Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Can coarse-grained force field parameters be transferable? MALGORZATA KOWALIK, Department of Chemical Engineering, 121 Fenske Laboratory, University Park, Pennsylvania 16802, USA, JANNA K. MARANAS, Department of Chemical Engineering, 107 Fenske Laboratory, University Park, Pennsylvania 16802, USA — We present results from molecular dynamics simulations of self-assembled copolymers in explicit coarse-grained water. Our goal is to provide intermolecular potentials for coarse-grained beads that are mixture independent. With such transferable potentials, forming new combinations of copolymers and adding new polymers is relatively straightforward. In this approach, each coarse-grained bead (polymer as well as water) is assigned mixture independent Lennard-Jones parameters. We use generic combining rules, with a pair-independent scaling parameter for interactions between hydrophilic and hydrophobic beads. We succeed in describing six coarse-grained beads system using only six intermolecular parameters, to describe 15 individual interactions. We conclude that a transferable set of intermolecular parameters is possible.

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Date submitted: 28 Nov 2012 Electronic form version 1.4