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Quantifying Fluctuation Effects on the Order-Disorder Transition of Symmetric Diblock Copolymers JING ZONG, QIANG (DAVID) WANG, Department of Chemical and Biological Engineering Colorado State University — How fluctuations change the order-disorder transition (ODT) of symmetric diblock copolymers is a classic yet unsolved problem in polymer physics.[1] Here we unambiguously quantify the fluctuation effects by direct comparisons between fast off-lattice Monte Carlo (FOMC) simulations[2] and mean-field theory using exactly the same model system (Hamiltonian), thus without any parameter-fitting. The symmetric diblock copolymers are modeled as discrete Gaussian chains with soft, finite-range repulsions as commonly used in dissipative-particle dynamics simulations. The effects of chain discretization and finite-range interactions on ODT are properly accounted for in our mean-field theory.[3] Our FOMC simulations are performed in a canonical ensemble with variable box lengths to eliminate the adverse effects of fixed box sizes on ODT.[4] Furthermore, with a new order parameter for the lamellar phase, we use replica exchange and multiple histogram reweighting to accurately locate ODT in our simulations.

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