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Invited Talk: pH-responsive polymer-grafted nanoparticles: From colloidal monolayer to Pickering emulsion

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Responsive nanoparticles at fluid interfaces offer great potential for realizing controllable self-assembly that can benefit various applications, ranging from 2D nanomaterials synthesis, switchable emulsions and microdroplet reactor. Herein, we apply electrostatic dissipative particle dynamics (DPD) simulations to study nanoparticle monolayers formed at planar water-oil interface, and probed the direct interactions among emulsions stabilized with active nanoparticles. The model nanoparticle is functionalized with weak polyelectrolytes to render the pH-sensitivity, which permits further manipulation of the monolayer properties. Qualitative and quantitative analysis of the monolayer microstructure shows a disorder-order phase transition, which is driven by the modulation of long-range electrostatic interactions subject to pH changes. Different regimes of particle self-diffusion in the monolayer were identified and correlated with the structural transition. We further modeled the head-on collision and coalescence of two droplets covered by pH-responsive polymer-grafted nanoparticles. The maximal resistance forces were measured to quantitatively discriminate the efficacy of particles in stabilizing emulsions at different degrees of ionization. Moreover, the influence of ionization state was studied in various surface coverage regimes and shows two different mechanisms of preventing coalescence. The findings of these numerical simulations provide greater insight into the interfacial behavior of active polymer-grafted nanoparticles and the stability of Pickering emulsions.