

Abstract Submitted
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Conformation of a Lennard-Jones Chain in Explicit Solvent: A Solvation Potential Approach¹ SHISHIR ADHIKARI, MARK TAYLOR, Dept. of Physics, Hiram College — The conformation of a polymer chain in solution is intrinsically coupled to the chain's local solvent environment. In much of the theoretical work on polymers in solution the effects of solvent are treated implicitly and explicit chain-solvent coupling is ignored. Although a formally exact treatment of chain-solvent coupling can be constructed, the required many-body solvation potential is not practical to compute. Following on our work with hard-sphere and square-well chain-in-solvent systems [1] here we show that for Lennard-Jones (LJ) systems this many-body solvation potential can be made tractable via an “exact” decomposition into a set of two-site potentials. We use these exact short chain results, combined with the pure solvent potential of mean force, to construct approximate two-site solvation potentials for long LJ-chains. Monte Carlo simulations for full chain-in-solvent systems verify the accuracy of our solvation potential mapping across the full LJ-solvent phase diagram.

[1] J. Chem. Phys. 127, 184901 (2007); J. Polym. Sci., Part B: Polym. Phys. 45, 3319 (2007).

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Mark Taylor
Dept. of Physics, Hiram College

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