Abstract Submitted
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Large-scale nanocomposites simulations using hybrid particle/SCFT simulations[1] SCOTT SIDES, Tech-X Research — Preliminary results from 2D simulations of block copolymer nanocomposites (Phys. Rev. Lett. Vol 96, 250601 (2006) have been performed using a hybrid self-consistent field theory (SCFT) algorithm. While these simulation results showed that the presence of nanoparticles could induce changes in block copolymer morphologies, quantitative agreement with experiments for the particle densities at this transition are not yet possible. A feature missing in the 2D hybrid simulations is the packing behavior of real, three-dimensional spherical particles embedded in lamellar layers or hexagonally packed cylinders formed by linear diblock chains. In order to carry out these hybrid particle/SCFT 3D simulations a new object-oriented SCFT framework has been developed. The object-oriented design enables the hybrid/SCFT simulations to be performed in a framework that is both numerically efficient and sufficiently flexible to incorporate new SCFT models easily, In particular, this new framework will be used to investigate the distribution of particle positions in diblock lamellar layers as function of nanoparticle density to study the interplay of patterning due to diblock domain structure and the chain depletion interaction between spherical particles.

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