SCHOOL OF CHEMICAL, BIOLOGICAL & MATERIALS ENGINEERING

And

UNIVERSITY OF OKLAHOMA BIOENGINEERING CENTER

100 E. Boyd, Sarkeys Energy Center, T-335 405-325-5811 The University of Oklahoma Norman, Oklahoma 2009 – 2010 Seminar Series

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Will present a seminar on

"SIMULATIONS OF SELF-ASSEMBLY IN SURFACTANT, NANOPARTICLE AND BLOCK COPOLYMER SYSTEMS"

In this seminar, I plan to present recent work on self-assembly of (a) ionic surfactant into micelles (b) nanoparticles with attached chains to sheets and strings and (c) cylinders and spheres in thin films of diblock copolymers. The importance of electrostatic interactions on self-assembly of surfactants and biological systems has been widely acknowledged. Most theoretical approaches for these systems are based on mean-field approximations that neglect higher order correlations that are particularly important for multivalent ions and in environments of low dielectric permittivity. We have developed implicit-solvent ionic surfactant models and have used them in Grand Canonical Monte Carlo simulations to investigate the critical micelle concentration, aggregation number and micellar shape in the presence of explicit salt. We illustrate the importance of ion correlation effects by comparing these results with a Yukawa-type surfactant model that incorporates electrostatic screening implicitly. For diblock copolymer self-assembly under shear, the morphologies of the film vary with composition, segregation strength, and the strength of the shear field. We find that a critical shear rate, films self-assemble into cylindrical micelles with orientation parallel to the shear direction, in agreement to experimental observations.

THURSDAY, APRIL 15, 2010
COOKIES AND COFFEE -- 2:45 P.M.
SEMINAR -- 3:00 P.M.
SARKEYS ENERGY CENTER, ROOM M-204

THIS IS A REQUIRED SEMINAR FOR CHE 5971