Schedule for the 8th Mid-Atlantic Soft Matter workshop, December 9, 2010

National Institute of Standards and Technology, NIST Center for Neutron Research.

8:15 am

Registration and Breakfast

8:50 am

Opening Remarks (Dan Neumann, Daniel Blair)

9:00 am

Klaus Gawrish (NIH): *Structure and function of G protein-coupled membrane receptors - a topic for soft matter research*

9:40 am

Sound-bite Session I

10:20 am

Coffee Break, K04

10:40 am

Yilong Han (Hong Kong Univ. of Sci. and Tech.): *Glass transitions and solid-solid transitions in colloidal thin films*

11:20 am

Sound-bite Session II

12:00 pm

Lunch

1:20 pm

NCNR tour

2:00 pm

Magdaleno Medina-Noyola (Autonomous Univ. of San Luis Potosi): *Theory of Slow-equilibration and Aging of Glass-forming Liquids*

2:40 pm

Sound-bite Session III

3:20 pm

Break, K04

3:40 pm

Thomas Epps (Univ. of Delaware): *Using Interfacial Manipulations to Generate Functional Materials from Nanostructured Polymers*

4:20 pm

Sound-bite Session IV

5:00 pm

Quick Break

5:10 pm

Gil Toombes (NIST/University of Delaware): *Effects of Neuronal Membrane Geometry on Ion Channel Distribution, Mobility and Activity*

Klaus Gawrish, NIH
Structure and function of G protein-coupled membrane receptors - a topic for soft matter research
G protein-coupled membrane receptors (GPCR) are located in the plasma membrane of cells where they transmit extracellular signals elicited by compounds like neural transmitters, hormones, odorants, or light to the cell interior where they activate GTP-binding proteins (G proteins). This large superfamily of heptahelical molecules comprises receptors for dopamine, serotonin, epinephrine, opioids, and cannabinoids, just to mention a few. The proper function of GPCR is critical for all higher forms of life. GPCR are the known target of over 25% of all pharmaceuticals on the market and of an estimated 60% of all drugs that are currently under development. It has been shown that GPCR require a fluid lipid matrix of proper composition for their function.

My lab conducts structural and functional studies on two reconstituted GPCR of class A, bovine rhodopsin and recombinantly expressed cannabinoid receptor CB2. We investigate GPCR at close to functional conditions, in a fluid lipid matrix with a biologically relevant composition of lipids, with particular emphasis on polyunsaturated lipids as found in brain. There is evidence that neuronal GPCR may require high concentrations of lipids with polyunsaturated hydrocarbon chains for full activation. Lipids with polyunsaturated hydrocarbon chains are distinctly different from saturated and monounsaturated chains in their structure and motional properties, a topic to which studies by neutron scattering have made a major contribution.

Yilong Han, Hong Kong Univ. of Sci. and Tech.
Glass transitions and solid-solid transitions in colloidal thin films
Colloids are excellent model systems for the study of phase transitions. Significant insights about glass transitions have been obtained from experiments on colloidal glasses composed of isotropic particles, but much less effort has been expended to study glasses composed of anisotropic particles. We measured the dynamics of a monolayer of colloidal ellipsoids by video microscopy and revealed that the rotational and translational motions become glassy at different densities; thus an intermediate "orientational glass" with glassy-rotational dynamics and liquid-like translational dynamics has been found. This intermediate phase was predicted to exist in 3D, but has never been observed. Interestingly, the fastest translating and rotating particles are anticorrelated in space. A crossover to a nematic phase for large aspect ratio particles and a crossover to a "rotator" phase for small aspect ratio particles are expected. In the second set of experiment, we studied the nucleation of a solid-solid transition between triangular and square lattices in microgel colloidal thin films. When the mother phase is a crystal, its nonzero strain energy and precursor defects can induce new behaviors in the nucleation process. We observed a surprising two-step nucleation: a liquid nucleus was first generated from a square lattice and then became a solid nucleus with triangular lattice. These results provide new challenges in theory and simulation.

Magdaleno Medina-Noyola, Autonomous Univ. of San Luis Potosi
Theory of Slow-equilibration and Aging of Glass-forming Liquids
The self-consistent generalized Langevin equation (SCGLE) theory of colloid dynamics and dynamic arrest [1,2] has been recently been extended [3] to describe the irreversible evolution of the static structure factor and of the intermediate scattering function of a liquid in response to changes in the external macroscopic control parameters. This non-equilibrium theory has been applied to the description of the aging processes occurring in a suddenly quenched model colloidal liquid with hard-sphere plus short-ranged attractive interactions, whose structure and dynamics evolve irreversibly from the initial conditions before the quench to a final, dynamically arrested state [4]. Here we also apply the same theory to the description of the slow dynamics of incompletely equilibrated glass-forming liquids. For this, we consider the equilibration process of a hard-sphere fluid prepared in a non-equilibrium state with the desired final volume fraction phi but with a prescribed non-equilibrium static structure factor $S_o(k;\phi)$ different from the equilibrium structure factor $S_{eq}(k;\phi)$. The evolution of the alpha-relaxation time tau(k)

and of the long-time self-diffusion coefficient D_L as a function of the evolution time t_w is then monitored for an array of volume fractions. For a given waiting time the plot of tau(k;t_w,ϕ) as a function of phi exhibits two regimes corresponding to samples that have fully equilibrated within this waiting time $\phi < \phi_c(t_w)$ and to samples for which equilibration is not yet complete $\phi > phi_c(t_w)$. This two-regime scenario is observed in molecular dynamics simulations of incompletely equilibrated hard-sphere. In soft-sphere systems a similar scenario is also found to occur as a function of the pressure-to-temperature ratio.

[1] R. Juarez-Maldonado, P.E. Ramirez-Gonzalez, M. A. Chavez-Rojo, and M. Medina-Noyola, Phys. Rev. E 76 (2007) 062502.

[2] L. E. Sanchez-Diaz, A. Vizcarra-Rendon, and R. Juarez-Maldonado, Phys. Rev. Lett. 103, 035701 (2009).

[3] P. Ramirez-Gonzalez and M. Medina-Noyola, J. Phys.: Condens. Matter 21 (2009) 504103; ibid Phys. Rev. E 82, 061503 (2010).

[4] P. Ramirez-Gonzalez and M. Medina-Noyola, Phys. Rev. E 82, 061504 (2010).

Thomas Epps, Univ. of Delaware

Using Interfacial Manipulations to Generate Functional Materials from Nanostructured Polymers

As future technological progress necessitates the design and control of nanoscale devices, new methods for the facile creation of smaller features must be discovered. One sub-class of soft material, block copolymers, provides the opportunity to design materials with attractive chemical and mechanical properties based on the ability to assemble into periodic structures with nanoscale domain spacings. To employ block copolymers in many applications, it is essential to understand how interfacial energetics influence copolymer morphologies. Two areas of recent research in the group involve: (1) probing the effects of interfacial composition on block copolymer self-assembly using tapered block copolymers, and (2) generating gradient substrate and "free" surfaces for thin films block copolymer studies. In the first area, we are manipulating the interfacial region between blocks to control ordering transitions in tapered diblock copolymers and triblock copolymers. As an example of recent work, our normal and inverse tapered diblock copolymers show measurable decreases in the order-disorder transition temperature (TODT) relative to the corresponding non-tapered diblock copolymers; with the inverse tapered materials showing the greatest deviation in TODT. In the second area, we are manipulating polymer thin film interfacial interactions using discrete gradient methods to control the free surface interactions, and gradient arrays of assembled monolayers to influence the substrate surface interactions. In particular, our chlorosilane monolayer gradients and solvent vapor gradients permit rapid screening of the surface/polymer interactions necessary to induce the desired nanostructure orientations in many block copolymer systems.

Gil Toombes, NIST/University of Delaware

Effects of Neuronal Membrane Geometry on Ion Channel Distribution, Mobility and Activity

Neuronal activity depends upon the precise localization and concentration of a multitude of ion channel and receptor types, yet the individual molecules are surprisingly mobile. How do neurons modulate receptor diffusion to control synaptic strength? Could the high curvature of synaptic and dendritic membranes influence channel distribution or activity? To isolate the role of neuronal membrane geometry, we developed a biomimetic system based on cell-sized Giant Uni-lamellar Vesicles (GUVs) containing voltage-gated ion channels. With the GUV body acting as the neuronal "soma", an "axon" was formed by extracting a membrane tube from the GUV. Single particle tracking was then used to measure the diffusion of individual ion channels in the tubular membrane. Channels moved more slowly in membrane tubes with smaller radii (up to a 5-fold slowdown) and this reduced mobility was consistent with a hydrodynamic theory that extends the Saffman and Delbruck model to cylindrical geometries. Work is ongoing to understand how membrane curvature, composition and tension influence ion channel distribution and activity.

Soundbite Talks: *MASM8*

Session I

1. Sarah Mastroianni (University of Delaware)
   Nanostructured photovoltaic materials using block copolymer assemblies
2. Kerstin Nordstrom (University of Maryland)
   Impact Dynamics in a 3D Granular Bed
3. Anindita Basu (University of Pennsylvania)
   Rheology and Jamming in Soft Colloids
4. Angela Holmberg (University of Delaware)
   Fabrication of Fluoro-efficient Polymers for Omniphobic Surfaces
5. Wei-Fan Kuan (University of Delaware)
   Interfacial modification in self-assembled triblock copolymers
6. Thomas Smart (University of Delaware)
   Stabilization of non-equilibrium block copolymer assemblies
7. Bin Wei (University of Delaware)
   Synthesis and phase behavior of tapered block copolymers
8. Jillian Emerson (University of Delaware)
   Homopolymer Blend/Nanoparticle Films for Application in Organic Photovoltaic Devices
9. Elizabeth Kelley (University of Delaware)
   Synthesis and self-assembly of bio-responsive block copolymers
10. Ming Luo (University of Delaware)
    Investigation of ABA triblock copolymer thin film morphology using substrate and thickness gradients
11. Paul Douglas Godfrin (University of Delaware)
    Efficient Modelling of Cluster Lifetime and Stability in Mixed Potential Systems
12. John R. Royer (New York University)
    Spherical and Non-Spherical Particles under Cyclic Shear
13. Flor Mitre (Georgetown University)
    Cristalization of dispersions of candelilla wax in safflower oil. Its behavior and simulation under stirring conditions.

Session II

1. Xin Bian (Technical University, Munich, Germany)
   Smoothed dissipative particle dynamics simulation of colloidal suspensions
2. Jung Min Kim (University of Delaware)
   Effect of particle size on the dynamical arrest of sticky hard spheres
3. Prasad Sarangapani (MedImmune)
   Development of an accurate microfluidic viscometer for high-throughput analysis of protein solutions
4. Bum Jun Park (University of Pennsylvania)
   Equilibrium configuration of non-spherical Janus particles at fluid-fluid interfaces
5. Joon Ho Roh (University of Maryland)
   The role of electrostatic interactions on the dynamics of RNA
6. Xin Zhang (University of Maryland)
   Amphiphilic Block Copolymer Self-Assembly and Pattern Transfer

7. Sudeep Dutta (Georgetown University)
   Droplet Rearrangement in Flowing Emulsions

8. Richard Arevalo (Georgetown University)
   Stress Propagation in Sheared Collagen Networks

9. Yuli Wei (University of Pennsylvania)
   Clogging of Hard and Soft Particles in 2D Porous Media

10. Frederick R. Phelan Jr. (NIST)
    Biased Diffusion of a Polymer Chain in a Nanofluidic Staircase

11. Peter Yunker (University of Pennsylvania)
    Particle-Shape-Dependent Effects During Evaporation of Colloidal Drops in Confined Geometries

12. Charles Thomas (University of Pennsylvania)
    Exploring the Clogging Transition with a Quasi-2D Hopper

Session III

1. Daniel B. Allan (Johns Hopkins University)
   Interfacial Microrheology of Lysozyme Layers at the Air-Water Interface

2. Pramukta Kumar (Georgetown University)
   Mechanisms of Shear Thinning in a Suspension of Rigid Rods

3. Armstrong Mbi (Georgetown University)
   Displacements Distribution of Particles in a Sheared Colloidal Glass

4. Aaron Eberle (NIST)
   Flow-SANS investigation of shear induced structural reorganization in particulate gels

5. Edward Van Keuren (Georgetown University)
   Synthesis of multicomponent nanoparticles

6. Albert J. Jin, Ph.D (NIBIB/NIH)
   Biomedical Studies and Cellular Imaging via Atomic Force Microscopy

7. Ted Brzinski (University of Pennsylvania)
   X-ray Fluoroscopy of Sedimentation in Viscoelastic Fluids

8. Antonio Faraone (NIST Center for Neutron Research)
   Neutron Spin Echo Spectroscopy at the NIST Center for Neutron Research

9. Jennifer Rieser (University of Pennsylvania)
   Dynamics in cohesive granular flow

10. Joel Rovner (Johns Hopkins University)
    Elastic Torque on a Ferromagnetic Disk within a Nematic Liquid Crystal

11. NI YAN (Department of Chemistry, Georgetown University)
    Pyrene-Integrated Low Molecular Mass Gelators Based on Sugar: Special Self-Assembly Properties in Organic Solvents and Water

12. Marcus Cicerone (NIST)
    Short-time dynamics and transport in molecular glasses

13. Adam Roth (University of Pennsylvania)
    Coarsening of Two Dimensional Foam on a Curved Surface

Session IV

1. Kathryn Whitaker (University of Delaware)
   Thermoreversible, Fluorescent, Hollow Silica Particles for Microrheology of Gels and Glasses

2. Daniel Blair (Georgetown University)
   Shear induced fibrillogenesis in pure silk dope

3. Lilian (State University of Campinas)
   "5α-Cholestan-3β-yl N-(2-Aryl)carbamates organogelators as a model systems to study petroleum additives mechanism of action"

4. Madhu Sudan Tyagi (University of Maryland and NIST Center for Neutron Research)
   The Dynamics of Unfolded versus Folded tRNA

5. Eric Yearley (University of Delaware/NIST)
   Small-Angle Scattering Studies of Monoclonal Antibody Self-Associations at High Concentrations

6. Kathryn Krycka (NCNR)
   Polarized SANS Capabilities

7. Whirang Cho (University of Delaware/NIST)
   Phage-templated synthesis of organic crystals

8. Peter Beltramo (University of Delaware)
   Polarization of colloidal suspensions in electric fields

9. Justin Stimatze (Georgetown University)
   Simulating fiber motion in shear flow using Dissipative Particle Dynamics

10. Amrita Pal (Georgetown University)
    Salt, pH and thermoresponsive hydrogel of N-(4-n-alkyloxybenzoyl)-L-carnosine.

11. Anand Banerjee (NIH)
    Stochastic model of clathrin-coated pit assembly