

Abstract Submitted
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A molecular view of latex-water interfaces¹ ZIFENG LI, KRISTEN FICHTHORN, SCOTT MILNER, Department of Chemical Engineering, Pennsylvania State University, FANG YUAN, RONALD LARSON, Department of Chemical Engineering, University of Michigan — Latex paints and coatings are colloidal suspensions, in which amorphous polymer particles are dispersed in an aqueous phase. The polymer-water interface plays a key role in the stability and rheology of the suspension. To obtain a molecular level view of this interface, atomistic simulations were performed for a slab of poly(methyl methacrylate)-poly(butyl acrylate) random copolymer in water, focusing on polymer and water density profiles, the hydrogen bonding of water with polymer carbonyl groups, and surface tension. The carbonyl groups at the interface were found to orient significantly towards water. We also calculated the temperature dependence of the surface tension between the polymer/water and polymer/ vacuum interfaces, including tail corrections for cut-off dispersion interactions, and we predict the contact angle of a water droplet at room temperature.

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