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Quantifying Fluctuations/Correlations in Polymer Brushes QIANG WANG, XINGHUA ZHANG, Department of Chemical and Biological Engineering, Colorado State University, PENGFEI ZHANG, BAOHUI LI, Institute of Physics, Nankai University — Fast lattice Monte Carlo (FLMC) simulations with multiple occupancy of lattice sites and Kronecker δ-function interactions give 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] Using FLMC simulations with Wang-Landau – Transition-Matrix sampling, we have studied polymer brushes in both an implicit and explicit solvent. The various quantities obtained from simulations (including the internal energy, Helmholtz free energy, constant-volume heat capacity, segmental distribution, and chain sizes) are compared with predictions from the corresponding lattice self-consistent field theory and Gaussian fluctuation theory that are based on the same Hamiltonian as in FLMC simulations (thus without any parameter-fitting) to unambiguously and quantitatively reveal the effects of system fluctuations and correlations neglected or treated only approximately in the theories.

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

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