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Three-body Interactions in Polymer Nanocomposites AMALIE L. FRISCHKNECHT, Sandia National Laboratories, ARUN YETHIRAJ, University of Wisconsin — We use the modified iSAFT density functional theory (DFT) to calculate interactions among nanoparticles immersed in a polymer melt. Because a polymer can simultaneously interact with more than two nanoparticles, three-body interactions are important in this system. We treat the nanoparticles as spherical surfaces, and solve for the polymer densities around the nanoparticles in three dimensions. The polymer is modeled as a freely-jointed chain of spherical sites, and all interactions are repulsive. The potential of mean force (PMF) between two nanoparticles displays a minimum at contact due to the depletion effect. The PMF calculated from the DFT agrees nearly quantitatively with that calculated from self-consistent PRISM theory. From the DFT we find that the three-body free energy is significantly different in magnitude than the effective three-body free energy derived from the two-particle PMF. [This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility at Los Alamos National Laboratory (Contract DE-AC52-06NA25396) and Sandia National Laboratories (Contract DE-AC04-94AL85000).]

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