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Studying Soft Materials with Soft Potentials – Fast Monte Carlo Simulations JING ZONG, XINGHUA ZHANG, Department of Chemical and Biological Engineering, Colorado State University, PENGFEI ZHANG, YUHUA YIN, BAOHUI LI, Institute of Physics, Nankai University, Tianjin, P. R. China, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — The basic idea of fast Monte Carlo (FMC) simulations[1] is to use soft potentials that allow particle overlapping, instead of hard repulsions (e.g., the Lennard-Jones potential in continuum or the self- and mutual-avoiding walks on a lattice) used in conventional molecular simulations. This gives orders of magnitude faster/better sampling of configurational space. In addition, since soft potentials are commonly used in polymer field theories, using the same Hamiltonian in both FMC simulations and the theories thus allow stringent test of the latter, without any parameter-fitting, to unambiguously and quantitatively reveal the consequences of theoretical approximations. Here we use several systems, ranging from small-molecule liquid crystals to homopolymer solutions and brushes, to demonstrate these great advantages of FMC simulations performed both in continuum and on a lattice.

[1] *Q. Wang and Y. Yin*, **J. Chem. Phys., 130**, 104903 (2009); *Q. Wang*, **Soft Matter, 5**, 4564 (2009).

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