Abstract Submitted
for the OSF05 Meeting of
The American Physical Society

Computational studies of model polymers in solution SAYURI ICHIDA, TYSON PAPAY, GREGORY PETERSEN, MARK TAYLOR, Dept. of Physics, Hiram College — The conformation of a polymer molecule in solution is strongly dependent on the "quality" of the solvent. In a good solvent a chain is expanded or swollen relative to an isolated chain while in a poor solvent a chain is in a compact or collapsed state. In this work we present a series of Monte Carlo simulation studies of a single interaction-site polymer in an explicit monomeric solvent. In particular, we have studied both a hard-sphere chain and a hard-sphere ring in a hard-sphere solvent, a hard-sphere chain tethered to a surface in a hard-sphere solvent, and a square-well chain in a square-well solvent. In all cases, the hard sphere solvent is found to compress the hard sphere polymer thus acting as a poor solvent. For the square-well system both chain expansion and chain compression are observed as the solvent quality changes from poor to good with decreasing temperature. Application of these results to developing accurate solvation potentials for polymer-in- solvent systems will be discussed.

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Date submitted: 28 Sep 2005 Electronic form version 1.4