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Polymer-mediated structure of nanoparticles in dense melts: transferability and an effective one-component approach RAJARSHI CHAKRABARTI, Post Doctoral Research Associate, Material Science and Engineering, University of Illinois at Urbana Champaign, KENNETH SCHWEIZER, G. Ronald and Margaret H. Morris Professor of Materials Science and Engineering, University of Illinois at Urbana Champaign — Two component PRISM theory is used to investigate the dependence of polymer-mediated interactions between the sites of complex nanoparticles on filler shape. Dilute limit potential-of-mean force (PMF) calculations for spheres, diatomics, 4-site rods and disks, and a tetrahedron are compared under depletion, steric stabilization, and bridging conditions. The PMFs are only weakly dependent on filler shape (good transferability), and scale nearly linearly with filler to monomer site diameter ratio. The question of a whether a reliable one component nanoparticle model can be constructed based on the dilute limit polymer-mediated PMF as input to the HNC integral equation theory is explored for spherical nanoparticles. Compared to the full 2-component theory results, stronger depletion and steric stabilization, but weaker bridging, is predicted, trends due to the qualitatively different spatial organization of polymers in the three regimes of interfacial cohesion. However, overall the structural behaviors predicted by the one-component approach are qualitatively reliable.

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