Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Fast Off-Lattice Monte Carlo Simulations with Soft Potentials
JING ZONG, DELIAN YANG, Colorado State University, YUHUA YIN, Nankai University, XINGHUA ZHANG, QIANG (DAVID) WANG, Colorado State University — Fast off-lattice Monte Carlo simulations with soft 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 the hard-sphere or Lennard-Jones repulsion).[1] Here we present our fast off-lattice Monte Carlo simulations ranging from small-molecule soft spheres and liquid crystals to polymeric systems including homopolymers and rod-coil diblock copolymers. The simulation results are compared with various theories based on the same Hamiltonian as in the simulations (thus without any parameter-fitting) to quantitatively reveal the consequences of approximations in these theories.

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

Jing Zong
Colorado State University

Date submitted: 29 Dec 2010 Electronic form version 1.4