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Fast Lattice Monte Carlo Simulations of Inhomogeneous Polymers QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University, PENGFEI ZHANG, Institute of Physics, Nankai University, XINGHUA ZHANG, DELIAN YANG, Department of Chemical and Biological Engineering, Colorado State University, BAOHUI LI, Institute of Physics, Nankai University — Fast lattice Monte Carlo (FLMC) simulation with multiple occupancy of lattice sites and Kronecker δ-function interactions gives orders of magnitude faster/better sampling of the configurational space of multi-chain systems than conventional lattice MC simulations with self- and mutual- avoiding walks and nearest-neighbor interactions.[1] It also enables direct comparisons with the corresponding polymer field theories based on the same Hamiltonian (thus without any parameter-fitting) to unambiguously and quantitatively reveal the effects of fluctuations and correlations neglected or treated only approximately in the theories. Here we present our FLMC simulations of inhomogeneous polymeric systems including grafted and confined polymers, as well as the comparisons with lattice self-consistent field theory and Gaussian fluctuation theory to quantitatively reveal the consequences of approximations in these theories.

[1]Q. Wang, **Soft Matter, 5**, 4564 (2009).

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