

Abstract Submitted
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Demixing of Charged Nanoparticle-Polymer Mixtures: A Simulation Study¹ BEN LU, ALAN R. DENTON, North Dakota State University — The phase behavior of mixtures of charged nanoparticles and neutral polymers is studied by computer simulation. Adapting the classic Asakura-Oosawa-Vrij model, the polymers are modeled as coarse-grained effective spheres that are mutually ideal (theta solvent), but can overlap the nanoparticles with a penetration energy that mimics a loss of chain conformational entropy. Although monodisperse in chain length, the polymers fluctuate in radius of gyration in response to the nanoparticles. Within the primitive model of charged colloids, the nanoparticles are modeled as charged hard spheres, governed by effective electrostatic interactions, including a repulsive screened-Coulomb (Yukawa) pair potential and a one-body volume energy. To investigate demixing behavior, constant-NPT Gibbs ensemble Monte Carlo simulations are performed over ranges of nanoparticle-polymer size ratio, nanoparticle charge, and salt concentration. In the limit of neutral nanoparticles, simulation results are compared with predictions of density-functional theory.

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