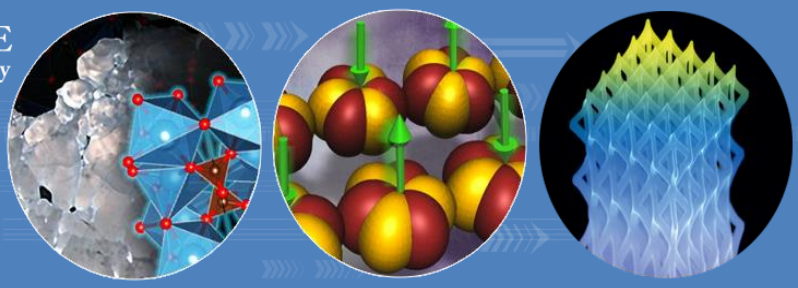

Active Matter at the Center for Nanophase Materials Sciences

Monday, July 31, 2017

Organizers:
Miguel Fuentes-Cabrera (fuentescabma@ornl.gov)
Bobby G. Sumpter (sumpterbg@ornl.gov)

Active Matter is a new and exciting field of Materials Science. In Active Matter, the systems are out of equilibrium, consuming energy that is translated into a variety of emergent phenomena, including collective motion and dynamic self-assembly (shape-changing polymers, granular matter and self-propelled particles are classical examples of active matter). Understanding of the underlying collective properties of active matter, including how to distinguish and classify its different states, is very challenging, yet it may hold the key to grasping the mechanics and statistics of living systems. Indeed, work in active matter is expected to have applications in soft condensed matter, robotics, microbiology, and biotechnology, to mention a few. To enable advancing in those directions, it is necessary to have a comprehensive approach in which theory and experiment work together to design and effectively explore active matter.

This workshop will bring together users and CNMS staff experts in the field of collective motion and dynamic self-assembly with the goal of identifying the major roadblocks that hinder our advance in Active Matter and developing synergies between experiment and theory.

Invited Speakers:

- Alexander Alexeev, *Georgia Institute of Technology*
- Qian Chen, *University of Illinois at Urbana-Champaign*
- Oleg Gang, *Brookhaven National Laboratory*
- David Hu, *Georgia Institute of Technology*
- Cynthia J. Reichhardt, *Los Alamos National Laboratory*

***Active Matter* at the Center for Nanophase Materials Sciences**

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Tentative Agenda

8:30AM **Welcome – Bobby Sumpter, CNMS Deputy Director and Group Leader**

9:00AM Qian Chen, University of Illinois at Urbana-Champaign
"*Imaging Phase Transition Dynamics at the Nanoscale*"

9:45AM Alexander Alexeev, Georgia Institute of Technology
"*Using Computer Simulations to Design Active Suspensions of Synthetic Micro-Swimmers*"

10:30AM Break

10:45AM David Hu, Georgia Institute of Technology
"*Fire Ants Build a Raft in Two Minutes, Grubs Eat a Pizza in Two Hours"*

11:30AM Lunch

12:30PM Cynthia J. Reichhardt, Los Alamos National Laboratory
"*Jamming and Clogging of Passive and Active Particles in Disordered Media*"

1:15PM Oleg Gang, Brookhaven National Laboratory
"Designed Nanoscale Systems via Self-Assembly"

2:00PM Break

2:15PM TBD

3:00PM Roundtable Discussion

See following pages for abstracts.

Abstracts

Imaging Phase Transition Dynamics at the Nanoscale

Qian Chen
University of Illinois at Urbana-Champaign, IL, United States

Self-assembly of nanoscale building blocks is an efficient strategy to construct complexity in biology and engineering, which produces extremely rich phases, reconfigurability and associated functions. Yet the quantitative prediction of their ensemble architectures and formation kinetics remains a challenge due to technical impediments. Here we use a new nanoscopic imaging technique, liquid phase transmission electron microscopy, to directly image the self-assembly of colloidal nanoparticles in solution, one-by-one in real-time. Depending on solvent conditions, a single type of anisotropic nanoparticles can lead to a wide variety of final structures not previously predicted: linear and cyclic “polymeric” chains, hierarchical plastic crystals, and highly ordered solids. In-situ monitoring of the dynamic pathways together with computation reveals interesting and novel phenomena in these systems due to inherent many-body coupling and discreteness at the nanoscale. We expect our study to open new opportunities in understanding the conformation, phase behaviors and collective dynamics on the nanometer length scale that is not accessible using other means.

Using Computer Simulations to Design Active Suspensions of Synthetic Micro-Swimmers

Alexander Alexeev
George W. Woodruff School of Mechanical Engineering
Georgia Institute of Technology

Advances in polymer science have led to the development of novel materials that can reversible change the shape controlled by external stimuli. Bi-layered hydrogel sheets with nanoscale thickness exhibit rapid out-of-plane deformation defined by the mismatch in stimuli-responsiveness of composing layers. We use computational modeling to examine how such stimuli-responsive synthetic materials that can undergo complex and reversible shape transformations can be used to design self-propelling microscopic swimmers. Our X-shaped micro-swimmers are made of a bi-layered hydrogel sheet that reversibly bends and straightens controlled by a periodical application of an external stimulus. We first use dissipative particle dynamics to model hydrogel swimmer and explore the physics of its propulsion through a viscous solvent. Using this model, we investigate how material properties affect swimming speed to optimize swimmer performance. We then employ lattice Boltzmann simulations to investigate the collective behavior of suspensions of these swimmers. We probe swimming of the synthetic micro-swimmers in an unbounded environment to examine their collective velocity and self-organization. We then probe how this behavior changes when swimmer suspensions with different concentrations are enclosed in a confined space. Finally, we probe how the swimmers interact with neutrally buoyant spherical particles to understand how the swimmers can be harnessed to transport a cargo in a microfluidic environment.

Fire Ants Build a Raft In Two Minutes, Grubs Eat A Pizza In Two Hours

David Hu
Georgia Tech

The world can be a dangerous place, especially if you are an insect. In the wetlands of Brazil, fire ants link their bodies together to build waterproof rafts. The rafts can bounce off rocks or flow around twigs, exhibiting both liquid and solid behavior from the ants rearranging their bodies. Rearrangement is also important for black soldier fly larvae, which are the dominant scavengers of animal carcasses. These grubs can eat an entire pizza in two hours. We film insects using time-lapse video, and measure their forces using rheometers and force platforms. The speed and versatility of these biological materials may provide inspiration for synthetic systems.

Jamming and Clogging of Passive and Active Particles in Disordered Media

Cynthia Reichhardt
Theoretical Division, Los Alamos National Laboratory

There has been tremendous growth in studying nonequilibrium systems of particle assemblies which can exhibit jamming effects. In general jamming has been studied in the absence of quenched disorder. Here we examine the dynamics of active and passive matter systems interacting with random or periodic substrates and obstacle arrays, and show that it is possible to make a clear distinction between jammed systems and clogged systems. For non-active systems of particles flowing through random obstacle arrays, when the particle density is well below that at which an obstacle free system would jam, we find that the system can reach a clogged state. The clogged states can be distinguished from jammed states in that they are spatially heterogeneous, are fragile, and have a pronounced memory effect. In contrast, jammed states are much more homogeneous, robust, and have much weaker memory effects. We outline a possible scenario in which jamming is dominated by a diverging length scale associated with a critical density at point J, while clogging is associated with the coarsening of a dense area across the sample. We have also investigated clogging and jamming in active matter or self-motile particle systems. Such dynamics can effectively describe certain biological systems such as run-and-tumble bacteria or crawling cells, as well as non-biological systems such as self-driven colloids or artificial swimmers. For active matter systems driven over random disorder we find that for intermediate amounts of self-motility the system does not clog; however, for increasing self-propulsion of the particles there is a strong reduction of the mobility due to a self-clogging or self-clustering in the system that resembles the "faster is slower" effect found in certain pedestrian panic models.

Designed Nanoscale Systems via Self-Assembly

Oleg Gang
Department of Chemical Engineering and Department of Applied Physics and Applied Mathematics, Columbia University
Center for Functional Nanomaterials, Brookhaven National Laboratory

In the last decades nanoscale inorganic objects emerged as a novel type of matter with unique functional properties and a plethora of prospective applications. Although a broad range of nano-synthesis methods has been developed, our abilities to organize these nano-components into designed static and reconfigurable architectures are quite limited. An incorporation of bio-molecules into a nano-object allows establishing selective interactions between the components of nano-systems. Such encoding may permit programming of complex and dynamically tunable systems via self-assembly: biomolecules act as site-specific scaffolds, smart assembly guides and reconfigurable structural elements.

I will discuss our advances in addressing the challenge of programmable assembly using the DNA platform, in which a high degree of addressability of nucleic acids is used to direct the formation of structures from nanoscale components. Our work investigates the major leading parameters determining a structure formation and explores new concepts for creating targeted nano-architectures. The principles and practical approaches developed by our group allow for assembly of well-defined three-dimensional superlattices, two-dimensional membranes and finite-sized clusters from the multiple types of the nano-components. Our recent progress on the development of by-design assembly strategies will be illustrated by the novel DNA-nanoparticle framework lattices and clusters with prescribed architectures. Finally, I will discuss the dynamically controlled assemblies, where selective triggering allows for system transformations and cascade reactions.