Multi-Scale Modeling of the Structure and Rheology of Surfactant Solutions and Polymer-Colloidal Networks

Ronald G. Larson

Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109

Continuum-level thermodynamic and transport properties can now be computed from molecular-scale interactions using multi-scale molecular dynamics (MD) simulations and Brownian dynamics (BD) simulations, along with biasing methods, such as umbrella sampling, and forward flux sampling. We demonstrate the power of these methods by computing the dynamics and rheology of surfactant solutions and colloid-polymer mixtures used in consumer products, such as shampoos, paints, and drug-release formulations. The complex structures of these solutions require multi-scale modeling that includes atomistic and coarse-grained molecular simulations, as well as colloidal scale simulations to connect rheological properties to chemical composition. We compare the predicted results to experimental data, and extract information, such as micelle length and breakage time, that is unavailable, or not easily available, from experiments.