

Abstract Submitted
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Understanding Fluctuation/Correlation Effects on the Order-Disorder Transition of Symmetric Diblock Copolymers with a Density-Functional Theory JING ZONG, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — How fluctuations change the order-disorder transition (ODT) of symmetric diblock copolymers (DBC) is a classic yet unsolved problem in polymer physics.¹ Taking a model system of discrete Gaussian chains interacting with soft, finite-range repulsions as commonly used in dissipative-particle dynamics simulations we formulate a density-functional theory (DFT) based on the polymer integral equation theories,² which includes the system fluctuations and correlations neglected by the mean-field theory (i.e., the widely applied self-consistent field theory) and can be reduced to the latter under the mean-spherical approximation. We then unambiguously reveal the fluctuation/correlation effects on the ODT of symmetric DBC by direct comparisons among the mean-field theory, DFT, and fast off-lattice Monte Carlo simulations,³ all using exactly the same model system (Hamiltonian) and thus without any parameter-fitting.

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