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Field-theoretic nanocomposite simulations: preliminary results of hybrid particle/SCFT simulations SCOTT SIDES, Tech-X Corporation, GLENN FREDRICKSON, University of California at Santa Barbara — Using block copolymers as mesoscale templates for organic/inorganic nanoparticles has the potential to create patterned particle aggregates that could be used as magnetic storage media and semiconductor materials. More generally, polymer nanocomposites such as these are being investigated for the potential to develop materials with specifically tailored optical, electrochemical, thermal and mechanical properties. The overall behavior of the nanocomposite system depends on the morphology of the polymer chains as well as the arrangement of the particles in the polymer matrix. Self-consistent field theory (SCFT) for dense polymer melts has been highly successful in describing complex morphologies in block copolymers. Field-theoretic simulations such as these are able to access large length and time scales that are difficult or impossible for particle-based simulations such as molecular dynamics, while still incorporating more realistic polymer models than many macroscopic, continuum simulations. In this talk I will outline the SCFT method, discuss some efficient methods of numerically solving the SCFT equations and present results for spherical nanoparticles embedded in an AB diblock copolymer melt. These results have been obtained using a hybrid particle/SCFT approach that treats the polymer in a field theory framework while explicitly retaining the individual nanoparticle coordinates as degrees of freedom.

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