Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Theoretically Informed Coarse-Grained Simulations of Polymer Nanogels PRATEEK JHA, JOS ZWANIKKEN, Northwestern University, FRANCOIS DETCHEVERRY, JUAN DE PABLO, University of Wisconsin - Madison, MONICA OLVERA DE LA CRUZ, Northwestern University — Nanoscale finite-sized polymer networks (nanogels) are smart responsive materials that undergo large reversible volume changes with moderate changes in environmental conditions such as temperature, pH, light, and electric field. We develop a coarse-grained model of nanogels in terms of experimentally measurable physical quantities, and perform a theoretically informed Monte Carlo simulation that combines ideas from both the particle and continuum approaches of polymer physics. The elastic interactions are treated through beads connected by harmonic springs ("particles"), and the van der Waals and electrostatic interactions are treated by weighted densities ("fields"). Our simulations predict high degrees of swelling and a discontinuous volume phase transition in ionic nanogels, in contrast to moderate swelling and a continuous volume phase transition for the non-ionic case. We analyze the effects of mesh-size, polymer charge fraction, ionic strength, and solvent quality, on the swelling behavior of nanogels. A comparison is made with the results of a simplified continuum model, where the electrostatic interactions are treated using the Poisson-Boltzmann approximation.

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Date submitted: 16 Dec 2010 Electronic form version 1.4