Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Novel and Efficient Methods for Calculating Pressure in Polymer Lattice Models PENGFEI ZHANG, QIANG WANG, colorado state university — Pressure calculation in polymer lattice models is an important but nontrivial subject. The three existing methods – thermodynamic integration, repulsive wall, and sedimentation equilibrium methods – all have their limitations and cannot be used to *accurately* calculate the pressure at *all* polymer volume fractions φ. Here we propose two novel methods. In the first method, we combine Monte Carlo simulation in an expanded grand-canonical ensemble with the Wang-Landau – Optimized Ensemble (WL-OE) simulation to calculate the pressure as a function of polymer volume fraction, which is very efficient at low to intermediate φ and exhibits negligible finite-size effects. In the second method, we introduce a repulsive plane with bridging bonds, which is similar to the repulsive wall method but eliminates its confinement effects, and estimate the two-dimensional density of states (in terms of the number of bridging bonds and the contact number) using the $1/t$ version of Wang-Landau algorithm. This works well at all φ, especially at *high* φ where all the methods involving chain insertion trial moves fail.

Pengfei Zhang
colorado state university

Date submitted: 15 Nov 2013 Electronic form version 1.4