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Interactions between Nanoparticles and Polymer Brushes: Molecular Dynamics Simulations and Self-consistent Field Theory Calculations[1] SHENGFENG CHENG, CHENGYUAN WEN, Virginia Polytechnic Institute and State University, SERGEI EGOROV, University of Virginia — Molecular dynamics simulations and self-consistent field theory calculations are employed to study the interactions between a nanoparticle and a polymer brush at various densities of chains grafted to a plane. Simulations with both implicit and explicit solvent are performed. In either case the nanoparticle is loaded to the brush at a constant velocity. Then a series of simulations are performed to compute the force exerted on the nanoparticle that is fixed at various distances from the grafting plane. The potential of mean force is calculated and compared to the prediction based on a self-consistent field theory. Our simulations show that the explicit solvent leads to effects that are not captured in simulations with implicit solvent, indicating the importance of including explicit solvent in molecular simulations of such systems. Our results also demonstrate an interesting correlation between the force on the nanoparticle and the density profile of the brush.

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