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Parameterization and Adsorption Study of Hydrophobic Ethoxylated Urethane (HEUR) using Coarse-Grained MD Simulations with Implicit Water SHIHU WANG, RONALD G. LARSON, Chemical Engineering Department, University of Michigan, VALERIY V. GINZBURG, The Dow Chemical Company, Midland, Michigan — We parameterize a coarse-grained (CG) model using implicit water for a model Hydrophobic Ethoxylated Urethane (HEUR) composed of poly(ethylene oxide) (PEO) endcapped with hydrocarbon tails. Our model matches predictions using a CG Martini model with explicit water for PEO in water. We illustrate the strong adsorption of PEO onto hydrocarbon surfaces in water and obtain parameters for PEO at hydrocarbon/water interfaces. As a validation, we simulate the self-assembly of alkyl poly(ethylene glycol) surfactants and observe the transition from a lamellar phase to cylindrical micelles upon varying EO length, a result in agreement with previous studies. Lastly, we study the adsorption of HEURs onto hydrophobic surfaces. We observe bridge formation between two surfaces, interconnected flower-like micelles and their subsequent adsorption, in equilibrated systems. We discuss the influence of hydrophobe length and HEUR volume fraction on the adsorption process and the equilibrium adsorption. These results provide important insights for HEURs adsorption and are useful for comparisons with Self-Consistent Field Theory.

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