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Simulation of Fluctuations in Diblock Copolymer Melts: Testing an Alternative to the Fredrickson-Helfand Theory JIAN QIN, CEMS at Univerisyt of Minnesota, DAVID MORSE, CEMS at University of Minnesota — Simulations of a bead-spring model of disordered diblock copolymer melts have been conducted to test a renormalized one-loop (ROL) theory of composition fluctuations recently proposed by the authors. The simulations use hybrid Monte Carlo (MC) / Molecular Dynamics (MD), reptation and double-rebriding moves, combined with replica exchange, to relax chain conformations. The quantitative comparison of simulation results with theory relies on a procedure that uses perturbation theory to independently identify the self-consistent-field (or RPA) interaction parameter. For the modest chain lengths accessible to simulations ($N \leq 64$ here), results for the maximum $S(q^*)$ of the structure factor are quite different from both RPA and Fredrickson-Helfand predictions, but agree very well with renormalized one-loop predictions.

Jian Qin
CEMS at Univerisyt of Minnesota

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