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Accurate fluctuation-corrected phase diagrams of high-molecular-weight block-copolymer melts KRIS DELANEY, GLENN FREDRICKSON, UC Santa Barbara — We describe a theoretical framework for accurately computing fluctuation-corrected phase diagrams of block polymer melts. The method is based on complex Langevin sampling of a UV regularized field-theoretic model, with Helmholtz free energies computed using thermodynamic integration. UV regularization ensures that the free energies thus computed do not have an arbirary reference; they can be compared between incommensurate phases, permitting for the first time the explicit computational determination of order-order transitions with fluctuation corrections included. We further demonstrate that free energies are accurate in the disordered phase by comparing to perturbation theory on the one-loop level. We note that our method uses no uncontrolled approximations beyond the initial definition of a coarse-grained molecular model for the polymer melt. The method can be applied straightforwardly to melts and solutions containing multiple species with diverse polymer architectures.

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