Abstract Submitted
for the NWS11 Meeting of
The American Physical Society

Thermodynamic Consistency in Highly Coarse-Grained Models of Polymer Melts JAMES MCCARTY, MARINA GUENZA, University of Oregon — One of the main obstacles to the widespread application of coarse-graining methods in materials science is the lack of thermodynamics consistency between various hierarchical levels of description. Oftentimes, effective potentials that are optimized to reproduce one property of the system, such as the pair distribution function, fail to reproduce other properties of interest. Here we present a quantitative coarse-grained model of a polymer melt that preserves thermodynamic consistency and reproduces the correct equation of state of the system. Comparison is made to molecular dynamics simulations of various models and to results from integral equation theory. We also discuss some of the implications coarse-graining has for the entropy and free energy of the system due to a reduction of the degrees of freedom in the model.

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Date submitted: 16 Sep 2011 Electronic form version 1.4