MAR11-2010-000677

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

"Hairy" Nanoparticles in Block Copolymers and Homopolymers: Modeling using Hybrid Self-Consistent Field Theory

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Today, dispersed nanoparticles play important role in various applications (toughened plastics, healthcare, personal care, etc.) Mesoscale simulations and theory are important in understanding what governs the morphology of nanoparticles under various conditions. In particular, for nanoparticle/block copolymer mixtures, two popular simulation methods are Self-Consistent Field/Density Functional Theory (SCF-DFT) (Thompson, Ginzburg, Matsen, and Balazs, Science 292, 2469 [2001]), and Hybrid Self-Consistent Field Theory (HSCFT) (Sides et al., Phys Rev Lett 96, 250601 [2006]). The two methods are shown to be very similar in their assumptions and end-results; the choice of the method to be used can depend on the specific problem. Here, we use modified HSCFT to explicitly account for the complicated role of short-chain ligands grafted onto nanoparticles to promote dispersion. In particular, we discuss the phase diagrams of such "hairy" nanoparticles in diblock copolymers as function of diblock composition, nanoparticle volume fraction, and ligand length. Depending on the particle size and ligand coverage, particles could segregate into favorable domain, stay close to the interface, or phase-separate from the block copolymer altogether. We also consider the dispersion of "hairy" nanoparticles in a homopolymer and analyze the morphologies of particle clusters as function of ligand length. The results could have interesting implications for the design of new nanocomposite materials.