Nov 20, 2019

Shengfeng Cheng, Assistant Professor at Department of Physics, Center for Soft Matter and Biological Physics, and Macromolecules Innovation Institute, Virginia Polytechnic Institute and State University

Title: Drying of Soft Matter Solutions

Abstract:

The drying process of a soft matter 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) leaves a ring-like deposit at its perimeter after drying. As another example, novel stratification phenomena have recently been discovered in thin films of polydisperse particle suspensions that undergo rapid drying. In all these processes, the interplay of solvent evaporation, fluid dynamics, diffusion, phoresis, wetting, and capillarity leads to far-from-equilibrium settings where rich phenomena emerge. In this colloquium, I will describe efforts of using large scale molecular dynamics (MD) simulations to study various soft matter solutions undergoing drying, including solutions and suspensions 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 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 as well as drying mixtures of liquids with different volatility, the formation of a variety of dry structures in evaporating films or droplets, and ways to control these structures via tuning drying conditions.