Abstract Submitted
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Fast Lattice Monte Carlo Simulations of Polymers QIANG WANG, PENGFEI ZHANG, Colorado State Univ — The recently proposed fast lattice Monte Carlo (FLMC) simulations (with multiple occupancy of lattice sites (MOLS) and Kronecker δ-function interactions) give much faster/better sampling of configuration space than both off-lattice molecular simulations (with pair-potential calculations) and conventional lattice Monte Carlo simulations (with self- and mutual-avoiding walk and nearest-neighbor interactions) of polymers.[1] Quantitative coarse-graining of polymeric systems can also be performed using lattice models with MOLS.[2] Here we use several model systems, including polymer melts, solutions, blends, as well as confined and/or grafted polymers, to demonstrate the great advantages of FLMC simulations in the study of equilibrium properties of polymers.

[1]Q. Wang, **Soft Matter 5**, 4564 (2009); **6**, 6206 (2010).
[2]P. Zhang and Q. Wang, **Soft Matter 9**, 11183 (2013).

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