

**Schedule for the 21<sup>th</sup> MASM: The Mid-Atlantic Soft Matter Workshop**  
Institute for Bioscience and Biotechnology Research, Rockville, MD  
February 15, 2019

**8:45 am**

Opening Remarks

**8:50 am**

Enrico Malito (Glaxo Smith Kline):

*Structure-based design and optimization of vaccine candidates*

**9:30 am**

Soundbite Session I

**10:30 am**

Coffee Break

**10:50 am**

Srinivasa Raghavan (University of Maryland):

*Nature-Inspired Multicompartment and Multilayered Structures*

**11:30 am**

Soundbite Session II

**12:20 pm**

Lunch

**1:30 pm**

Amish Patel (University of Pennsylvania):

*Characterizing Protein Hydration to Inform its Interactions*

**2:10 pm**

Soundbite Session III

**3:00 pm**

Coffee Break

**3:20 pm**

Silvia Muro (University of Maryland):

*Parametric Control of Nanocarriers to Optimize Drug Transport Across the Blood-Brain Barrier*

**4:00 pm**

Soundbite Session IV

**4:50 pm**

Coffee Break

**5:05 pm**

Alexander Andrianov (IBBR):

*Self-Assembling Polyphosphazenes and Their Biomedical Applications*

**5:45 pm**

End of Meeting

**Srinivasa Raghavan**, University of Maryland  
*Nature-Inspired Multicompartment and Multilayered Structures*

This talk will describe the design and synthesis of new soft materials inspired by architectures found in nature. In one case, the inspiration comes from the architecture of the eukaryotic cell, which has multiple inner compartments (organelles), each with a distinct function. To mimic this, we have created biopolymer-based multicompartment capsules (MCCs) using an oil-free microfluidic technique. Our approach exploits the electrostatic complexation of oppositely charged polymers dissolved in aqueous media. We can control the overall size of the MCCs, the sizes of the inner compartments, and the number of inner compartments. More importantly, we can encapsulate different payloads in each of the inner compartments, including colloidal particles, enzymes, and microbial cells. A hallmark of biological cells is the existence of cascade processes, where products created in one organelle are transported and used in another. We will show examples of such cascade processes using our MCCs.

Next, we draw inspiration from the multilayered structure of onions, eggs, embryos, and body parts like blood vessels and the spinal disc. Each layer of these structures typically has a unique composition and thereby a distinct function. The synthesis (morphogenesis) of these structures in nature typically proceeds in an inside-out fashion, where a core is formed initially, followed by a first shell and then additional shells. In the same vein, we have developed an inside-out technique to synthesize multilayered polymeric materials. Each polymer shell is an aqueous gel formed by free-radical polymerization. A given shell grows outward from the surface of the previous shell; thus, the shell thickness steadily increases with time and can be controlled. Using this technique, we have synthesized multilayered capsules, tubes, and surfaces. The multilayered tubes exhibit spontaneous changes in tube diameter in response to the properties of the flowing liquid, which is reminiscent of blood vessels.

**Enrico Malito**, GlaxoSmithKline  
*Structure-based design and optimization of vaccine candidates*

Structural biology facilitates the rational design of vaccines by enabling an atomic-level control of their antigenic and immunogenic properties. Recent examples of the impact of structural biology on vaccine design and development are the insights that our group at GSK Vaccines gained from studying the structures of protein antigens of the meningococcal vaccine

4CMenB (*Bexsero*), of the human cytomegalovirus (HCMV) Pentamer and of the respiratory syncytial virus (RSV) pre-fusion F antigens in complex with potentially neutralizing antibodies. By combining 3D structural determination and biophysical methods with computational tools to design engineered molecules containing or displaying desired functionalities, or mutated to enhance stability, we show how structure-based antigen design can be used to identify, generate, and characterize novel vaccine antigens, thus guiding the early stages of high-quality antigen development.

Disclosure: This work was sponsored by GlaxoSmithKline Biologicals SA. Enrico Malito is an employee of the GSK group of companies.

**Amish Patel**, University of Pennsylvania  
*Characterizing Protein Hydration to Inform its Interactions*

The extent to which the inherent structure of water is perturbed by complex molecules, such as proteins, peptides, and surfactants, influences the thermodynamics and the kinetics of their assembly. However, accurately characterizing this perturbation is challenging, because the manner in which proteins disrupt the inherent structure of water depends not only on the chemistry of the underlying protein surface, but also on the precise topographical and chemical pattern displayed by the protein. Nevertheless, understanding the role of water in protein interactions is essential to understanding, predicting, and eventually controlling such interactions, which play a crucial role in the development of therapeutic strategies and in protein separations. In this presentation, I will discuss our recent successes in quantitatively characterizing the disruption of water structure in the hydration shell of proteins, and in using this information to predict the interfaces through which proteins interact with one another and self-assemble. Our approach also informs strategies for optimally modulating protein interactions, and facilitates the design of ligands that will bind to proteins of interest with high affinity and specificity. We hope that these advances will pave the way for the discovery of novel therapeutics that specifically target proteins of interest, and the rational design chromatographic ligands for challenging protein separations.

**Silvia Muro**, University of Maryland

*Parametric Control of Nanocarriers to Optimize Drug Transport Across the Blood-Brain Barrier*

Accessing the brain is key to study its function and pathology, and for diagnostic and therapeutic purposes. Yet, this remains a great challenge due to the blood-brain barrier (BBB). To overcome this, novel nanovehicles are being designed to cross this interface, without much translational success. A prime obstacle is the lack of knowledge on the biological regulation of these devices, as most efforts have been devoted to controlling their chemical and physical properties, otherwise necessary tasks. Research in our group is focused on bridging this gap of knowledge. For this purpose, we have designed model nanovehicles targeted to receptors of the main routes of transcytosis across endothelial barriers (clathrin, caveolae, and cell adhesion molecule -CAM- identified by our lab), to compare their properties and BBB transport ability in cellular and animal models, using fluorescent and radioactive tracers. Engagement of receptors of the three routes by drug nanocarriers coated with targeting antibodies resulted in vesicular transport across the endothelial lining. The CAM pathway, in contrast to clathrin and caveolar routes, was effective across a broad spectrum of carrier sizes and targeting valencies. This is reminiscent of the CAM function, which contributes to transcellular leukocyte migration. We observed this is because the CAM route associates with a precise remodeling of the lipid composition of the endothelial plasmalemma and reorganization of the actin cytoskeleton. Surprisingly, biophysical parameters of the drug carrier which improve binding and uptake by the endothelium not always result in more efficient transcytosis, where an elusive balance must be met in order to optimize transport. As a result of said optimization, therapeutic cargoes such as enzyme for inherited neurodegenerative conditions were delivered to the brain in an active form after intravenous administration in mouse models. Improved delivery of therapeutics across the BBB in vivo illustrates the potential of nanodevices addressed to transcytosis routes as translational tools to improve CNS treatment.

**Alexander Adrianov**, IBBR

*Self-Assembling Polyphosphazenes and Their Biomedical Applications*

Ionic polyphosphazenes represent a distinct class of polyelectrolytes with unique structural characteristics and the ability to undergo hydrolytic degradation under physiological conditions. Their potential applications in life sciences span from immunostimulation and vaccine delivery to biodegradable nanoparticulate encapsulation systems based on ionotropic hydrogels. Many biologically relevant properties of these macromolecules stem from their ability to interact with biological targets on molecular and cellular levels. This presentation summarizes current knowledge on the self-assembly behavior of ionic polyphosphazenes in aqueous solutions and discusses potential role of supramolecular systems in the development of new biomedical applications of these versatile macromolecules.

## Soundbite Talks: *MASM 21*

### *Session I*

1. Doug Henderson (University of Maryland)  
*Structural Ordering in Highly Concentrated Gels of Cellulose and Ionic Liquid*
2. Yu-Jiun (Nate) Lin (University of Delaware)  
*Microfluidic aerosol of viscoelastic hydrocolloids through complex geometries*
3. Niti Agrawal (University of Maryland)  
*Self Assembly of Wormlike Micelles in the Polar Organic Solvents*
4. Chong Shen (Lehigh University)  
*Failures of defining Effective temperature in an active colloidal system*
5. Adrian P. Defante (NIST)  
*The influence of the metal interface on drug formulation stability*
6. Ting-An Chen (Georgetown University)  
*Synthesis and characterization of gels from branched polyethylenimine and carbon dioxide as gellant*
7. Yu-Fan Lee (University of Delaware)  
*Characterizing and Tuning Shear Thickening of Waterborne Titanium Oxide Slurry*
8. Avanish Bharati (NIST)  
*Characterizing the Structure of Complex Soft Materials in Dynamic and Industrially Relevant Environments using  $\mu$ RheoSANS*
9. Xin Zhang (University of Maryland)  
*Oligomeric Cellulose Synthesis and Crystallization*
10. Martyna Habdas (Saint Joseph's University)  
*Effectiveness and localization of novel porphyrin complex on B16 mouse melanoma cells*
11. Louis Poon (Georgetown University)  
*Synthesis and FT-IR characterization of poly(dimethyl)siloxane-based polyelectrolyte complexes*
12. Alexandros Chremos (NIST)  
*Hidden Hyperuniformity in Soft Polymeric Materials*
13. Wengang Zhang (NIST)  
*The Relationship Between Unstable Localized Vibrational Modes and Dynamical Heterogeneity in Glass Formers*
14. So Hyun Ahn (University of Maryland)  
*Single-Step Synthesis of Alginate Microbeads with Polymer Shell*

## *Session II*

1. Abhay Goyal (Georgetown University)  
*Counter-ion and solvent mediated electrostatic interactions*
2. Xiangwen Lai (Georgetown University )  
*Shear thickening of silica rod suspension*
3. Yuyin Xi (University of Delaware)  
*Porous particle gel induced by solvent segregation*
4. Michael Jenkins (Saint Joseph's University )  
*Autonomous Particle Tracking using Neural Networks*
5. Nicholas Posey (NIST)  
*Enhancing Polymer-Protein Interactions*
6. Sai Nikhil Subraveti (University of Maryland)  
*Interfacial polymerization of thermoplastic shells around hydrogels*
7. Girishma Grover (Georgetown University)  
*Mechanical studies on amino-acid based gelator in different solvent system.*
8. Rebecca Fedderwitz (University of Maryland)  
*Functionalized Iron Based Nanoparticle Ink For 3D Printed & Flexible Electronics*
9. Leah Borden (University of Maryland)  
*Electrical Suturing of Polyelectrolyte Hydrogels to Reseal Cut or Damaged Tissues*
10. Andrea Giuntoli (NIST)  
*Universal scaling in shear thinning liquids*
11. Yun Liu (NIST)  
*Colloidal systems with both a short-range attraction and long-range repulsion: phase diagrams, structures, and dynamics*

### *Session III*

1. Debra Audus (NIST)  
*Complex Coacervate Core Micelles*
2. Yimin Luo (University of Delaware)  
*One-step, in-situ simulated drying rheology measurements*
3. Minaspi Bantawa (Georgetown University)  
*The Role of Network Topology in Soft Gels*
4. Rui Zhang (Villanova University)  
*Constant force microrheology*
5. Yimin Mao (UMD/NIST)  
*Furan-2,5-dicarboxylic acid, a promising platform molecule: monomer, polymer, and MOF*
6. Nathan Mahynski (NIST)  
*Symmetry-based discovery of multicomponent colloidal crystals*
7. Danielle Beaupre (Georgetown University)  
*Thiol-Disulfide Exchange as a Means to Redox-Reversible Gels: Design and Synthesis of Small Molecule and Polymer Gelators*
8. Francis Snyder (Saint Josephs University)  
*Microrheology of Colloidal Gels*
9. Samim Ali (NIST)  
*Polyelectrolyte complex: Understanding phase behavior, viscoelasticity and interfacial properties*
10. Joseph JIang (Lehigh University)  
*Stress distribution detection near shear bands*
11. Matan Mussel (NICHD, NIH)  
*Similarities between action potentials and acoustic pulses in lipids*

## *Session IV*

1. Claudia Dessi (Georgetown University)  
*Active microtubules are special active swimmers in rheology fluids*
2. Cesar Torres (University of Maryland)  
*The Role of Catanionic Aggregates on Extending Drug Release from Soft Contact Lenses*
3. Hema Choudhary (University of Maryland)  
*Synthesis of Hemostatic Foams*
4. Feng Jiang (University of Maryland)  
*Supramolecular Luminescent Triblock Copolymer Thermoplastic Elastomer via Metal-Ligand Coordination*
5. Kimberly Dennis (University of Delaware)  
*Characterizing paint drying dynamics and structure development using diffusing wave spectroscopy*
6. Luis Gustavo Duarte (Georgetown University/UNICAMP)  
*A novel benzothiazole-salophen derivative for the assembly of all-solution-processed white organic light-emitting diodes*
7. Leopold Torres (NIST)  
*A Fast and Simple Method to Fabricate Angle-Independent and Transferable Structurally Colored Films*
8. Hojin Kim (University of Delaware)  
*Anisotropic Phononic Bandgaps of Colloidal Crystals*
9. Abhishek Shetty (Anton Paar USA)  
*A lab scale Rheo-SAXS setup for multi-scale characterization.*
10. Mehdi Molaei (University of Pennsylvania)  
*surface pressure and interfacial rheology of soft glassy interfaces*
11. Ryan P. Murphy (NIST)  
*Capillary Rheo-SANS: Measuring the nanostructure and rheology of soft matter at high velocity*