The Department of Chemical and Biomolecular Engineering at The Johns Hopkins University

Presents

The 2008

John C. and Florence W. Holtz Lecture

Thursday, March 6, 2008

Seminar at 10:30 A.M……..…….Maryland Hall (Room 110)

Refreshments at 10:00 A.M. …….....Maryland Hall (Room 220)

Carol K. Hall

Department of Chemical and Biomolecular Engineering
North Carolina State University

Self-Assembly of Dipolar Particles: Designing Smart Materials Using Computer Simulation

Colloid particles with dipolar interactions that self-assemble into pre-defined microstructures have the potential to serve as the foundation for a new generation of micro- and nano-structures of remarkable complexity and precision. Dipolar colloidal particles self-assemble into a rich variety of microstructures ranging from co-crystals of novel symmetry, to open networks (gels) of cross-linked chains of particles. We use discontinuous molecular dynamics computer simulation to explore the self assembly, structure, crystallization and/or gelation of systems of colloid particles with permanent dipole moments. Several different types of phases are found. . At high packing fractions we find ordered phases including face centered cubic (FCC), hexagonal close packed (HCP) and body centered tetragonal (BCT). At low packing fractions we find fluid, string-fluid and gel phases. The very low volume fraction gel phases and the well ordered crystal phases are promising for materials applications. We study how the kinetics and thermodynamics of the assembly process is affected by particle size, concentration, particle size ratio (for mixtures), dipole moment, and location of the dipole within the particle. The results of this study should help guide our experimental colleagues in their quest to design and engineer “smart” gels and materials.

The Holtz Lecture will be held in Maryland Hall Rm.110 a t 10:30 a.m.
Continental Breakfast in Maryland Hall Rm. 220 at 9:45 a.m.
For additional information contact the Seminar Chair German Drazer at drazer@jhu.edu