Abstract Submitted
for the OSF09 Meeting of
The American Physical Society

**Conformation of a Lennard-Jones Chain in Explicit Solvent: A Solvation Potential Approach**[1] SHISHIR ADHIKARI, MARK TAYLOR, Hiram College — Computer modeling of polymer systems is important both for developing new materials and understanding how biological macromolecules function. This type of modeling is made difficult by the large system sizes required to study a polymer chain in solvent. The problem can be formally simplified by mapping the "many-body" chain-in-solvent system to a single chain plus a "few-body" effective potential that mimics the role of the solvent. This few-body potential (where few = the number of chain monomers) depends on the instantaneous conformation of the chain and is, in general, not practical to compute. Thus, one generally assumes a two-site decomposition of this potential. Here we use Monte Carlo simulation techniques to study a Lennard-Jones chain-in-solvent system. We construct a set of "exact" two-site solvation potentials for a 5-mer chain thereby demonstrating the validity of the two-site approximation. We then construct approximate solvation potentials for long chains, which combine exact short chain results with the pure solvent potential of mean force. Our solvation potential results compare well with simulation results for the full chain-in-solvent systems.

[1]Financial support was provided NSF grant DMR-0804370 and Hiram College.

Mark Taylor
Hiram College

Date submitted: 18 Sep 2009 Electronic form version 1.4