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Field Theoretic Simulations of Polymer Nanocomposites JASON KOSKI, HUIKUAN CHAO, ROB RIGGLEMAN, University of Pennsylvania — Polymer nanocomposites (PNCs) are materials comprised of nanoparticles immersed in a polymer matrix. PNCs are used in a broad range of industries due to the enhanced properties achieved from the coexistence between the polymer and nanoparticle. A global understanding of the physical principles that dictate the equilibrium morphologies of these systems would greatly assist further development of PNCs. While polymer field theory has long been an efficient method to model equilibrium morphologies of inhomogeneous polymer systems, extensions to incorporate nanoparticles are often limited by their accuracy, computational expense, or their restriction to mean-field descriptions. In this talk, I will present a method in which nanoparticles are incorporated into a polymer matrix using a pure field theoretic approach. I provide results that indicate our approach captures correlations in the particle positions that agree identically with particle-based simulations of the same model. Additionally, our method can be applied in a fully-fluctuating field theoretic simulation where the field fluctuations are sampled using complex Langevin dynamics. Finally, I will show demonstrative calculations of the distribution of spherical and cylindrical particles embedded in a diblock copolymer melt.

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