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**Structure and Diffusion of Nanoparticles at the Liquid-Vapor Interface** SHENGFENG CHENG, GARY GREST, Sandia National Laboratories — Large-scale molecular dynamics has been used to simulate a layer of nanoparticles diffusing on the surface of a liquid. Both a low viscosity liquid, represented by Lennard-Jones monomers, and a high viscosity liquid, represented by linear homopolymers, are studied. The organization and diffusion of the nanoparticles are studied as the coverage and the contact angle between the nanoparticles and liquid are varied. Results are compared to simulations of identical nanoparticles in two-dimensions. We show that when the interaction between the nanoparticles and liquid is reduced the contact angle increases and the nanoparticles ride higher on the liquid surface, which enables them to diffuse faster. In this case the short range order is also reduced as seen in the pair correlation function. For low contact angles, nanoparticles diffuse into the liquid for high coverages.

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