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Calculating Pressure and Surface Tension of Lattice Polymers QIANG WANG, PENGFEI ZHANG, Department of Chemical and Biological Engineering, Colorado State University — Calculating pressure and related surface tension of polymeric systems in lattice Monte Carlo simulations is an important but nontrivial subject. Here we propose several novel, efficient, and accurate methods. In the first method, we combine chain insertion/deletion with the Wang-Landau – Optimized Ensemble (WL-OE) simulation, which is very efficient at low to intermediate polymer volume fractions φ. 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. This method works especially well at *high* φ where all the methods using chain insertion/deletion fail. Finally, we combine the above two methods, which gives complete thermodynamics over the *entire* range of continuous and exact φ-values with negligible finite-size effects. To demonstrate our methods, we apply them to calculate the bulk pressure and surface tension of nano-confined homopolymers.

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