NANO HIGHLIGHT
Surfactant Self-Assembly on Nano-Structured Surfaces: Multi-Scale Computational Prediction and Design

NSF NIRT GRANT 0403633

PIs: **K. E. Gubbins[1], J. Bernholc[1], D.W. Brenner[1] and S.C. Glotzer[2]**
[1]North Carolina State University and [2]University of Michigan

A central problem in developing realistic computational methods for the prediction of property behavior and design of polymers, surfactant solutions, self-assembled nano-structures, protein solutions and colloidal suspensions (examples of 'soft matter') is the development of so-called coarse graining schemes to connect the atomistic description of matter with the so-called meso-scale treatment (in which matter is considered to be made up of 'blobs' of matter, each consisting of a number of atoms). Such a connection is needed because computers are as yet too slow for us to access the necessary length and time scales needed for the study of soft matter. Such coarse graining involves the definition of 'effective forces' between the meso-scale blobs of matter, which has proved very difficult; previous attempts used approximate coarse graining methods, that are specific to one type of property or system and not applicable to others. We have developed a rigorous procedure for doing this that guarantees that the meso-scale model yields the same thermodynamic and structural properties as for the more detailed atomistic model [1].

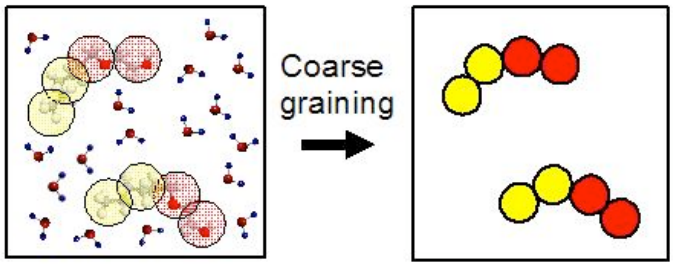

Figure 1. The proposed coarse-graining procedure going from the fully atomistic system of surfactant molecules (molecules that have a hydrophilic and a hydrophobic end, shown as a chain molecule with groups of atoms enclosed by spheres) in water to a meso-scale model.

Our coarse graining procedure is now being tested for increasingly complex systems of self-assembled surfactants. If it proves successful it would open the way to understanding how to design surfactant systems that would self-assemble to form a wide range of nano-structured materials for particular applications, including electronic devices, photonics, catalysts, biosensors, bioelectronic materials. Moreover, these same or very similar procedures could provide a way to realistically model and design other soft matter systems, including polymers, colloidal suspensions, and solutions of biological molecules such as proteins, DNA, RNA, etc.

[1] N. Chennamsetty, H. Bock, and K. E. Gubbins, *Mol. Phys.* **103**, 3185 (2005)