PHYSICS COLLOQUIUM

DR. SHENGFENG CHENG

DEPARTMENT OF PHYSICS, CENTER FOR SOFT MATTER AND BIOLOGICAL PHYSICS, AND MACROMOLECULES INNOVATION INSTITUTE, VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY

WATCHING PAINT DRY IS SURPRISINGLY INTERESTING

SEPTEMBER 27 | 2:00 PM

130 HAHN HALL NORTH

The drying process of a soft matter solution such as a colloidal suspension or a polymer solution provides an excellent playground to explore nonequilibrium physics. One famous example is the coffee ring effect, where a spill of coffee (a particle-laden drop) after drying leaves a ring-like deposit at its perimeter. As another example, novel stratification phenomena have recently been discovered in polydisperse particle suspension films that undergo rapid drying. In all these processes, the interplay of solvent evaporation, fluid dynamics, diffusion, phoresis, and capillarity leads to far-from-equilibrium settings where rich phenomena emerge. In this talk, I will describe our effort of using large scale molecular dynamics (MD) simulations to study various soft matter solutions undergoing drying, including solutions of colloids, polymers, and their mixtures. The solvent is first modeled explicitly as a Lennard-Jones liquid. For bidisperse particle suspensions, a state diagram of stratification outcome is determined and the counterintuitive "small-on-top'" stratification, with an enrichment of the smaller particles at the receding liquid-vapor interface during fast drying, is observed. The diagram is compared to the predictions of several theoretical models recently proposed on the basis of diffusiophoresis. An approach to control stratification via thermal gradients and associated thermophoresis is proposed and validated with MD simulations. The explicit solvent is further mapped to an implicit, uniform, viscous medium by matching the diffusion coefficients of the particles as well as their pair correlation functions. A consistent stratification behavior is observed in both explicit and implicit solvent models under the same drying condition. We also apply our models to investigate the drying process of solutions of polymers and particle-polymer mixtures. Our results reveal a new strategy of unfirmly dispersing nanoparticles into a polymer matrix using fast solvent evaporation, interesting stratification phenomena in drying polyelectrolyte solutions, the formation of a variety of dry structures in drying films or droplets, and ways to control these structures via tuning drying conditions.

COLLEGE OF SCIENCE PHYSICS VIRGINIA TECH