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Silica-Based Janus Nanoparticles at the Water-Decane Interface[1]

HENG FAN, ALBERTO STRIOLO, The University of Oklahoma, School of Chemical, Biological and Materials Engineering — It is well known that solid particles adsorb at water-oil interfaces to reduce the contact area between the two immiscible phases. Stable emulsions are obtained when the particles strongly adsorb at the interfaces. We report herein all atom molecular dynamics simulation results for silica-based nanoparticles functionalized with hydrophobic moieties at the decane-water interface. The simulation results are quantified in terms of contact angle at the water-nanoparticle-decane interface, mobility of the nanoparticles, association of multiple nanoparticles at the interface, and free-energy landscapes that dictate the nanoparticle adsorption at the interface. The results are discussed based on the chemical features of the nanoparticle surface. Comparison with experimental data, including but not limited to TEM and cryo-TEM images of water-oil emulsions, are provided.

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