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Modeling Hairy Nanoparticle Assemblies: Effect of Surface Adsorption Strength on Canopy Entanglements and Dynamics JEFFREY ETHIER, LISA M. HALL, Ohio State Univ - Columbus — Neat hairy nanoparticles (polymer-grafted nanoparticles) exhibit unique mechanical, dielectric, and optical properties while avoiding dispersion challenges found in traditional polymer nanocomposites. On surfaces, such HNPs can form ordered arrays with controlled interparticle spacing whose properties depend on interpenetration or entanglement of the polymer canopies. We use coarse-grained molecular dynamics (MD) simulations to model individual or small groups of HNPs with various grafting densities, graft lengths, and surface adsorption strengths. Specifically, particles and monomers are modeled as spherical beads which can adsorb on a flat surface; the particle diameter is ten times that of the monomer. We validate our model by comparing our height profiles to those from recent experiments as a function of bead-surface adsorption strength. As expected, the canopy height decreases with increasing surface adsorption strength, and the polymer spreads out to maximize its contact with the surface. For various grafting densities and graft lengths, we analyze the polymer dynamics as a function of distance from the substrate and NP surface. We also examine the entanglement density between neighboring adsorbed HNPs.

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