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Fast Off-Lattice Monte Carlo Simulations with a Novel Soft-Core Spherocylinder Model JING ZONG, XINGHUA ZHANG, QIANG (DAVID) WANG, Colorado State University — Fast off-lattice Monte Carlo simulations with soft-core repulsive potentials that allow particle overlapping give orders of magnitude faster/better sampling of the configurational space than conventional molecular simulations with hard-core repulsions (such as in the Lennard-Jones potential).[1] Here we present our fast off-lattice Monte Carlo simulations on the structures and phase transitions of liquid crystals and rod-coil diblock copolymers based on a novel and computationally efficient anisotropic soft-core potential that gives exact treatment of the excluded-volume interactions between two spherocylinders (thus the orientational interaction between them favoring their parallel alignment). Our model further takes into account the degree of overlap of two spherocylinders, thus superior to other soft-core models that depend only on their shortest distance. It has great potential applications in the study of liquid crystals, block copolymers containing rod blocks, and liquid crystalline polymers.

[1] *Q. Wang and Y. Yin*, **J. Chem. Phys., 130**, 104903 (2009).

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