Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A new lattice Monte Carlo method for simulating dielectric inhomogeneity[1] XIAOZHENG DUAN, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, ZHEN-GANG WANG, Division of Chemistry and Chemical Engineering, California Institute of Technology, ISSEI NAKAMURA, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — We present a new lattice Monte Carlo method for simulating systems involving dielectric contrast between different species by modifying an algorithm originally proposed by Maggs et al. The original algorithm is known to generate attractive interactions between particles that have different dielectric constant than the solvent. Here we show that such attractive force is spurious, arising from incorrectly biased statistical weight caused by the particle motion during the Monte Carlo moves. We propose a new, simple algorithm to resolve this erroneous sampling. We demonstrate the application of our algorithm by simulating an uncharged polymer in a solvent with different dielectric constant. Further, we show that the electrostatic fields in ionic crystals obtained from our simulations with a relatively small simulation box correspond well with results from the analytical solution. Thus, our Monte Carlo method avoids the need for the Ewald summation in conventional simulation methods for charged systems.

[1]This work was supported by the National Natural Science Foundation of China (21474112 and 21404103). We are grateful to Computing Center of Jilin Province for essential support.

State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese A

Date submitted: 03 Nov 2015 Electronic form version 1.4