

**Schedule for the 16<sup>th</sup> MASM: The Mid-Atlantic Soft Matter Workshop**  
The National Institutes of Health, Bethesda, MD  
January 29, 2016

**8:20 am**

Registration and Light Refreshments

**8:45 am**

Opening Remarks

**8:50 am**

Carole Parent (NIH/NCI):

*Live imaging of signal relay during chemotaxis and its relevance to inflammation*

**9:40 am**

Sound-bite Session I

**10:25 am**

Coffee Break

**10:40 am**

Clifford Brangwynne (Princeton University):

*Measuring the intracellular dew point: phase transitions in cells*

**11:30 am**

Sound-bite Session II

**12:15 pm**

Lunch

**1:30 pm**

Eleni Katifori (University of Pennsylvania):

*The evolution of efficient fluid flow*

**2:20 pm**

Sound-bite Session III

**3:05 pm**

Break

**3:20 pm**

Darrin Pochan (The University of Delaware):

*Material Construction through Peptide Solution Assembly*

**4:10 pm**

Sound-bite Session IV

**4:55 pm**

Break

**5:05 pm**

Kenneth Yamada (NIH/NIDCR):

*Cell, Tissue, and Matrix Dynamics in Three-dimensional Environments*

**5:55 pm**

End of Workshop

**Carole Parent**, NIH/NCI

*Live imaging of signal relay during chemotaxis and its relevance to inflammation*

The property of sensing and initiating directional migration in response to external cues is a fundamental property of biological systems. My research program aims to understand how cells detect and respond to external chemotactic signals and, in particular, how the spatial and temporal relay of chemotactic signals between cells impact single and group cell migration. The cornerstone of our approach to studying this paradigm is the tagging of signaling protein effectors with the green fluorescent protein (GFP) to visualize where, when and how relevant cascades are activated in live cells. Along with several other experimental tools, the outcome of our live imaging efforts led us to propose novel mechanisms to explain how chemotactic gradients are transduced and amplified in simple and complex biological settings. Our studies of chemotaxis involve three distinct model systems with complementary virtues: the social amoebae *Dictyostelium discoideum*, mammalian neutrophils, and breast cancer metastatic cell lines. In addition to combining biochemical, cell biological and genetic approaches, we benefit from a long-standing collaboration with physicists to quantitatively describe the movements, with single cell resolution, of large groups of cells, and extract metrics that are relevant to the biological responses being studied. Our findings provide insight into understanding signal transduction pathways in complex physiological settings, and directly translate to clinically important processes such as inflammation, immune responses, tissue repair, and cancer metastasis.

**Clifford Brangwynne**, Princeton University

*Measuring the intracellular dew point: phase transitions in cells*

Increasing evidence suggests that phase transitions play an important role in the internal organization of living cells. We have shown

that a number of membrane-less RNA and protein rich organelles, known as RNP bodies, represent condensed liquid phase droplets, which assemble by liquid-liquid phase separation. The nucleolus is a liquid-like nuclear body, which plays an important role in cell growth and size homeostasis. Using the reductive cell divisions of early *C.elegans* embryos, we show that a simple phase threshold model explains striking features of the intrinsic coupling of nucleolar assembly to cell size. Building on these findings, we develop a Cahn-Hilliard model for nucleolar liquid-liquid phase separation, which can quantitatively account for the dynamics of nucleolar assembly, for both an in vitro reconstituted system, and within living cells. We use a custom microfluidics platform to test these models in growing *C.elegans* worms, where we find that the nucleolus grows proportional to cell and organism growth. Concentration-dependent phase transitions allow the cell to read-out its size, and could provide a novel biophysical feedback mechanism for cell growth control.

**Eleni Katifori**, The University of Pennsylvania

*The evolution of efficient fluid flow*

Complex life above a certain size depends on a circulatory system for oxygen and nutrient delivery. The size of organisms relying exclusively on molecular diffusion to deliver oxygen to their body is severely limited: by diffusion alone, oxygen would not be able to travel more than  $100\mu\text{m}$  in the tissue. Both plants and animals have developed circulatory systems of striking complexity to solve the problem of nutrient delivery and waste removal.

Typically, the circulatory system has to satisfy competing demands: minimizing building costs and the amount of veins created, and maximizing efficiency in transport but also ensuring robustness to damage and the ability to operate under fluctuating demands. These competing demands have resulted in complex and heterogeneous vascular structures that exhibit evolutionary adaptations that span several orders of magnitude in size, from the detailed anatomy of each individual vessel to the overall topology of the whole network. In this talk we will present and discuss some

specific examples where these adaptations become evident. First, using fluid flow simulations we explore the adaptive advantage of the secondary wall thickenings of individual xylem vessels in plants and their effect on sap flow. Then, using laminar flow network simulations, we investigate plant strategies for the connectivity of individual xylem vessels in the vascular bundle and of individual veins in the whole leaf. Finally, in an example more relevant to animal vascular systems, we show how simple local adaptive rules produce a network that is optimally connected.

**Darrin Pochan**, The University of Delaware

#### *Material Construction through Peptide Solution Assembly*

Self-assembly of molecules into materials is an attractive materials construction strategy primarily due to its simplicity in application. By considering properly designed peptidic molecules in the bottom-up materials solution assembly process, one can take advantage of inherently biomolecular attributes; intramolecular folding events, secondary structure, and electrostatic interactions; in addition to more traditional self-assembling molecular attributes such as amphiphilicity, to define hierarchical material structure and consequent properties. Additionally, computational tools are being developed to aid in molecule design for the formation of desired, predetermined nanostructure so that one can take advantage of the vast complexity possible with peptide primary structure. We are using biomimicry and theory-guided design to create new soft matter through peptide self-assembly in solution.

First, a class of beta-sheet molecules that form robust, nanofibrillar network hydrogels will be discussed. The local nanostructure control is realized through proper peptide molecule design as well as desired solution assembly pathway. One-dimensional fibril growth is accomplished with the designed beta-hairpin peptides with hinges in the assembling peptide molecules being manifested in the supramolecular fibril structure. If properly designed, hydrogel networks can be formed from the peptide assembly. Examples of nanostructure control as well as control of overall hydrogel network structure, and

resultant shear-thinning and rehealing viscoelastic and cell-level biological properties, will be presented. In addition, peptide fibrils can be used to template the growth of inorganic materials as well as the assembly of inorganic nanoparticles.

Second, theoretical efforts afford the construction of arbitrary peptide nanostructures not observed in natural proteins. Initial examples of targeted materials include two-dimensional sheets with targeted, non-natural, symmetry of peptide packing within the sheets. Initial experimental results of the theory-defined sequences and the subsequent nanostructures formed through solution assembly will be presented.

Cryo transmission electron microscopy (cryoTEM), transmission electron microscopy (TEM), small angle neutron or x-ray scattering (SANS, SAXS), atomic force microscopy, oscillatory rheology, and spectroscopy have all been used to characterize the nano-through-microstructure and material properties of the above self-assembled systems and will be included in the presentation.

**Kenneth Yamada**, NIH/NIDCR

#### *Cell, Tissue, and Matrix Dynamics in 3D Environments*

Although numerous studies of cells on regular, flat two-dimensional tissue culture surfaces have provided valuable knowledge about many biological processes, living organisms are three-dimensional (3D). Direct visualization studies of the real-time motility of cells, tissues, and extracellular matrix in 3D environments by new microscopy approaches are providing novel biological insights spanning multiple spatial and temporal scales. On the length scale of matrix fibers and the cell attachments to them termed cell adhesions, features such as local stiffness, elasticity, and cell/matrix movements are important for cell migration. In tissues, cell movements and matrix remodeling are involved in sculpting organs. Visualizing such dynamics by real-time approaches will provide extensive data that can ultimately be used for studies of the roles of physical forces and architecture in cell and tissue motility relevant to embryonic development and cancer.

## Soundbite Talks: *MASM 16*

### *Session I*

1. John J. Williamson (Georgetown University)  
*Flip-flop and symmetry-breaking fields in lipid bilayers*
2. Jin-Song Pei (University of Oklahoma)  
*A New Mathematical Model for Mullins Effect*
3. Yun Liu (NIST/University of Delaware)  
*Investigating protein structures in concentrated solutions*
4. Greg Alushin (NHLBI/NIH)  
*Mechanosensing via Cytoskeletal Strain*
5. Jerome Irianto (University of Pennsylvania)  
*Invasion - Mutation: Cell migration through stiff constrictions causes mutations and damages the nucleus*
6. Hawa Racine Thiam (NIH/NHLBI)  
*Spatiotemporal regulation of cell-ECM adhesions during the cell cycle.*
7. Charlotte Pfeifer (University of Pennsylvania)  
*Segregation of mobile nuclear proteins away from chromatin when the nucleus is constricted*
8. Vikram Rathee (Georgetown University)  
*Shear Thickening using Boundary Stress Microscopy*
9. Javen Weston (Georgetown University - NIST)  
*Deconvolution of  $\mu$ RheoSANS Scattering Data: A Comparison with Traditional RheoSANS*
10. Zoey Davidson (University of Pennsylvania)  
*Finding structural signatures of dynamic heterogeneity with machine learning*
11. Ralph Nossal (National Institutes of Health)  
*Activation Energies Associated with Physiological Processes Indicate Temperature-dependent State Changes in the Lipid Bilayers of Higher Organisms*

### *Session II*

1. Marcus Cicerone (NIST)  
*The nature of relaxation in non-crystalline condensed phase matter*
2. Tamoghna Das (NIST & University of Maryland)  
*Searching for universality in complex fluids*

3. Nathan Mahynski (NIST)  
*Structure-directing soft matter agents: a new paradigm for colloidal assembly*
4. David Green (University of Virginia)  
*Ligand Phase Separation on Nanoparticle Surfaces.*
5. John Royer (NIST)  
*A rheological signature of frictional interactions in shear thickening suspensions*
6. Rachel Lee (University of Maryland)  
*Quantifying Collective Migration during Cancer Progression*
7. Debbie Audus (NIST)  
*Coupling of phase separation and self-assembly in patchy particle solutions*
8. Markus Bleuel (NIST/UMD)  
*USANS at NIST/NCNR*
9. Christina Stuelten (NIH/NCI)  
*LPA converts metastatic breast cancer cells to an epithelial phenotype as evidenced by increased cell directionality, decreased cell speed and increased E-Cadherin membrane staining*
10. Doug Henderson (University of Maryland)  
*Small Angle Neutron Scattering of TEMPO-oxidized Cellulose*
11. Jack Douglas (NIST)  
*Quantifying Collective Motion in Proteins Using Tools Drawn From Glass Physics*

### *Session III*

1. Pinar Gurel (NHLBI, NIH)  
*Direct observation of force-induced conformational transitions in F-actin*
2. Piotr Habdas (Saint Joseph's University)  
*Spatially Heterogeneous Dynamics in Dense Colloidal Suspensions with Short-Range Interparticle Forces*
3. Subhasish Chatterjee (CCNY/CUNY)  
*What can solid-state NMR tell us about fungal melanin assembly?*
4. Meijin Li (Georgetown University)  
*Synthesis and studies of pyrene-substituted poly(isobutylene-alt-maleic anhydride) (Py-PIMA)*
5. Anthony Kotula (NIST)  
*The Rheo-Raman Microscope: Simultaneous Conformational, Rheological and Optical Characterization of Soft Matter*

6. Robert Bradbury (Indiana University)  
*Charge effect on the Viscoelastic Properties of Surfactant Bilayers*
7. Teresa Duncan (Georgetown University )  
*Addition of Glycol Ethers to Poly(vinyl acetate)-Borate Networks for Cleaning Painted Surfaces*
8. Alexandros Chremos (NIST)  
*Clouds of Counter-ions around Polyelectrolytes*
9. Peiran Jin (Georgetown University)  
*A model for structure change of reconstituted fibroin gels in deformation*
10. Pasha Tabatabai (Georgetown University)  
*Protein gelation kinetics near the overlap concentration*
11. Daniel Seeman (NIST/NCNR)  
*Development of micro-RheoSANS at the NIST Center for Neutron Research*

#### *Session IV*

1. Anna Coughlan (Johns Hopkins University)  
*Assembly and Phase Behavior of Magnetic Particles with and without Depletion*
2. Jeffrey Toretzky (Georgetown University)  
*Phase separation in cancer*
3. Hongyu Guo (NIST-NCNR/UDel)  
*A universal method of size selective purification of Nanoparticles*
4. Wei-Shan (NIST)  
*Study Adsorption Properties of Shale Gas in Porous Materials by Small-Angle Neutron Scattering*
5. Yimin Mao (University of Maryland, NIST-NCNR)  
*Crystal Structure Determination of Poly(ethylene furanoate) using X-ray Fiber Diffraction*
6. Xin Zhang (University of Maryland)  
*Cellulose Ionic Liquid Solvents Dissolution and Phase Diagrams*
7. Vishwas V (Georgetown University)  
*Transient shear banding phenomenon in dense emulsions*
8. Mohan Zhang (Georgetown University)  
*Mechano-responsive, Thermo-reversible, Luminescent Organogels Derived from a Long-chained, Naturally-occurring Fatty Acid*

9. zhiyuan wang (NCNR & Tsinghua University)  
*Attraction interaction between colloidal particles in binary solvent of 2,6-lutidine and water*
10. Paul Salipante (NIST)  
*Reversible adsorption kinetics of near surface dimer colloids*
11. Rui Lu (University of Maryland)  
*Thin Films of Blends of Cellulose and Polyacrylonitrile*
12. Matthew Hartings (American University)  
*Protein-based, micrometer-sized ferrogels*