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Molecular Dynamics Simulations of Nanoparticles Coated with Charged Polymers CHENGYUAN WEN, SHENGFENG CHENG, Virginia Polytechnic Institute and State University — Polymer coating is frequently used to stabilize colloidal and nano-sized particles. We employ molecular dynamics simulations to study nanoparticles coated with polymer chains that contain ionizable groups. In a polar solvent, the chains become charged with counterions dissociated. In the computational model, we treat the solvent as a uniform dielectric background and use the bead-spring model for the polymer chains. Counterions are explicitly included as mobile beads. The nanoparticle is modeled as a layer of sites uniformly distributed on a spherical surface with a certain fraction of sites serving as the tether points of the grafted polymer brush. We vary the grafting density and calculate the distribution of polymer beads and counterions around the nanoparticle. Our results indicate that charged chains adopt extended conformations because of their mutual repulsions. We further study the interactions between two polymer-coated nanoparticles and obtain the potential of mean force. We also find an interesting transition of a confined single layer of such polymer-coated nanoparticles into two layers when the confinement is removed. Results show that the brush-brush contact has a nonuniform distribution and the nanoparticles tend to form dipole-like structures.

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