355g A Molecular Dynamics Study of the Wetting of Hydrophobic Substrates by Aqueous Surfactant Solutions

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Many industrial processes rely on conventional surfactants to increase the wetting of hydrophobic substrates by aqueous solutions. For instance, organic surfactants are added to herbicide solutions in order to achieve a larger wetted area when the solution is applied to the leaf of a plant, which due to the Epicuticular wax is a difficult-to-wet surface. For over three decades it has been known that trisiloxane alkoxylate surfactants or superspreaders are far more effective than conventional surfactants. However, superspreaders are photosensitive, toxic, and relatively expensive. Classical molecular dynamics simulations are being conducted to determine the mechanism by which organic and silicon surfactants increase the spreading of aqueous droplets on hydrophobic surfaces. Sessile water drops containing either low-molecular-weight alcohols or polyoxyethylene surfactant molecules have been simulated at 298 K on an atomistic graphite lattice. During the course of the simulation surfactant molecules tend to the three-phase contact line where the headgroups are found to interact strongly with water and the tailgroups are directed radially outward and displaced from the droplet. An implementation of the fast multipole algorithm is used for the rapid evaluation of long-range electrostatic forces. Complementary sessile drop wetting experiments are being conducted by our research group.