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Modeling pH-Responsive Adsorption of Polyelectrolytes at Oil-Water Interfaces[1] SHIYI QIN, XIN YONG, Binghamton Univ — We use dissipative particle dynamics (DPD) to discover the interfacial adsorption of pH-responsive polyelectrolytes in oil-water binary systems under different pH values. The electrostatic interactions between charged beads and the dielectric discontinuity across the interface are modeled by exploiting a modified Particle-Particle-Particle-Mesh (PPPM) method, which uses an iterative method to solve the Poisson equation on a uniform grid. We first model the adsorption behavior of a single linear polyelectrolyte from the aqueous phase. The Henderson-Hasselbalch equation describes the relation between pH and the degree of ionization of the modeled polyelectrolytes. Through changing the degree of ionization, we explore the influence of pH on the adsorption behavior and show that the electrostatic interactions significantly modulate the adsorption. Time evolutions of the position and conformation of the polyelectrolytes and the variation in the oil-water surface tension will be measured to characterize the adsorption behavior. Furthermore, we model the pH-dependent adsorption behavior of polyelectrolytes with more complicated structures, namely, branched polyelectrolytes with hydrophobic backbones and hydrophilic side chains. We also find that the addition of salts in the medium and the lengths of the backbone and ionized side chain affect the adsorption.

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