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Modeling Interfacial Adsorption of Polymer-Grafted Nanoparticles XIN YONG, Binghamton University — Numerous natural and industrial processes demand advances in our fundamental understanding of colloidal adsorption at liquid interfaces. Using dissipative particle dynamics (DPD), we model the interfacial adsorption of core-shell nanoparticles at the water-oil interface. The solid core of the nanoparticle encompasses beads arranged in an fcc lattice structure and its surface is uniformly grafted with polymer chains. The nanoparticles bind to the interface from either phase to minimize total surface energy. With a single nanoparticle, we demonstrate detailed kinetics of different stages in the adsorption process. Prominent effect of grafted polymer chains is characterized by varying molecular weight and polydispersity of the chains. We also preload nanoparticles straddling the interface to reveal the influence of nanoparticle surface density on further adsorption. Importantly, these studies show how surface-grafted polymer chains can alter the interfacial behavior of colloidal particles and provide guidelines for designing on-demand Pickering emulsion.

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