

**Tentative Schedule for the 14<sup>th</sup> Mid-Atlantic Soft Matter workshop**  
Georgetown University, Institute for Soft Matter Synthesis and Metrology I(SM)<sup>2</sup>  
January 16, 2015

**8:30 am**

Registration and Breakfast

**8:50 am**

Opening Remarks

**9:00 am**

Emanuela Del Gado (Georgetown University):

*Assembly of nano-objects at liquid interfaces: crowding, ordering and rearranging at the interface upon out-of-equilibrium adsorption*

**9:50 am**

Sound-bite Session I

**10:10 am**

Coffee Break

**10:30 am**

Clare Waterman (National Institutes of Health):

*The molecular clutch that drives cell migration*

**11:20 am**

Sound-bite Session II

**12:00 pm**

Lunch

**1:20 pm**

Tom Lubensky (University of Pennsylvania):

*Isostatic Lattice: From Jamming to Topological Surface Phonons*

**2:10 pm**

Sound-bite Session III

**2:40 pm**

Break

**3:00 pm**

Kalman B. Migler (National Institute of Standards and Technology):

*Kinetics of Early Stage Crystallization of Polyethylene as Probed by Raman Spectroscopy*

**3:50 pm**

Sound-bite Session IV

**4:20 pm**

Break

**4:40 pm**

Piotr Habdas (St. Joseph's University):

*Collective particle motion in dense colloidal suspensions*

**5:30 pm**

End of Workshop

**Emanuela Del Gado**, Georgetown University

*Assembly of nano-objects at liquid interfaces: crowding, ordering and rearranging at the interface upon out-of-equilibrium adsorption*

The adsorption at liquid interfaces is a powerful way to drive the self-assembly of nanoparticles because the adsorbed objects can still move and rearrange to form various 2-dimensional structures. Applications range from nano-porous filtering devices to nano-scale sensors. When high coverages and relatively fast self-assembly of the particle-laden interface needs to be achieved, the emerging dynamics of the objects at the interface may affect the adsorption kinetics and the final patterns.

To address these issues we have developed a numerical approach that, in spite of a few simplifications, allows us to account for the irreversible nature of the adsorption process, to follow the adsorption kinetics and to elucidate its interplay with the particle dynamics at the interface. Inspired by a series of experiments on core-shell nanoparticles at oil-water and air-water interfaces, our numerical studies have shown that, in presence of soft repulsive interactions, the adsorption may be slowed down by the crowding of the particles at the interface and that the adsorption kinetics and/or the size polydispersity can be used to tune the degree of ordering and the amount of defects at the interface. We have computed the effective interactions at the interface for polymer shell nanoparticles, as a function of the solvent quality, we have started to gain new insight into the role of hydrodynamic interactions, and analyzed the effect of the out-of-equilibrium adsorption in the assembly of protein fibrils at air-water interfaces.

**Clare Waterman**, NIH/NHLBI

*The molecular clutch that drives cell migration*

TBA

**Tom Lubensky**, University of Pennsylvania

*Isostatic Lattice: From Jamming to Topological Surface Phonons*

Frames consisting of nodes connected pairwise by rigid rods or central-force springs, possibly with preferred relative angles controlled by bending forces, are useful models for systems as diverse as architectural structures, crystalline and amorphous solids, sphere packings and granular matter, networks of semi-flexible polymers, and protein structure. The rigidity of these networks depends on the average coordination number  $z$  of the nodes: If  $z$  is small enough, the frames have internal zero-frequency modes, and they are floppy; if  $z$  is large enough, they have no internal zero modes and they are rigid. The critical point separating these two regimes occurs at a rigidity threshold, which corresponds closely to what is often referred to as the isostatic point, that for central forces in  $d$ -dimensions occurs at coordination number  $z_c = 2d$ . At and near the rigidity threshold, elastic frames exhibit unique and interesting properties, including extreme sensitivity to boundary conditions, power-law scaling of elastic moduli with  $(z - z_c)$ , and diverging length and time scales.

This talk will explore elastic and mechanical properties and mode structures of model periodic lattices, such as the square and kagome lattices with central-force springs, that are just on verge of mechanical instability. It will discuss the origin and nature of zero modes of these structures under both periodic (PBC) and free boundary conditions (FBC), and it will derive general conditions [1] (a) under which the zero modes under the two boundary conditions are essentially identical and (b) under which phonon modes are gapped with no zero modes in the periodic spectrum but include zero-frequency surface Rayleigh waves in the free spectrum. In the former situation, lattices are generally in a type of critical state that admits states of self-stress in which there can be tension in bars with zero force on any node, and distortions away from that state give rise to surface modes under free boundary conditions whose degree of penetration into the bulk diverges at the critical state.

The gapped states have a topological characterization, similar to that of topological insulators, that define the nature of zero-modes at the boundary between systems with different topology.

[1] K. Sun, A. Souslov, X. M. Mao, and T.C. Lubensky, PNAS 109, 12369-12374 (2012).

[2] C.L. Kane and T.C. Lubensky, Nature Physics 10, 39-45 (2014)

**Kalman B. Migler**, NIST/MS&E

*Kinetics of Early Stage Crystallization of Polyethylene as Probed by Raman Spectroscopy*

The kinetic pathway by which a molten polymer transforms into a multi-length scale semi-crystalline structure upon cooling is an unsolved problem in polymer physics, yet it is critical to the processing, properties and ultimate performance of these materials. Here we utilize Raman spectroscopy to probe the early stage crystallization kinetics of a high-density polyethylene during low undercooling and shear. The importance of Raman as a tool stems from its ability to measure the mass fraction of conformations that are in consecutive trans sequences (locally straight) but are not in an orthorhombic configuration, which we demonstrate on the n-alkane, C<sub>21</sub>H<sub>44</sub>. We then apply this concept to early stage crystallization of polyethylene and find that the Raman peaks indicative of this local non-orthorhombic chain straightening precede the appearance of the peak which indicates orthorhombic crystallinity. We analyze the spectra within the context of a three-state model to extract the mass fractions of the orthorhombic and the non-orthorhombic continuous-trans (NOCT) states as crystallization proceeds. Concomitant birefringence and turbidity measurements indicate that this NOCT state can be understood as a separate mesomorphic phase which emerges from the melt state and precedes crystallization.

**Piotr Habdas**, St. Joseph's University

*Collective particle motion in dense colloidal suspensions*

The viscosity of a glass-forming liquid diverges when its temperature is lowered. This divergence is typically attributed to emerging domains of particles that move in a correlated fashion. The size and shape of these cooperative rearrangement regions are thought to be closely related to the macroscopic properties of glasses. Moreover, the presence of cooperative motion of molecules or particles across a wide range of disordered molecular matter has prompted search for universal explanations of glass formation. However, some properties of glasses depend on the details of constituent interparticle potentials. For example, repulsive colloidal glasses form when the packing fraction of particles with a hard-sphere interparticle potential is made sufficiently large. Whereas, an addition of a small short-range attraction to particle potential in a repulsive glass leads to the formation of attractive glasses, which exhibit many new properties. Exploration of the similarities and differences between glasses composed of particles with attractive versus repulsive interactions could help to reveal universal aspects of the glass transition and could lead to development of new methods for manipulating properties of glassy materials.

In this talk I will report on our studies of colloidal particle dynamics in a model glass system as the sample evolves from a hard-sphere glass to a system with attractive interparticle interactions. The transition from the repulsive glass to attractive systems is induced by short-range depletion forces. We use confocal microscopy to study colloidal suspensions with single-particle resolution. The dynamical and structural behaviors of the resulting colloidal suspensions will be discussed.

## Soundbite Talks: *MASM 14*

### *Session I*

1. Lauren Graham (Royal Society of Chemistry)  
*Greetings from 'Soft Matter' at the RSC*
2. Joel Clemmer (Johns Hopkins University)  
*Critical scaling with strain rate in overdamped sheared disordered solids*
3. Sebastian Hurtado Parra (Saint Joseph's University)  
*Active microrheology of dilute Brownian colloidal suspensions*
4. SangHo Jee (University of Maryland)  
*Encapsulation of Hydrophobic Dyes as Model Drugs in Hybrid Assemblies of Inorganic Nanoparticles*
5. Mohan Zhang (Georgetown University)  
*Correlations of Gelation Abilities and Structures of Dihydroxylated Derivatives of Long-chained and Unsaturated Fatty Acids*
6. Zoey Davidson (University Of Pennsylvania)  
*Liquid Crystals in Cylindrical Confinement with a Symmetry Breaking Twist*
7. Bob Leheny (Johns Hopkins University)  
*Echoes in x-ray speckles track nanometer-scale plastic events in concentrated colloidal gels under shear*

### *Session II*

1. Anthony Kotula (NIST)  
*Polyethylene crystallization during shear probed by Raman spectroscopy*
2. Peter Olmsted (Georgetown University)  
*Spontaneous curvature in polar chiral filaments near surfaces*
3. Tingting Li (Georgetown University)  
*Creating Charge Transfer Nano Co-crystals using Reprecipitation*
4. Tristan Sharp (Johns Hopkins University)  
*Loss of Superlubricity in Elastic Single-Asperity Contacts*
5. Thomas Rosch (NIST)  
*NIST's Chemical Workbench: Application to Coarse-Grained Simulations of Crystallization*
6. Teresa Duncan (Georgetown University)  
*Poly(vinyl acetate)-Borate Networks with Glycol Ethers for Cleaning Objects of Cultural Heritage*

7. Matt Harrington (University of Maryland)  
*Characterizing arbitrary 3D particle-scale rotations in granular flows*
8. Takuma Hoshino (Tokyo Metropolitan University)  
*Correlated phase separation in stacked membranes*
9. Axel Stuermer (Georgetown University)  
*Measuring the mechanical properties of keratin/actin composite networks*
10. Thomas C. O'Connor (Johns Hopkins University)  
*AIREBO-M: A reactive model for hydrocarbons at extreme pressures*
11. Mehdi Bouzid (Georgetown University )  
*Non-local rheology of dense granular flows*
12. Doug Godfrin (University of Delaware)  
*Influence of Clusters on Dynamics and Viscosity*
13. Debra Audus (NIST)  
*Interplay of Isotropic and Directional Interactions in a Spot Model of Proteins*

### *Session III*

1. Eleni Katifori (UPenn)  
*Folding of naturally curved shells*
2. Brian Utter (James Madison University)  
*Erosion and flow of hydrophobic granular materials*
3. Richard Wool (University of Delaware)  
*Does Entangled Polymer Soft Matter become Harder or Softer in Nanoconfinement?*
4. Sudeep Dutta (Georgetown University)  
*Droplet Motion in a Flowing Emulsion*
5. Marguerite Braun (Georgetown University)  
*Dynamics of Entangled DNA*
6. Matthew Hartings (American University)  
*Gold nanoparticles trapped in fibers of unfolded proteins: Hydrophilic proteins show a higher propensity for aggregation than hydrophobic proteins*
7. Yan Zhang (Georgetown University)  
*Ultrasound-responsive gelation*
8. Zhongyu Mou (Georgetown University)  
*Aggregation modes on a series of Phenalenyls*
9. Paul Salipante (NIST)  
*Model colloid system for interfacial kinetics*

## *Session IV*

1. Chen Zhao (Department of Physics)  
*Effect of molecular weight on particle formation in nanoprecipitation*
2. Michelle Calabrese (University of Delaware)  
*The rheology and microstructure of branched micelles under shear*
3. Zachery Brown (Saint Joseph's University )  
*Achieving a Homogeneous Mixture in Dense Colloidal Suspensions*
4. John Kerin (Georgetown University)  
*Effects of Finite Temperature on a Model Colloidal Gel Network Under Oscillatory Shear*
5. Claudio Resta (Universit di Pisa, Georgetown University)  
*Design and Investigation of new Amino Acid Functionalized Conjugated Polymers*
6. Stephanie Lam (NIST)  
*Characterization of Complex Solution-Nanotube Interfaces using AUC and SANS*
7. Jingjing Li (Georgetown University)  
*Effects of Salt on the Gelation Mechanism of Hydrogels*
8. Elizabeth Kelley (NIST)  
*Probing the structure and dynamics of lipid bilayers using neutron scattering*
9. Lin Guo (Johns Hopkins University)  
*Boundary Condition for Fluid Flow at curved Surfaces*
10. Rana Ashkar (NIST/UMD)  
*Peering into polymer dynamics in carbon nanocomposites*