

Molecular Modeling of Nano-particle / Copolymer and Surfactant Systems

Shekhar Jain, Adam Bymaster, Chris Emborsky, ZhengZheng Feng, Kenneth Cox and Walter Chapman^{C, S}
Rice University, Houston, TX, U.S.A.

Many novel applications of copolymer and surfactant systems take advantage of their unique microstructure and phase behavior. Example applications include performance polymers, stabilizers for pharmaceutical suspensions, templates for nano-materials, and water-based coatings. The challenge in molecular level design of such systems lies in having predictive models that include the physics that emerges from finite-size effects, varying dimensionality, surface forces and interplay of multiple length scales. We present a novel molecular theory for multi-scale modeling of complex fluid assemblies. This computationally efficient classical density functional theory can predict the effects of molecular size, branching and functional groups on interfacial properties and microstructure. Predictions of the theory are in agreement with molecular simulation results and experiment for phenomena such as polymer depletion, potential of mean force between nano-colloids, and surface-induced segregation – key elements in polymer-colloid systems and in coatings of polymer blends.