Theory of effective interactions and dispersion of soft nanoparticles in polymer melts JIAN YANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — Integral equation theory is employed to investigate the consequences of nanoparticle softness (surface fluctuations) and corrugation (discrete roughness) on the equilibrium behavior of polymer-particle mixtures in the dilute filler limit. Monomer-particle pair correlations exhibit qualitatively different features relative to hard spheres which depend on both roughness and softness. Under athermal nonadsorbing polymer conditions, depletion effects on the interparticle potential-of-mean-force (PMF) are qualitatively modified by surface corrugation and/or fluctuations. As particle softness increases, monomer-scale PMF oscillations are destroyed, and the strongest attraction occurs at a particle separation and attraction depth that depends sensitively on surface fluctuation amplitude, as does the dependence on monomer-nanoparticle size asymmetry ratio (R). For corrugated particles, the most attractive nanoparticle separation does not occur at contact, and is far weaker and less sensitive to R than for hard spheres. Second virial coefficient calculations are performed to estimate how particle softness/roughness modifies miscibility in chemically matched blends. How surface corrugation and softness modifies bridging and sterically stabilized states has also been studied..

Jian Yang
University of Illinois at Urbana-Champaign

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