33d Molecular Simulations of Surfactant-Assisted Spreading

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The effects of surfactant additives on the spreading of liquid drops on partially-wetting solid surfaces is investigated using molecular dynamics simulations. The solvent, solid and surfactant are modeled as coexisting atomic species, with Lennard-Jones or SPC/E models for non-polar and aqueous solvents, respectively, a tethered atom model for the solid, and a united atom model with standard force fields and appropriate bond-length and bond-angle interactions for the surfactant. In the simulations, an initially-spherical drop of water containing dissolved surfactant is allowed to spread freely on a clean substrate. In addition to drop shape, the molecular configurations and hydrodynamic flow fields are monitored. A particular focus in this study is to understand the mechanism for the unusual"superspreading" behavior of trisiloxane surfactants, which can yield complete wetting of aqueous solutions on hydrophobic surfaces. The formation of surfactant bilayers in the precursor film of a spreading drop appears to be a key ingredient.