Abstract Submitted
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Dispersion of small nanoparticles in random copolymer melts DEBAPRIYA BANERJEE, KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign, BOBBY SUMPTER, Oak Ridge National Laboratory, MARK D. DADMUN, University of Tennessee and ORNL — Microscopic PRISM integral equation theory is applied to study the structure and miscibility of extremely small nanoparticles (e.g., C60 buckyballs) dissolved at low concentrations in a chemically heterogeneous random AB copolymer melt. The effects of polymer stiffness, melt isothermal compressibility, and the strength and spatial range of polymer-particle, polymer-polymer, and filler-filler attractions on the miscibility of the nanoparticles are studied. Complex, subtle and highly nonuniversal behavior is found. Appropriate tuning of the chemical interactions can result in the emergence of an intermediate range of random copolymer compositions where miscibility is maximized and larger than in either homopolymer limit. The physical origin involves a competition between depletion, steric stabilization, and bridging polymer-mediated interactions. When the direct interaction between the small fillers is tuned to model fullerenes, the potentials of mean force exhibit a competition between contact aggregation and bridging, and miscibility is enhanced with decreasing contact aggregation until the onset of bridging. Qualitative comparisons to recent experiments have been performed using attractive interaction strengths motivated by quantum chemical calculations.

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