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Predicting the dynamics and thermodynamics of nanoparticles in block copolymers

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In applications involving polymer nanocomposites, controlling the dispersion of the nanoparticles is one of the most critical aspects of their design. For example, optimal mechanical properties are typically found when particles are maximally dispersed, while varying the interparticle spacing on the nm length scale can tune the optical properties of a composite. In all of these cases, the distribution of nanoparticles is a complex interplay of entropic and energetic interactions between the matrix polymers, nanoparticles, particle surface-grafted polymers, and even the processing conditions. Recently, my group has been extending the polymer field theory framework to enable the study of inhomogeneous polymer nanocomposites. The framework has the advantage of being computationally efficient and able to treat anisotropic particles (nanorods) and explicit surface chemistry, such as grafted nanoparticles. In this talk, I will describe some of our recent results with the method studying the distribution and interactions between nanoparticles in block copolymer matrices. First, I will show how we have quantified the interactions between nanoparticles and block copolymer grain boundaries. Second, I will describe our more recent efforts using non-equilibrium methods to study the role of processing, such as solvent annealing, on the distribution of nanoparticles in block copolymer thin films.