Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Effective Pair Potentials and Mesoscale Simulations of Binary Polymer Blends JAMES MCCARTY, MARINA GUENZA, Department of Chemistry, University of Oregon, Eugene, Oregon — Macromolecular mixtures are complex fluids characterized by an extended range of relevant length scales, such as the diverging length scale of concentration fluctuations, which develops when two chemically distinct polymers in a blend approach the spinodal. Such macroscopic phenomena readily exceed box sizes commonly used to model polymer ensembles, yet depend specifically on local interactions between monomers. To overcome this problem, we present an implementation of our analytical coarse-graining procedure, which maps a binary mixture of polymers into a system of interacting colloidal particles. By utilizing the hypernetted-chain closure, we derive a "soft" effective potential acting between coarse-grained units, which is explicitly parameter dependent. From computer simulations of various polymer systems under different thermodynamic conditions we calculate pair correlation functions and show that our mesoscale simulations capture the relevant trends expected for demixing as the thermodynamic conditions are changed.

James McCarty
University of Oregon

Date submitted: 17 Nov 2009 Electronic form version 1.4