Abstract Submitted
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Predicting the Phase Behavior of Polymer Nanocomposites using Field-Based Simulations[1] JASON KOSKI, ROBERT RIGGLEMAN, University of Pennsylvania — Polymer nanocomposites (PNCs) have been shown to improve mechanical, electric, and optical properties, which are not achievable with polymers or nanoparticles alone. The parameter space associated with PNCs is vast and having efficient tools to study and characterize PNCs is critical to understand parameter-structure-property relationships. In recent years, we have extended the powerful polymer field theory framework to capture particle correlations and allow for efficient characterization of PNCs. We have made numerous strides in extending the class of PNC systems that are able to be studied with polymer field theory; namely, nanospheres, nanorods, complex grafted particles, and liquid crystals. In this talk, I provide details in developing this framework and illustrate its potential by demonstrating its applicability to bulk polymer nanocomposite systems where we can relax the mean-field approximation, study systems with several nanoparticles, and systems that can macro- or microphase separate (e.g. polymer blends or block copolymers). I will also discuss recent advances we have made in incorporating dynamics into our framework which has exciting implications in understanding the phase behavior of PNCs.

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