAYA KOBAYASHI, Y ITO, F NAGAI, S MATSUMOTO, T KAMBE, Y BENINO, T NAMBA, Okayama University — FeSe is one of the iron-based superconductors that have the simplest structure. Its superconducting properties are easily modulated by chemical and mechanical method, such as alkali metal intercalation and thinning down to monolayer. The synthesis of copper intercalation by melt method brought the structural change of the system in increasing the copper amount. To investigate the superconducting property of the system, we have synthesized copper intercalated FeSe single crystal. The decrease of superconducting transition temperature observed here is discussed in relation to its modulation on to electronic state of iron.
M1.00366 Boson Sampling with Trapped Ions. KATHERINE COLLINS, Univ of Maryland-College Park. KENNETH WRIGHT, CHRISTOPHER RICKERD, CHRISTOPHER MONROE. Univ of Maryland-College Park and Joint Quantum Institute — A classical computer is limited in its ability to solve certain types of problems. A quantum computer might be able to solve some of these problems more efficiently. Calculating the permanent of an N×N matrix is an example of a problem that cannot be efficiently solved by a classical computer. Computing the permanent of an N×N matrix is an example of a problem that cannot be efficiently solved by a classical computer. Computing the permanent of an N×N matrix scales on the order of N!. A quantum device that is able to compute an N×N permanent through boson sampling represents a physical device that can evaluate a problem not efficiently solvable by a classical system. Some experiments have already demonstrated boson sampling with photons for a small number of bosonic modes, but it is difficult to increase the number of bosons in such experiments. One way to demonstrate a larger-scale boson sampling problem is to use the phonon excitations of a trapped ion chain. We present our progress towards experimentally demonstrating boson sampling with trapped ions.


M1.00367 Block Copolymer-Based Supramolecular Elastomers with High Extensibility and Large Stress Generation Capability1. ATSUKI NORO, MIKIHIRO HAYASHI, Nagoya University — We prepared block copolymer-based supramolecular elastomers with high extensibility and large stress generation capability. Reversible addition fragmentation chain transfer polymerizations were conducted under normal pressure and high pressure to synthesize several large molecular weight polystyrene-b-[poly(butyl acrylate)-co-polyacrylamide]-b-polystyrene (S-Ba-S) block copolymers. Tensile tests revealed that the largest S-Ba-S with middle block molecular weight of 3140k achieved a breaking elongation of over 2000% with a maximum tensile stress of 3.6 MPa and a toughness of 28 MJ/m3 while the reference sample without any middle block hydrogen bonds, polystyrene-b-poly(butyl acrylate)-b-polystyrene with almost the same molecular weight, was merely viscous and not self-standing. Hence, incorporation of hydrogen bonds into a long soft middle block was found to be beneficial to attain high extensibility and large stress generation capability probably due to concerted combination of entropic changes and internal potential energy changes originating from the dissociation of multiple hydrogen bonds by elongation.

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M1.00368 Continued Growth on Graphene Edges. ZHENGTANG LUO. Hong Kong Univ of Sci & Tech — Previously, we have shown that the large-size single crystal graphene can be obtained by suppressing the nucleation density during Chemical Vapor Deposition (CVD) growth. Here we demonstrate that the graphene single crystal can be amplified by a continued growth method. In this process, we used a mild oxidation step after the first-growth, which lead to the observed formation of oxides at the vicinity of graphene edges, which allows the graphene growth at seed edges due to reduced activation energy. Consequently, we successfully grown a secondary single-crystal graphene structures with the same lattice structure, orientation on the graphene edges. This amplification method would enable the production of graphene electronics with controlled properties.

M1.00369 Nonlinear Transport and Noise Properties of Acoustic Phonons. KAMIL WALCZAK, Pace University — We examine heat transport carried by acoustic phonons in molecular junctions composed of organic molecules coupled to two thermal baths of different temperatures. The phononic heat flux and its dynamical noise properties are analyzed within the scattering (Landauer) formalism with transmission probability function for acoustic phonons calculated within the method of atomistic Green’s functions (AGF technique). The perturbative computational scheme is used to determine nonlinear corrections to the acoustic heat flux and its noise power spectral density with up to the second order terms with respect to temperature difference. Our results show the limited applicability of ballistic Fourier’s law and fluctuation-dissipation theorem to heat transport in quantum systems. We also derive several noise-signal relations applicable to nanoscale heat flow carried by phonons, but valid for electrons as well. We also discuss the extension of the perturbative transport theory to higher order terms in order to address a huge variety of problems related to nonlinear thermal effects which may occur at nanoscale and at strongly non-equilibrium conditions with high-intensity heat fluxes.

2 This work was supported by Pace University Start-up Grant.

M1.00370 Spectroscopic study of some diatomic molecules via the proper quantization rule. B. FALAYE, IPN, Mexico City, Mexico — Spectroscopic techniques are very essential tools in studying electronic structures, spectroscopic constants and energetic properties of diatomic molecules. These techniques are also required for parametrization of new method based on theoretical analysis and computational calculations. In this research, we apply the proper quantization rule in spectroscopic study of some diatomic molecules by solving the Schrödinger equation with two solvable quantum molecular systems-Tietz-Wei and shifted Deng-Fan potential models for their approximate nonrelativistic energy states via an appropriate approximation to the centrifugal term. We show that the energy levels can be determined from its ground state energy. The beauty and simplicity of the method applied in this study is that, it can be applied to any exactly as well as approximately solvable models. The validity and accuracy of the method is tested with previous techniques via numerical computation for H2 and CO diatomic molecules. The result also include energy spectrum of 5 different electronic states of NO and 2 different electronic state of I2.

M1.00371 “Dual Society Ever Precedes through Trevor SWAN & Wassily Leontief”. WH-MAKSOED, Prodi of Physics UI, Depok 16424- INDONESIA — “Dual Society” introduced by E.F. Schumacher are classified as non-stable society who easy to be shaken by politics uncertainties. In Robert J. Barro & X. Sala-i-Martin: “Convergence” states: “a key economic issue is whether poor countries or regions tend to grow faster than rich ones”. For growth models comprises Roy Forbes Herrod & Essey-Domar, three assumptions described by Eduardo Ley are[(U+2639)i]. output is proportional to capital,(ii). Investment ex ante equals saving & (iii) saving proportional to output. Underlines Trevor SWAN, developing countries differ significantly among themselves. Economic growth models comprises Herrod-Domar growth model, Solow growth model & endogenous growth model. Further, for five stages of economic growth from Rostov of Leontief technology, ever retrieves the Jens Becker: “Institutional Isomorphism revisited: Convergence & Divergence in Institutional Change” instead Frumkin’s “Institutional Isomorphism & Public Sector Organizations”.

1 Acknowledgment devotes to the Lates HE. Mr. Brigadier General-TNI[rtd]. Prof. Ir. HANDOJO
2a Devotes to Robert J. Barro & Xavier Sala-i-Martin:”ECONOMIC GROWTH” whose design depict coincidences with Salvador Dali painting: “The Persistence of Memory”
M1.00372 “the human BRAIN & Fractal quantum mechanics”

M1.00373 “From Fundamental Motives to Rational Expectation Equilibrium[REE, henceworth] of Indeterminacy”

M1.00374 Can we judge an oxide by its cover? The case of the metal/oxide interface from first principles

M1.00375 Carbon nanotube transistor based high-frequency electronics

M1.00376 Gate Opening Transition of Zeolitic Imidazolate Framework – 8 in Xenon adsorption and Carbon Monoxide Adsorption

M1.00377 Majorana fermion mean field study of two-dimensional inequivalent bipartite kondo lattice
M1.00378 A universal scaling law for the evolution of granular gases, MATHIAS HUMMEL, JAMES CLEWETT, MARCO G. MAZZA, Max Planck Institute for Dynamics and Self-Organization — Dry, freely evolving granular materials in a dilute gaseous state coalesce into dense clusters only due to dissipative interactions. This clustering transition is important for a number of problems ranging from geophysics to cosmology. Here we show that the evolution of a dilute, freely cooling granular gas is determined in a universal way by the ratio of inertial flow and thermal velocities, that is, the Mach number. Theoretical calculations and direct numerical simulations of the granular Navier–Stokes equations show that irrespective of the coefficient of restitution, density, or initial velocity distribution, the density fluctuations follow a universal quadratic dependence on the system’s Mach number. We find that the clustering exhibits a scale-free dynamics but the clustered state becomes observable when the Mach number is approximately of O(1). Our results provide a method to determine the age of a granular gas and predict the macroscopic appearance of clusters.

M1.00379 Development, Selection, and Validation of Tumor Growth Models, AMIR SHAHMOADI, ERNESTO LIMA, J. TINSLEY ODEN, The University of Texas at Austin — In recent years, a multitude of different mathematical approaches have been taken to develop multiscale models of solid tumor growth. Prime successful examples include the lattice-based, agent-based (off-lattice), and phase-field approaches, or a hybrid of these models applied to multiple scales of tumor, from subcellular to tissue level. Of overriding importance is the predictive power of these models, particularly in the presence of uncertainties. This presentation describes our attempt at developing lattice-based, agent-based and phase-field models of tumor growth and assessing their predictive power through new adaptive algorithms for model selection and model validation embodied in the Occam Plausibility Algorithm (OPAL), that brings together model calibration, determination of sensitivities of outputs to parameter variances, and calculation of model plausibilities for model selection.

M1.00380 Evidence for quantization and topological states in spin Hall conductivity of low-dimensional systems, SEBASTIAN KUEFNER, LARS MATTHES, JUERGEN FURTHMUELLER, FRIEDHELM BECHSTEDT, FSU Jena — Ab initio relativistic band structure calculations are performed for the frequency-dependent spin Hall conductivity of two-dimensional atomically thin crystals and one-dimensional nanoribbons. We study the influence of topology, quantization and topological edge states. As model systems, fully halogenated germanene, Gel, and its Gel nanoribbons are investigated. Gel represents a topological insulator due to strong spin-orbit interaction and, hence, band inversion. We demonstrate the quantization of the static spin Hall conductivity. It is hardly influenced by temperature variation but significantly by Fermi level shift. The frequency dependence of the conductivity is governed by the band-structure details. Topological edge states influence the conductivity mainly for vanishing frequencies.

M1.00381 Ultrafast spectroscopy of exciton and exciton dynamics in mono and few layers of WS2, SUDIKSHA KHADKA, SHROUQ ALEITHAN, MAX LIVSHITS, JEFFREY J. RACK, MARTIN KORDESCH, ERIC STINAFF, Ohio University — Single layer of Transitional metal dichalcogenides (MX2) are 2D semiconductors that have a direct band gap in visible spectrum and fill the gap in between 2D metallic and insulating materials. They have possible application in optoelectronic devices, photovoltaics and photodetection, molecular sensing, ‘valleytronics’, and flexible transparent electronics. Tungsten disulphide (WS2), one of the member of MX2 family, has a direct band gap of 2.2 eV and a large valley splitting of about 0.4 eV. Here, we present a detailed study of exciton states and their decay mechanisms in mono and few layer WS2 using femtosecond transient absorption spectroscopy. We report a new peak at 3.010.1 eV whose origin in k space is believed to be at or around K point and further investigation is under way. The exponential fitting of decay curve of the exciton A reveals three time components as 1.70.3 ps, 33.510 ps and 67015 ps, most likely corresponding to carrier-carrier scattering, carrier-phonon scattering, and radiative relaxation respectively.

M1.00382 Enhanced TC in granular and thin film Al-Al2O3 nanostructures, J. S. HIGGINS, R. L. GREENE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland — It is known since the 1970s that the superconducting transition temperature of granular aluminium films can be as high as two to three times the transition temperature of bulk aluminium, depending on the grain size and how strongly the nanometer size grains are connected1,2. As the strength of the grain connectivity becomes increasingly weak, the enhanced TC is suppressed. The mechanism behind this enhancement is still under debate. Recent work on larger aluminium nanoparticles (18nm) embedded in an insulating Al2O3 matrix showed an onset of the superconducting transition as high as three times that of bulk aluminium1. In this situation, the Al grains are electronically disconnected and in a regime far removed from that of the granular films. Here we compare the two situations through electronic and thermal measurements in order to help elucidate the mechanism behind the enhancements. 1S. Pracht, et al., arXiv:1508.04270v1 [cond-mat.supr-con] (2015). 2G. Deutscher, New Superconductors From Granular to High Tc, New Jersey: World Scientific, 2006, p. 72-74. 3V. N. Smolyaninova, et al., Sci. Rep. 5, 15777 (2015).

M1.00383 Substitution and “site-decoupled doping” in iron pnicnites, M. MERZ, P. SCHWEISS, P. NAGEL, M.-J. HUANG, A. PLOG, R. EDER, TH. WOLF, H. V. LÖHNEYSEN, S. SCHUPELLER, Karlsruhe Institute of Technology, Germany — The composition-dependent electronic structure of iron pnictides, in particular the question if and how charge carriers are introduced to the system upon substitution — by Sr or alkali metals, AM, for Ba; by transition metals, TM, for Fe; and/or by P for As – continues to provide surprises. Our ongoing systematic study of spatial structure and electronic states by x-ray diffraction and x-ray absorption, performed on a large number of compositions in the (Ba, Sr, AM)(Fe, TM)2(As, P)2 family of compounds, shows, for instance, that valences are rarely as expected, that doping can be “effective” or “slow” depending on substituent, and that most substitution effects may be more crucial to magnetism and superconductivity in iron pnictides than direct doping effects.

M1.00384 STM imaging of vortex cores states in superconducting graphene, YU JI, MAOZ OVADIA, Harvard University, JENNIFER HOFFMAN, University of British Columbia, GIL-HO LEE, PHILIP KIM COLLABORATION, WENJING FANG COLLABORATION, Graphene becomes superconducting via the proximity effect when it comes in good contact with a superconductor. In the presence of a magnetic field, superconducting vortices will form and will each contain Andreev bound states. If the normal electrons in the vortices have a Dirac dispersion and they are surface bound states, the zero modes of the Dirac dispersion are then Majorana fermions. We investigate the electronic properties of graphene on superconducting NbN and search for these vortex bound states using our home built low temperature scanning tunneling microscope.

1Harvard University
2MIT
M1.00386 Singular manifestaition of square-planar coordination of a iridate Na$_2$IrO$_4$. SUDIPTA KANUNGO, BINGHAI YAN, PATRICK MERZ, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, MARTIN JANSEN, Max-Planck-Institut for Solid State Research, Stuttgart, Germany — Local environments and valence electron counts primarily determine the electronic states and physical properties of transition metal complexes. For example, square-planar surroundings found in transition oxometalates such as Curprates, Nickaltes are usually associated with the $d^0$ or $d^2$ electron configuration. In this work, we address an experimentally observed exotic square-planar mono-oxoanion [IrO$_4$]$^{4-}$ in Na$_2$IrO$_4$ with Ir(IV) in d$^3$ (S=$\frac{5}{2}$ state) configuration, using ab-initio calculations. On contrary, in its 3d counterpart, Na$_2$CoO$_4$, Co(IV) is in tetrahedral coordination with S=$\frac{3}{2}$ high spin state. Our ab-initio calculations reveal that the on-site Coulomb interaction U is the essential factor for determining the stability of the local coordination as well spin state. We find that due to weak Coulomb repulsion of Ir-5d electrons, Na$_2$IrO$_4$ form in a square-planar coordination whereas for Na$_2$CoO$_4$, Co(IV) is in tetrahedral coordination in all mass densities at 3d Co site. Following the trend from 3d to 5d, we predict that the intermediate 4d material Na$_2$RbO$_4$, if synthesized, may favor tetrahedral coordination but with an S=$\frac{5}{2}$ low spin state.


M1.00387 Local electronic structure and ferromagnetic interaction in La(Co,Ni)$_3$O$_5$. MENG-JIE HUANG, PETER NAGEL, DIRK FUCHS, HILBERT VON LOEHNEYSEN, MICHAEL MERZ, STEFAN SCHUPLLETER, Karlsruhe Institute of Technology, Germany — Perovskite-related transition-metal oxides exhibit a wide range of properties from insulating to superconducting as well as many peculiar magnetic phases, and covalalties, have been known for their proximity to spin-state transitions. How this changes with partial substitution by Ni is the topic of the present study. The local electronic structure and the ferromagnetic interaction in La(Co$_{1-x}$Ni$_x$)$_3$O$_5$ has been studied by x-ray absorption (XAS) and x-ray magnetic circular dichroism (XMCD). XAS clearly indicates a mixed-valence state for both Co and Ni, with both valences changing systematically with Ni content, x. While the gradual spin-state transition of Co$^{3+}$ from low-spin (LS) to high-spin (HS) is preserved for low x it is suppressed in the high Ni-content samples. Regarding the spin configuration of Ni we find it stabilized in a “mixed” spin state, unlike the purely LS state of Ni in LaNiO$_3$. XMCD identifies the element-specific contributions to the magnetic moment and interactions. In particular, we find that it must be the coexistence of the HS state in both Co$^{3+}$ and Ni$^{3+}$ that induces t$_2g$-based ferromagnetic interaction via the double-exchange mechanism.

M1.00388 Tuning band gap of monolayer and bilayer SnS$_2$ by strain effect and external electric field: A first-principles calculations1, ABEERA RAHMAN, YOUNG-HAN SHIN, University of Ulsan — Recently many efforts have been paid to two-dimensional layered metal dichalcogenides (LMDs). Among them MoS$_2$ has become a prototype LMD, and recent studies show surprising and rich new physics emerging in other van der Waals materials such as layered SnS$_2$ [1-4]. SnS$_2$ is a semiconducting earth-abundant material and Sn is a group IV element replacing the transition metal in MoS$_2$. SnS$_2$ shows new possibilities in various potential applications. However, the knowledge on basic properties of layered SnS$_2$ is still not well understood. In this study, we consider two types of structures: 1T with P$^{3}$m1 (164) space group and 1H with P$^{6}_{3}$m (194) space group. Our first-principles calculations show that the 1T structure for SnS$_2$ is more stable than the 1H structure whereas latter is more stable for MoS$_2$. Moreover, in contrast to MoS$_2$, SnS$_2$ shows an indirect band gap both for 1T and 1H structures while 1T MoS$_2$ is metallic and 1H has a direct band gap. We also study strain effect in the range of 0-10% on the band structure for monolayer and bilayer SnS$_2$ (both for 1T and 1H structures). We find significant change in their band gaps. We also investigate the bilayer SnS$_2$ with and without out-of-plane strain.

2 This research was supported by Brain Korea 21 Plus Program and Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Science, ICT and future Planning (NRF-2014M3A7B4049367, NRF-2014R1A2A1A1105089).

M1.00389 Manipulating individual defects in graphene/BN heterostructures: a first-principles study. LEDE XIAN, ANGEL RUBIO, Univ. of the Basque Country — Recent experiments have demonstrated the possibility of manipulating defects in insulating hexagonal boron nitride (hBN) within a graphene/hBN heterostructure using scanning tunneling microscopy, opening a new pathway of manipulating individual defects of insulators at the nanoscopic scale. With first principle calculations, we are able to simulate this process and elucidate the relevant physics in experiments. Moreover, we calculate the band level alignments between graphene and possible defects states in hBN. Thus, we identify different defects observed in experiments and provide important reference for future experiments and applications.

M1.00390 CVD-based, photolithographically patterned, highly-sensitive graphene Hall elements on hexagonal BN. JOONGGYU KIM, Center for Integrated Nanostructure Physics, Institute for Basic Science, DOES, Sungkyunkwan University, MIN-KYU JOO, JI-HOON PARK, Center for Integrated Nanostructure Physics, Institute for Basic Science, DOES, Sungkyunkwan University, VAN LUAN NGUYEN, Center for Integrated Nanostructure Physics, Institute for Basic Science, DOES, Sungkyunkwan University, KI KANG KIM, Department of Energy and Materials Engineering, Dongguk University, YOUNG HEE LEE, DONGSEOK SUH, Center for Integrated Nanostructure Physics, Institute for Basic Science, DOES, Sungkyunkwan University — Graphene is known to have a high carrier mobility, and the carrier density can be minimized at the charge neutrality point (CNP). Because such features are suitable for Hall sensor measuring magnetic field, we examined the possibility of graphene Hall element (GHE) as a highly sensitive magnetic sensor. For the high-throughput production of GHE in the future, the material synthesized by a chemical-vapor-deposition (CVD) method and the fabrication processes based on photolithography were adopted to show its mass-production feasibility. Specifically, the CVD synthesized hexagonal BN (hBN) was tested as a protection layer of graphene from extrinsic doping driven by SiO$_2$ substrate, which causes the shift of CNP. In addition, post annealing sequences were also included between the growth step, such as the hBN attachment on SiO$_2$ and the graphene transfer on hBN/SiO$_2$ substrate followed by the PMMA removal. From this work, we can get minimum magnetic resolution around 10 mg/H$_{2.5}$ at 300 Hz.

M1.00391 Study of correlations from Ab-Initio Simulations of Liquid Water1, ADRIAN SOTO, MARIVI FERNANDEZ-SERRA, Stony Brook University, DEUYU LU, SHINJAE YOO, Brookhaven National Lab — An accurate understanding of the dynamics and the structure of H$_2$O molecules in the liquid phase is of extreme importance both from a fundamental and from a practical standpoint. Despite the successes of Molecular Dynamics (MD) with Density Functional Theory (DFT), liquid water remains an extremely difficult material to simulate accurately and efficiently because of fine balance between the covalent O-H bond, the hydrogen bond and the attractive the van der Waals forces. Small errors in those produce dramatic changes in the macroscopic properties of the liquid or in its structural properties. Different density functionals produce answers that differ by as much as 35% in ambient conditions, with none producing quantitative results in agreement with experiment at different mass densities [J. Chem Phys. 139, 194502(2013)]. In order to understand these differences we perform an exhaustive scanning of the geometrical coordinates of MD simulations and study their statistical correlations with the simulation output quantities using advanced correlation analyses and machine learning techniques.

1 This work was partially supported by DOE Award No. DE-FG02-09ER16052, by DOE Early Career Award No. DE-SC0003871, by BNL LDRD 16-039 project and BNL Contract No. DE-SC0012704.
M1.00392 Improved methods for determining the secondary structure of proteins using FTIR spectroscopy, DAVID NETO, Oklahoma State University — The determination of the secondary structure is vitally important in the study of proteins. An oft overlooked and underused method to probe the secondary structure of a protein is Fourier transform infrared (FTIR) spectroscopy. A great compliment to both X-ray and NMR techniques, the speed and relatively low cost of FTIR measurements provide a wealth of information about the structure of a protein. To enhance the accuracy of secondary structure calculations, improved methods in the fitting of absorbance spectra are needed. In this talk, we will explore the development of these methods and apply them to a few well studied proteins.


2:30PM P53.00001 The intestine is a blender, PATRICIA YANG, MORGAN LAMARCA, VICTORIA KRAVETS, DAVID HU, Georgia Institute of Technology — According to the U.S. Department of Health and Human Services, digestive disease affects 60 to 70 million people and costs over 140 billion annually. Despite the significance of the gastrointestinal tract to human health, the physics of digestion remains poorly understood. In this study, we ask a simple question: what sets the frequency of intestinal contractions? We measure the frequency of intestinal contractions in rats, as a function of distance down the intestine. We find that intestines contract radially ten times faster than longitudinally. This motion promotes mixing and, in turn, absorption of food products by the intestinal wall. We calculate viscous dissipation in the intestinal fluid to rationalize the relationship between frequency of intestinal contraction and the viscosity of the intestinal contents. Our findings may help to understand the evolution of the intestine as an ideal mixer.

2:42PM P53.00002 Confinement of Single Microswimmers in Circular Microfluidic Chambers, TANYA OSTAPENKO, THOMAS BOEDDEKER, CHRISTIAN KREIS, FABIAN SCHWARZENDAHL, MARCO G. MAZZA, OLIVER BAUEMCHEN, Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — The characteristics of active fluids, such as suspensions of biological microswimmers, may not only originate from the mutual interactions between the constituents, but also from interactions with interfaces and confining walls. In fact, the natural habitats of many living organisms are complex geometric environments, rather than bulk situations. The influence of interfaces on the dynamics was recognized as an important factor, and there are differences in the way that pusher-type swimmers (e.g. E. coli) and puller-type swimmers (e.g. C. reinhardtii) behave close to flat interfaces. Using experiments and simulations, we report on the dynamics of single puller-type swimmers in 2D circular microfluidic chambers. We find that the radial probability distribution of trajectories displays a characteristic wall hugging effect, where swimmers remain trapped at a concave interface for decreasing chamber size. For trajectories in the vicinity of the concave wall, an alignment of the local swimming direction with the local wall tangent is observed. In contrast, the swimmers tend to scatter off convex interfaces with short interaction times. Based on geometric arguments involving the swimmer’s persistence length, we explain this entrainment effect at concave interfaces.

2:54PM P53.00003 Mirror-symmetry breakings in human sperm rheotaxis, NORBERT STOOP, Massachusetts Inst of Tech-MIT, ANTON BUKATIN, IGOR KUKHTEVICH, Russian Academy of Sciences, St. Petersburg Academic University, JOERN DUNKEL, Massachusetts Inst of Tech-MIT, VASILY KANTSLER, University of Warwick — Rheotaxis, the directed response to fluid velocity gradients, has been shown to facilitate stable upstream-swimming of mammalian sperm cells along solid surfaces, suggesting a robust mechanism for long-distance navigation during fertilization. However, the dynamics by which a human sperm orientates itself w.r.t. ambient flows is poorly understood. Here, we combine microfluidic experiments with mathematical modeling and 3D flagellar beat reconstruction to quantify the response of individual sperm cells in time-varying flow fields. Single-cell tracking reveals two kinematically distinct swimming states that entail opposite turning behaviors under flow reversal. We constrain an effective 2D model for the turning dynamics through systematic large-scale parameter scans, and find good quantitative agreement with experiments. We present comprehensive 3D data demonstrating the rolling dynamics of freely swimming sperm cells around their longitudinal axis. Contrary to current beliefs, this analysis uncovers ambidextrous flagellar waveforms and shows that the cells turning direction is not defined by the rolling direction. Instead, the different rheotactic turning behaviors are linked to a broken mirror-symmetry in the midpiece section, likely arising from a buckling instability.

3:06PM P53.00004 Microorganism billiards in closed plane curves, MADISON KRIEGER, Brown University — Recent experiments and numerical simulations have demonstrated that many species of microorganisms reflect aspecularly from a solid surface — due to steric and hydrodynamic interactions with the walls, their outgoing angle is fixed and independent of the angle of incidence. Motivated by these results, we discuss theory and computation of the “aspecular billiard”, a modification of the classical billiard in which the outgoing angle is constant. We restrict our attention to closed plane curves, focusing on three canonical examples: the ellipse, the Bunimovich stadium, and the Sinai billiard. These systems can have a rich array of orbits, and the Lyapunov exponent is shown to be dependent on the billiard geometry and the outgoing angle. We apply these results to the design of tunable passive sorting mechanisms.

3:18PM P53.00005 Helicobacter pylori displays spiral trajectories while swimming like a corkscrew in solutions,1 MAIRA A. CONSTANTINO, JOSEPH M. HARDCASTLE, RAMA BANSIL, Boston University, MEHDI JABBARZADEH, HENRY C. FU, University of Nevada at Reno — Helicobacter pylori is a helical shaped bacterium that causes gastritis, ulcers and gastric cancer in humans and other animals. In order to colonize the harsh acidic environment of the stomach H. pylori in viscous media. However a yet unanswer question is if the helical cell shape influences bacterial swimming dynamics or confers any advantage when swimming in viscous solution. We will present measurements of H. pylori trajectories displaying corkscrew motion while swimming in solution obtained by tracking single cells using 2-dimensional phase contrast imaging at high magnification and fast frame rates and simultaneously imaging their shape. We observe a linear relationship between swimming speed and rotation rate. The experimental trajectories show good agreement with trajectories calculated using a regularized Stokeslet method to model the low Reynolds number swimming behavior. Supported by NSF PHY 1410798 (PET: RB)

3:30PM P53.00006 Investigating wake patterns and propulsive frequencies of a flat plate under pitching motion, JOSEPH MOUBOGHA MOUBOGHA1, JACQUES ANDRE ASTOLFI2, French Naval Academy Institute - IRENAV — Fundamental mechanisms of swimming are explored using a simple geometry device - flat plate - in pure-pitching motion in a hydrodynamic tunnel. The experiments are carried out at different Reynolds numbers based on the plate length c. Pitching motion is generated for reduced frequencies k between 0 and 2 and for an angular amplitude of 10 deg. Velocity fields are obtained in the wake of the plate using Particle Image Velocimetry and measurements of drag coefficients are estimated from mean velocity profiles. This study confirms the occurrence of a threshold oscillation frequency beyond which the plate enters a propulsive regime and the wake features organized structures. In this case an inversion of the typical Karman vortex street is observed. The evolution of mean transverse velocity profiles in the wake of the plate shows that the usual wake profile with velocity deficit - plate with drag - can be transformed into a jet - plate with thrust - above a certain reduced frequency.

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Continuous-flow Electrokinetic Particle Separation in a Bifurcating Microchannel. DI LI, XINYU LU, XIANGCHUN XUAN, Clemson University — Separating particles from a heterogeneous mixture is important and necessary in many engineering and biomedical applications. Electrokinetic flow-based continuous particle separation has so far been realized primarily by the use of particle dielectrophoresis induced in constricted and/or curved microchannels. We demonstrate in this talk that particles can be continuously separated by size when passing through a bifurcating microchannel. This sheathless label-free separation relies on the wall-induced electrical lift force that acts to focus particles to the center of the main-branch and deflect them to size-dependent flow paths in the two side-branches. We also develop a numerical model to predict and understand this separation.

Predator-prey model for the self-organization of stochastic oscillators in dual populations. SARA MORADI, Université Libre de Bruxelles, 1050 Brussels, Belgium, JOHAN ANDERSON, Department of Earth and Space Sciences, Chalmers University of Technology, SE-412 96 Gteborg, Sweden, OZGUR D. GRCAK, Ecole Polytechnique, CNRS UMR7648, LFP, F-91128, Palaiseau, France — A predator-prey model of dual populations with stochastic oscillators is presented. A linear cross-coupling between the two populations is introduced that follows the coupling between the motions of a Wilberforce pendulum in two dimensions: one in the longitudinal and the other in torsional plain. Within each population a Kuramoto type competition between the phases is assumed. Thus, the synchronization state of the whole system is controlled by these two types of competitions. The results of the numerical simulations show that by adding the linear cross-coupling interactions predator-prey oscillations between the two populations appear which results in self-regulation of the system by a transfer of synchrony between the two populations. The model represents several important features of the dynamical interplay between the drift wave and zonal flow turbulence in magnetically confined plasmas, and a novel interpretation of the coupled dynamics of drift wave-zonal flow turbulence using synchronization of stochastic oscillator is discussed.

Exploring the Spatiotemporal Dynamics of Covariant Lyapunov Vectors for Chaotic Convection. MU XU, MARK PAUL, Virginia Tech — Covariant Lyapunov vectors provide access to fundamental features of chaos in high-dimensional systems that are far driven-from-equilibrium. We explore the spatiotemporal dynamics of covariant Lyapunov vectors for chaotic Rayleigh-Bénard convection to provide new physical insights. We use the covariant Lyapunov vectors to quantify the transition from hyperbolic to non-hyperbolic dynamics, to determine the degree of Oseledect splitting exhibited by the dynamics, and to shed light upon upon the tangled nature of the Lyapunov vectors. In this talk, we will explore the spatiotemporal dynamics of the Lyapunov vectors and their relation with the chaotic pattern dynamics of the flow field. Our results suggest that the Lyapunov vectors contain two distinct spatiotemporal features consisting of highly localized regions near defect structures and a spatially distributed checkerboard pattern. We will explore the connection between these features and the ideas of physical and spurious modes that may compose the dynamics.

The role of the capillary force in the liquid distribution in porous media. BOJAN MARKICEVIC, Pall Corp — The dynamics of the liquid spreading in porous media occupied by gas is investigated numerically using the capillary network models. In the numerical solution, the flow at the free interface is fully resolved from the force balance at each pore along the interface allowing for local flows to fill or empty the pores. The flow is transient and the interface shape is determined at each time step. The liquid/solid interactions are investigated for whole range from fully wetting to fully non-wetting cases, and the spread of neutral fluid is also solved. For the neutral fluid, the interface irregularity are caused by pore varying volume with the interface of specific thickness separating fully saturated and gas occupied parts of porous medium. For the capillary interactions present, the interface thickness increases and due to the gas entrainment by spreading liquid, the saturation profiles develop in the direction of the liquid flow. The profiles depend on the capillary force as liquid spreads along the paths consisting of smaller pores for wetting, and larger pores for non-wetting interactions. Finally, the influence of the capillary force is counteracted by viscous force, where for faster flows, the saturation profiles vanish and the interface of limited thickness develops.

Numerical modeling and simulation of flow through porous fabric surface. ZHENG GAO, XIAO LIN LI, Stony Brook University — We designed a numerical scheme to model the permeability of the fabric surface in an incompressible fluid by coupling the projection method with the Ghost Fluid Method in the front tracking framework. The pressure jump condition is obtained by adding a source term to the Poisson’s equation in the projection step without modifications on its coefficients. The numerical results suggest that this approach has the ability to reproduce the relationship between pressure drop and relative velocity observed in the experiments. We use this algorithm to study the effects of porosity on the drag force and stability of parachutes during its inflation and deceleration.

Numerical Study of Shear Flow in Partially Vegetated Open Channels. JINGFANG QU, SUNY, Stony Brook, S CHEN, North Carolina State University, JIE YU, XIAO LIN LI, SUNY, Stony Brook — Shear flow at the interface between a porous layer and an open conduit is a problem of fundamental importance to problems ranging from natural to engineered flows. Such shear flows are known to be unstable, inducing waves and coherent vortices via Kelvin-Helmholtz instability. These coherent flow structures can strongly enhance the exchange of scalar variables and vector variable such as momentum in and out of the canopy, hence playing an important role in controlling environmental quality of these system. We developed a numerical model using finite difference method for flow in open channel occupied by a vegetation canopy. We apply the method to simulate the shear flow and compare with the experimental study by White and Nepf in 2007. Preliminary comparisons with the experimental data show good agreements.
interactions, cell polarity, and cell-cell interaction. The model will be applied to a variety of systems, including motion on micropatterned substrates and the cells, however, is challenging. Here, I discuss our efforts to build a comprehensive cell motility model that includes cell membrane properties, cell-substrate interactions, and substrate heterogeneities.

Modeling can provide useful insights into the fundamental mechanisms of collective cell motility. Constructing models that incorporate the physical properties of cellular forces and tissue stresses from experimentally accessible cell shapes and traction forces, hence providing the spatio-temporal distribution of stresses in tissues, is key to understanding cell behavior in various contexts. Voronoi tessellation with directed noisy cell motility and interactions governed by a shape energy that incorporates the effects of cell volume incompressibility, particle models and vertex models of confluent cell layers. In this model, referred to as self-propelled Voronoi (SPV), cells are described as polygons in a Voronoi diagram, and the motion of cells is governed by a shape energy that incorporates the effects of cell volume incompressibility and cell-substrate interactions. The model can be applied to a variety of systems, including motion on micropatterned substrates and the migration of border cells in Drosophila.

1. Geometrical confinement is one of the key external factors influencing large scale coordination during collective migration. Using a combination of in vitro experiments and numerical simulations, we show that the velocity correlation length, measured in unconfined conditions, provides a convenient length scale to predict the dynamic response under confinement. The same length scale can also be used to quantify the influence range of directional cues within the cell population.

2. Heterogeneity within motile cell populations is frequently associated with an increase in their invasive capability and appears to play an important role during cancer metastasis. Using in silico experiments, we studied the way cell invasion is influenced by both the degree of cell coordination and the amount of variability in the motile force of the invading cells. Results suggest that mechanical heterogeneity dramatically enhances the invasion rate through an emerging cooperative process between the stronger and weaker cells, accounting for a number of observed invasion phenotypes.

3. Effective convergent extension requires on a consistent orientation of cell intercalation at the tissue scale, most often in relation with planar cell polarity mechanisms to define the primary axes of deformation. Using a novel modelling approach for cells mechanical interactions, we studied the dynamics of substrate free motile cell populations. Ongoing work shows in particular that nematic order emerges from interacting cells without the need for biochemical cues setting tissue polarity.

4. This work was supported by NIH Grant No. P01 GM078586 and NSF Grant No. 1068869.

**Wednesday, March 16, 2016 2:30PM - 5:30PM**

**Session P55 DBIO DFD GSOFT: Active Fluids in Living Matter: Collective Cell Motility**

Hilton Baltimore Holiday Ballroom 6 - Yuhui Tu, IBM, Inc.

### 2:30PM P55.00001Collective dynamics of cell migration and cell rearrangements

**ALEXANDRE KABELA**
University of Cambridge —
Understanding multicellular processes such as embryo development or cancer metastasis requires to decipher the contributions of local cell autonomous behaviours and long range interactions with the tissue environment. A key question in this context concerns the emergence of large scale coordination in cell behaviours, a requirement for collective cell migration or convergent extension. I will present a few examples where physical and mechanical aspects play a significant role in driving tissue scale dynamics.

1. Geometrical confinement is one of the key external factors influencing large scale coordination during collective migration. Using a combination of in vitro experiments and numerical simulations, we show that the velocity correlation length, measured in unconfined conditions, provides a convenient length scale to predict the dynamic response under confinement. The same length scale can also be used to quantify the influence range of directional cues within the cell population.

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### 3:06PM P55.00002 Multicellular Streaming in Solid Tumours

**JOSEF KAS**, Leipzig University —
As early as 400 BCE, the Roman medical encyclopaedist Celsus recognized that solid tumours are stiffer than surrounding tissue. However, cancer cell lines are softer, and softer cells facilitate invasion. This paradox raises several questions: Does softness emerge from adaptation to mechanical and chemical cues in the external microenvironment, or are soft cells already present inside a primary solid tumour? If the latter, how can a more rigid tissue contain more soft cells? Here we show that in primary tumour samples from patients with mammary and cervix carcinomas, cells do exhibit a broad distribution of rigidities, with a higher fraction of very soft cells can still remain rigid. Moreover, in tissues with the observed distributions of cell stiffnesses, softer cells spontaneously self-organize into lines or streams, possibly facilitating cancer metastasis.

### 3:42PM P55.00003 Active unjamming of confluent cell layers

**M CRISTINA MARCHETTI**, Syracuse University —
Cell motion inside dense tissues governs many biological processes, including embryonic development and cancer metastasis, and recent experiments suggest that these tissues exhibit collective glassy behavior. Motivated by these observations, we have studied a model of dense tissues that combines self-propelled particle models and vertex models of confluent cell layers. In this model, referred to as self-propelled Voronoi (SPV), cells are described as polygons in a Voronoi tessellation with directed noisy cell motility and interactions governed by a shape energy that incorporates the effects of cell volume incompressibility, contractility and cell-cell adhesion. Using this model, we have demonstrated a new density-independent solid-liquid transition in confluent tissues controlled by cell motility and a cell-shape parameter measuring the interplay of cortical tension and cell-cell adhesion. An important insight of this work is that the rigidity and dynamics of cell layers depends sensitively on cell shape. We have also used the SPV model to test a new method developed by our group to determine cellular forces and tissue stresses from experimentally accessible cell shapes and traction forces, hence providing the spatio-temporal distribution of stresses in motile dense tissues.

### 4:18PM P55.00004 Modeling collective cell motility

**WOUTER-JAN RAPPEL**, Univ of California - San Diego —
Eukaryotic cells often move in groups, a critical aspect of many biological and medical processes including wound healing, morphogenesis and cancer metastasis. Modeling can provide useful insights into the fundamental mechanisms of collective cell motility. Constructing models that incorporate the physical properties of the cells, however, is challenging. Here, I discuss our efforts to build a comprehensive cell motility model that includes cell membrane properties, cell-substrate interactions, cell polarity, and cell-cell interaction. The model will be applied to a variety of systems, including motion on micropatterned substrates and the migration of border cells in Drosophila.

**This work was supported by NIH Grant No. P01 GM078586 and NSF Grant No. 1068869.**
4:54PM P55.00005 Water Dynamics in Living Cells and Tumor Cell Migration in Confined Microenvironments, SEAN SUN, Johns Hopkins University — More than 70% of the total mass in living cells is water. In most biological scenarios water serves as a passive medium responsible for solvation and proper functioning of proteins. However, it has been long recognized that there are situations where dynamic transport of water in cells is important. First, cells actively transport water in order to maintain its volume, and because cell volume directly influences cell shape and internal hydrostatic pressure, it is a critical aspect of cell mechanics. Furthermore, cell volume is coupled to protein synthesis which ultimately determines the cell size. Therefore water transport and cell volume dynamics ultimately impact cell growth and division. Second, epithelial cells in organs such as the eye and kidney actively transport water across the cell membrane and the epithelial layer. Indeed, water channels such as aquaporins increase water permeability of the membrane and facilitate this transport. Recent, we have shown that in confined microenvironments, active transport of water is responsible for actin-independent cell movement in confined spaces, especially for cancer cells. These results suggest that cells actively control its water content. The active regulation of water content is a crucial aspect of cell dynamics. We will discuss a theoretical model of cell pressure/volume control. Implications of this model for active cell dynamics in multi-cellular epithelial sheets will be discussed.

Thursday, March 17, 2016 11:15AM - 2:15PM —
Session S2 GSOFT DFD: Rheology of Dense Particulate Media Ballroom II - Ted Brzinski, North Carolina State University

11:15AM S2.00001 Flow of colloidal suspensions and gels, ROSEANNA ZIA, Cornell University — Our recent studies of yield of colloidal gels under shear show that yield in such gels occurs in distinct stages. Under fixed stress, yield follows a finite delay period of slow solid-like creep. Post yield, the gel fluidizes and may undergo long-time viscous flow or, in some cases, may re-solidify. Under imposed strain rate, the transition from equilibrium to long-time flow is characterized by one or more stress overshoots, signifying a yield process here as well. These rheological changes are accompanied by evolution in morphology and dynamics of the gel network. Similar regimes have been observed in gels subjected to gravitational forcing; the gel initially supports its own weight, or perhaps undergoes slow, weak compaction. This may be followed by a sudden transition to rapid compaction or sedimentation. Various models have been put forth to explain these behaviors based on structural evolution, but this detail is difficult to observe in experiment. Here we examine the detailed microstructural evolution and rheology of reversible colloidal gels as they deform under gravity, identifying the critical buoyant force at which yield occurs, the role played by ongoing gel coarsening, and similarities and differences compared to yield under shear.

We gratefully acknowledge the support of the NSF XSEDE Computational Resource, the NSF Early CAREER Program, and the Office of Naval Research Young Investigator Program.

11:51AM S2.00002 A unified description of the rheology of hard particles, MICHEIL HERMES, University of Edinburgh — No abstract available.

12:27PM S2.00003 Linking Microstructural Changes to Bulk Behavior in Shear Disordered Matter, DANIEL BLAIR, Georgetown University — Soft and biological materials often exhibit disordered and heterogeneous microstructure. In most cases, the transmission and distribution of stresses through these complex materials reflects their inherent heterogeneity. Through the combination of rheology and 4D imaging we can directly alter and quantify the connection between microstructure and local stresses. We subject soft and biological materials to precise shear deformations while measuring real space information about the distribution and redistribution of the applied stress. In this talk, I will focus on the flow behavior of two distinct but related disordered materials; a flowing compressed emulsion above its yield stress and a strained collagen network. In the emulsion system, I will present experimental and computational results on the dynamical response, at the level of individual droplets, that directly links the particle motion and deformation to the rheology. I will also present results that utilize boundary stress microscopy to quantify the spatial distribution of surface stresses that arise from sheared in-vitro collagen networks. I will outline our main conclusions which is that the strain stiffening behavior observed in collagen networks can be parameterized by a single characteristic strain and associated stress. This characteristic rheological signature seems to describe both the strain stiffening regime and network yielding.

NSF DMR: 0847490

1:03PM S2.00004 Nonlinear and nonlocal rheology of jammed matter, BRIAN TIGHE, TU Delft — Emulsions, foams, and grains all jam into a weakly elastic state when confined by pressure. By now the mechanics of jammed matter is well understood in the case of slow, weak, and homogeneous forcing — but in reality, it is rare for all of these assumptions to hold. Here we demonstrate the complex rheology that results when jammed materials are forced at finite rate, finite amplitude, and finite wavelength. Using computer simulations, we subject dense soft sphere packings to a host of rheological tests, including stress relaxation, flow start-up, oscillatory shear, and standing wave forcing. These allow us to tease apart the influence of viscous, nonlinear, and nonlocal effects, and also to probe the link between particle dynamics and bulk response. We identify strain, time, and length scales that depend critically on the distance to the jamming transition, and which govern the onset of shear thinning, strain softening, and gradient elasticity.

1:39PM S2.00005 Effects of confinement on nanoparticle flows, JACINTA CONRAD, University of Houston — The transport properties of nanoparticles that are dispersed in complex fluids and flowed through narrow confining geometries affect a wide range of materials shaping and forming processes, including three-dimensional printing and nanocomposite processing. Here, I will describe two sets of experiments in which we use optical microscopy to probe the structure and transport properties of suspensions of particles that are confined geometrically. First, we investigate the structure and flow properties of dense suspensions of submicron particles, in which the particles interact via an entropic depletion attraction, that are confined in thin films and microchannels. Second, we characterize the transport properties of nanoparticles, dispersed at low concentration in water or in aqueous solutions of high-molecular weight polymers, that are confined in regular arrays of nanoposts or in disordered porous media. I will discuss our results and their practical implications for materials processing as well as for other applications that require confined transport of nanomaterials through complex media.

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Thursday, March 17, 2016 2:30PM - 4:18PM —
Session V53 DFD: Fluid Mechanics - General Hilton Baltimore Holiday Ballroom 4
2:30PM V53.00001 Equivalence of Non-Equilibrium Ensembles and Representation of Friction in Turbulent Flows: The Lorenz 96 Model, VALERIO LUCARINI, University of Hamburg, Hamburg, Germany, GIOVANNI GALLAVOTTI, Sapienza University of Roma — We construct different equivalent non-equilibrium ensembles in the Lorenz ’96 model of atmospheric turbulence. The vector field can be decomposed into an energy-conserving, time-reversible part, plus a non-time reversible part, including forcing and dissipation. We construct a modified version of the model where viscosity varies with time, so that energy is conserved, and the dynamics is time-reversible. The statistical properties of the irreversible and reversible model are in excellent agreement, if in the latter the energy is kept constant at a value equal to the time-average realized with the irreversible model. The average contraction rate of the phase space of the time-reversible model agrees with that of the irreversible model, where it is constant by construction. We show that the phase space contraction rate obeys the fluctuation relation, and we interpret its finite time corrections. A local version of the fluctuation relation is explored and successfully checked. The equivalence between the two ensembles extends to the Lyapunov exponents. These results have relevance in motivating the importance of the chaotic hypothesis. In explaining that we have the freedom to model non-equilibrium systems using different but equivalent approaches.

2:42PM V53.00002 Optimum design of vortex generator elements using Kriging surrogate modelling and genetic algorithm, RITHWIK NEELAKANTAN, RAMAN BALU, ABHINAV SAJI, Ace College of Engineering — Vortex Generators (VGs) are small angled plates located in a span wise fashion aft of the leading edge of an aircraft wing. They control airflow over the upper surface of the wing by creating vortices which energise the boundary layer. The parameters considered for the optimisation study of the VGs are its height, orientation angle and location along the chord in a low subsonic flow over a NACA0012 airfoil. The objective function to be maximised is the L/D ratio of the airfoil. The design data are generated using the commercially available ANSYS FLUENT software and are modelled using a Kriging based interpolator. This surrogate model is used along with a Genetic Algorithm software to arrive at the optimum shape of the VGs. The results of this study will be confirmed with actual wind tunnel tests on scaled models.

2:54PM V53.00003 Predicting the Noise of High Power Fluid Targets Using Computational Fluid Dynamics, MICHAEL MOORE, Jefferson Lab, Old Dominion University, SILVU COVRGB DUSA, Jefferson Lab — The 2.5 kW liquid hydrogen (LH2) target used in the $Q_{\text{weak}}$ parity violation experiment is the highest power LH2 target in the world and the first to be designed with Computational Fluid Dynamics (CFD) at Jefferson Lab. The $Q_{\text{weak}}$ experiment determined the weak charge of the proton by measuring the parity-violating elastic scattering asymmetry of longitudinally polarized electrons from unpolarized liquid hydrogen at small momentum transfer ($Q^2 = 0.025$ GeV$^2$). This target satisfied the design goals of < 1% luminosity reduction and < 0.5% contribution to the total asymmetry width (the $Q_{\text{weak}}$ target achieved 2% or 55ppm). State of the art time dependent CFD simulations are being developed to improve the predictions of target noise on the time scale of the electron beam helicity period. These predictions will be bench-marked with the $Q_{\text{weak}}$ target data. This work is an essential component in future designs of very high power low noise targets like MOLLER (5 kW, target noise asymmetry contribution < 25 ppm) and MESA (4.5 kW).

3:06PM V53.00004 Fluid Dynamical Consequences of Current and Stress-Energy Conservation, DILLON SCOFIELD, Dept Physics, Oklahoma State University, PABLO HUQ, College of Earth, Ocean, and Environment, Univ. Delaware — The dynamical consequences of fluid current conservation combined with the conservation of fluid stress-energy are used to develop the geometrodynamical theory of fluid flow (GTF). In the derivation of the GTF, we highlight the fact the continuity equation, equivalently the conservation of current density, implies the existence of the fluid dynamical vortex field. The vortex field transports part of the stress-energy; the other part of the stress-energy is transported by the fluid inertia field. Two channels of energy dissipation are determined by the GTF. One is an analog of the Joule heating found in electrodynamics. This follows from the conservation of stress-energy. The other dissipation channel arises from mechanisms leading to complex-valued constitutive parameters described in the electrodynamical analogy as due to a lossy medium. The dynamical consequences of the continuity equation, combined with the conservation of total stress-energy, then lead to a causal, covariant, theory of fluid flow, consistent with thermodynamics for all physically possible flow rates.

3:18PM V53.00005 The Geometry and Dynamics of a Propagating Front in a Chaotic Flow Field, MARK PAUL, Virginia Tech — There are many important problems regarding transport in complex fluid flows with implications in science, nature, and technology. Examples include the combustion of pre-mixed gases in a turbulent flow, the complex patterns of reagents in a chemical system, the spread of a forest fire, and the outbreak of an epidemic. This talk explores the transport and dynamics of a reacting species in a chaotic fluid flow field. Large-scale parallel numerical simulations are used to explore the dynamics of propagating fronts in complex three-dimensional time-dependent fluid flows for the precise conditions of the laboratory. It is shown that a chaotic flow field enhances the front propagation when compared with a purely cellular flow field. This enhancement is quantified by computing measures of the spreading rate of the products and by quantifying the complexity of the three-dimensional front geometry for a range of chaotic flow conditions.

3:30PM V53.00006 Surface Acoustic Wave Transport and Mixing in Fluids in an Enclosed Nanoslit, MORTEZA MIANSARIGAVZAN, JAMES FRIEND, University of California, San Diego — Non-laminar fluid flow was generated in a nanoslit combining a 128 MHz surface acoustic waves. A novel acoustic nanofluidic device was fabricated by a unique room-temperature, high-strength bonding method combining a 128-YX lithium niobate (LN) substrate with a second LN substrate containing a 1-cm long, 50-300-nm thick, 400 μm-wide planar nanoslit. The nanoslit was verified to be extremely smooth (roughness < 5 nm) and possess a uniformly rectangular shape. Despite an exceptionally low (~ 10^-5) hydrodynamic Reynolds number within the nanoslit, acoustic streaming induced by the SAW is found to drive filling of the hydrophilic nanoslit of fluid, induce rapid mixing of fluid within, and drive nanoparticle and early evidence of molecular separation from the fluid at the nanoslit exit as the fluid passes through. The unique physical phenomena may prove to be useful across a broad range of applications where it facilitates the use of nanofluidics in chemistry and medicine. It illuminates an extraordinary ability to use sound at ever smaller scales to manipulate fluids and particles within in unexpected ways.

3:42PM V53.00007 Electroosmotic Entry Flow with Joule Heating Effects, RAMA PRABHAKARAN, AKSHAY KALE, XIANGCHUN XUAN, Clemson University — Electrokinetic flow, which transports liquids by electroosmosis and samples by electrophoresis, is the transport method of choice in microfluidic chips over traditional pressure-driven flows. Studies on electrokinetic flows have so far been almost entirely limited to inside microchannels. Very little work has been done on the electroosmotic fluid entry from a reservoir to a microchannel, which is the origin of all fluid and sample motions in microchips. We demonstrate in this talk that strong vortices of opposite circulating directions can be generated in electroosmotic entry flows. We also develop a two-dimensional depth-averaged numerical model of the entire microchip to predict and understand the fluid temperature and flow fields at the reservoir-microchannel junction.
3:54PM V53.00008 Accounting for anomalous energy-dissipation in guided flows, PABLO HUQ, College Earth, Ocean, and Environment, Univ. Delaware, DILLON SCOFIELD, Dept. of Physics, Oklahoma State University — The Navier-Stokes theory significantly underestimates energy-dissipation in time-dependent flows through flow guides such ones with helical geometry. We show the geometrodynamical theory of fluids (GTF) accounts for this anomalous energy-dissipation by predicting the excitation of transverse modes of flow leading to such dissipation. According to the GTF, the transverse modes are composed of vorticity and swirl fields which together constitute a vortex field F which is a function of the swirl and vorticity fields. Analysis shows the energy-dissipation depends on the wave energy, the dot product of the swirl and the vorticity, as well as their cross product. These lead to heating of the fluid at a rate proportional to the work the current does against the swirl field. For the constitutive parameters of the theory we find the values for water to be \( \lambda = 0.01/(\text{cm/s}) \), and \( \kappa = 1 \) [unitless]. A lower bound for the effective value of the speed of the first transverse modes is found to be 90 cm/sec. We determine that a dimensionless vortex number, \( R_v \), usefully delineates the excitation of the transverse mode flow regime.

4:06PM V53.00009 Effect of Curvature Parameter on Non-Darcy Mixed Convective Flow in a Vertical Annulus: A LTNE Approach, MOUMITA BHOWMIK, PREMANANDA BERA, Indian Institute of Technology Roorkee — The influence of curvature parameter on fully developed mixed convective flow in a vertical annulus filled with porous medium under local thermal non-equilibrium (LTNE) state has been addressed here. Since the curvature parameter \( C \) describes the size of the enclosure, therefore the main emphasize is given to understand its impact on other controlling parameters. Based on computational results, \( C \) has a significant impact on both heat transfer rate as well as flow profiles for stably stratified flow. It has a tendency to reduce the magnitude of the maximum velocity. It is also observed that depending on other parameters, increment in \( C \) may have tendency to make the velocity profile free from back flow. The heat transfer rate is obtained maximum at a small value of \( C \) which is independent of media permeability and converges asymptotically on increasing \( C \). At the end, the linear stability analysis based on normal mode technique has been used to verify the results obtained from basic flow study. Overall, from both basic flow as well as linear stability results, it is found that increment in \( C \) makes the flow profile smooth which means \( C \) has tendency to stabilize the flow.