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Nanoparticle Self-Assembly in a Polymer Matrix and Its Impact on Phase Separation

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The ubiquitous clustering of nanoparticles (NPs) in solutions and polymer melts depends sensitively on the strength and directionality of the effective NP-NP interactions, as well as on the molecular geometry and interactions of the dispersing fluid. Surface functionalization apparently can also lead to emergent anisotropic interactions that can influence NP dispersion. Since NP clustering can strongly influence the properties of polymer nanocomposites and NP solutions, we investigate the reversible self-assembly of model NPs into clusters under equilibrium conditions through a combination of simulation and analytic methods. First, we performed molecular dynamics simulations of polyhedral NPs in a coarse-grained dense bead–spring polymer melt and find a transition from a dispersed to clustered NP state, consistent with the thermodynamic models of equilibrium particle association such as equilibrium polymerization. We also describe the competition between self-assembly and phase separation in an analytic lattice model of a mixture of polymers and NPs. We then focus on the particularly interesting situation where the associating "monomeric" NP species form high molecular mass dynamic polymeric clusters and where the assembly process then transforms the phase boundary from a form typical of a polymer solution to one that more resembles a polymer blend with increasing association near the critical point for phase separation. The model calculations elucidate basic physical principles governing the coupling of self-assembly and phase behavior in these complex mixtures.