Joint Condensed Matter
and
Center for Soft Matter and Biological Physics
Seminar

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Evaporation of Liquids and Solutions

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304 Robeson Hall

Evaporation of a liquid is a ubiquitous phenomenon. It drives the water cycle and can be used for cooling. It is also a useful tool for materials fabrication such as evaporation-induced self-assembly of colloidal particles and thin-film deposition via spin coating. In the first part of this talk, we will present million-atom scale molecular dynamics (MD) simulations of the evaporation process of water. An enhancement of water density near the liquid-vapor interface is found during fast evaporation. The temperature profiles based on both translational and rotational degrees of freedom are calculated at different stages of evaporation and evaporative cooling of the liquid-vapor interface is observed, which accounts for the higher water density at the interface. The velocity distribution of water molecules in the vapor phase during evaporation is also computed at various distances relative to the interface and fit to the Maxwell-Boltzmann distribution. Results indicate that local thermal equilibrium holds in the liquid phase, though the whole system is driven out of equilibrium. In the second part of this talk, we will focus on evaporating behavior of polymer solutions. In particular, polyelectrolyte solutions show rich physical behavior because of electrostatic interactions. We use MD simulations to study the evaporation of a solution of polyanionic chains (sodium polystyrene sulfonate). The polymers are represented by MARTINI-type bead-spring chains. Water is included as an explicit solvent and described with a model taking into account polarization effects. Counterions and salts are also explicitly included as mobile single beads. Our results show that the polyelectrolyte chains form layered structures with alternating polymer-rich and counterion-rich layers, indicating that one-pot evaporation technique may be developed to fabricate multilayer polyelectrolyte films that are currently mainly produced via a layer-by-layer deposition process. We will discuss the effects of polymer concentration, salt concentration, and evaporation rate on the structure of the resulting film. Finally, we will also briefly discuss our recent study of the evaporation of polymer solutions containing both polyanionic and polycationic chains.