

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Fluctuation/Correlation Effects on the Phase Behavior of Incompressible Polymer Blends Quantified by Fast Lattice Monte Carlo Simulations PENGFEI ZHANG, QIANG WANG, colorado state university — Fast lattice Monte Carlo (FLMC) simulations [Q. Wang, **Soft Matter** **5**, 4564 (2009); **6**, 6206 (2010)] with multiple occupancy of lattice sites and Kronecker δ -function interactions give orders of magnitude faster/better sampling of configuration space for many-chain systems than conventional lattice MC simulations with the self- and mutual- avoiding walk and nearest-neighbor interactions. Adapting the cooperative motion algorithm to a lattice with multiple occupancy, we studied incompressible and symmetric binary polymer blends using FLMC simulations in a semi-grand canonical ensemble with replica exchange and multiple histogram reweighting, and performed finite-size scaling analysis of our simulation results. Comparing the critical point and binodal curve obtained from FLMC simulations with the predictions from the corresponding Flory-Huggins (FH) and Gaussian-fluctuation (GF) theories, all based on the same model system and thus without any parameter-fitting, we unambiguously quantified the effects of fluctuations/correlations neglected in FH theory and treated approximately in GF theory.

Pengfei Zhang
colorado state university

Date submitted: 15 Nov 2013

Electronic form version 1.4