

Abstract Submitted
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Solvent induced unfolding of a polymer chain¹ ELIZABETH BREEN, MARK TAYLOR, Dept. of Physics, Hiram College, Hiram, OH — Many bio-molecules fold into specific 3D shapes that are closely associated with their functions. For many small proteins this folding transition follows an all-or-none process analogous to a first-order phase transition. Here we study a simple homo-polymer model that undergoes a similar type of folding transition and thus may provide some insight into the underlying physics of protein and bio-molecule folding [1]. In particular we investigate solvent induced folding or unfolding of a chain in a dense solvent environment. We study a flexible square-well-sphere chain in an explicit solvent of hard spheres. There is an adjustable attractive interaction between the solvent and the chain that mimics the effects of changing the solvent pH or concentration of a chemical denaturant. Starting from conditions favoring a folded polymer, increasing the chain-solvent interaction causes the solvent molecules to "stick to" or solvate the chain. This solvation effect can disrupt the folded chain structure, driving the chain into an open, unfolded conformation. Here we use both Wang-Landau and Metropolis Monte Carlo simulation techniques to study this isothermal, solvent-driven chain unfolding process. [1] Taylor, Paul, and Binder, J. Chem. Phys. 145, 174903 (2016).

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