

Abstract Submitted
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Phase Transitions and Helix Formation of a Fused Square-Well-Sphere Chain¹ MICHAEL MROZ, MARK TAYLOR, Dept. of Physics, Hiram College — This study involves observing phase transitions of a flexible polymer chain made of $N = 20$ square-well-sphere monomers, with the hard-core diameter σ and square-well diameter $\lambda\sigma$, connected by bonds of fixed length $L < \sigma$. The density of states of the polymer is calculated using the Wang-Landau simulation technique. The density of states was then utilized to compute thermodynamic and average structural properties of the chain. A temperature-interaction range (T- λ) phase diagram was constructed for a chain of bond length $L = 0.625\sigma$. With decreasing temperature this chain undergoes a coil-globule (i.e., collapse) transition followed by one or more low temperature transitions to an ordered ground-state structure. For $\lambda > 1.25$ this ground state is a simple helix while for smaller λ the ground state is a wrapped structure, in which one end of the chain forms a linear core about which the rest of the chain is helically wound. The low temperature transition takes on a first-order character for $\lambda < 1.1$.

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Mark Taylor
Dept. of Physics, Hiram College

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