Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Surface Tension of Nano-Confined Lattice Polymers PENGFEI ZHANG, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — Surface tension at solid/liquid interface is a key concept in understanding many important surface and interfacial phenomena such as wetting and capillarity. It is, however, not trivial to accurately calculate surface tension in lattice Monte Carlo (LMC) simulations, which are much faster than simulations in continuum. Here we propose a novel, efficient, and accurate method for calculating the surface tension of polymers confined between two parallel and impenetrable surfaces in LMC simulations, and examine how surface tension varies with the degree of confinement (i.e., separation distance between the two surfaces). Direct comparisons between our LMC results and the corresponding lattice self-consistent field (LSCF) calculations also unambiguously and quantitatively reveal the fluctuation/correlation effects on surface tension neglected in LSCF theory. Keywords: Surface tension, lattice polymers, Monte Carlo simulations

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Date submitted: 14 Nov 2014 Electronic form version 1.4