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Modeling of self-assembly in diblock copolymer and particle mixtures using self-consistent field theory SEUNG HA KIM, ERIC COCHRAN, Iowa State University — We use self-consistent field theory (SCFT) to investigate the spatial preference of particle position in the self-assembly of lamellae-forming diblock copolymer and spherical nanoparticle mixtures. We calculate the free energy of the system, which is dependent on the interaction parameter between B segments and particles (χ_{BP}), the effective particle volume fraction (ϕ_{eff}), and the ratio of the particle diameter to block copolymer domain spacing (d_p/d_{BCP}). We show that both small and large particles segregate to the intermaterial dividing surface (IMDS), whereas only for intermediate values of d_p/d_{BCP} particles are located at the center of the domain. These results are interpreted as a subtle consequence of the competition between enthalpic polymer-particle interactions and the chain packing frustration imposed by the particulate inclusion. These findings are useful for understanding the mechanism of spontaneous assembly in block copolymer nanocomposites, and will assist in the rational design of systems where control of the particle placement is crucial.

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