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Theory of the Structure and Miscibility of Soft Filler Polymer Nanocomposites JIAN YANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — A new hybrid theory for soft filler polymer nanocomposites is constructed based on combining integral equation methods and small scale Monte Carlo simulation. The consequences of nanoparticle softness (surface fluctuations) and corrugation (discrete roughness) on the equilibrium behavior is investigated in the dilute filler limit. Under athermal (entropic) conditions, the monomer-particle pair correlations exhibit qualitatively different features relative to hard smooth spheres. Polymer-mediated depletion attractions in the particle potential-of-mean-force (PMF) are qualitatively modified by surface corrugation and/or fluctuations. With increasing particle softness, monomer-scale PMF oscillations are destroyed, and the interparticle separation and effective maximum attraction strength depend sensitively on surface fluctuation amplitude and monomer-nanoparticle size ratio. Second virial coefficient calculations are performed to estimate how particle softness/roughness modifies miscibility, and a mechanism is identified for entropically stabilizing rough nanofillers in the absence of a cohesive interface. Surface corrugation and softness is also found to significantly modify the bridging and sterically stabilized states associated with adsorbing polymers.

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