Abstract Submitted
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Polymer phase transitions in a dense solvent[1] RYOGO SUZUKI, MARK TAYLOR, Dept. of Physics, Hiram College — In this research, we investigate the physics of a model polymer in explicit solvent using computer simulations. In particular, we examine how the presence of explicit solvent affects the conformational phase transitions of a polymer chain between expanded, collapsed, and folded states. We study a flexible 16-bead square-well-sphere chain with short-range interactions in a hard sphere solvent across a range of solvent densities. Using the Wang-Landau algorithm we compute the single chain density of states for this system and thus are able to construct the canonical partition function. From the partition function we can determine all thermodynamic properties, including average energy, specific heat, and energy probability distribution functions. We find the dense hard sphere solvent acts to slightly stabilize the folded state of the chain and suppresses the polymer collapse transition.

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