Abstract Submitted
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Protein-like folding and other phase transitions of a single polymer chain[1] MARK TAYLOR, Dept. of Physics, Hiram College, WOLFGANG PAUL, Martin-Luther-Universitat, Halle, Germany, KURT BINDER, Johannes-Gutenberg-Universitat, Mainz, Germany — A single polymer chain can undergo a series of conformational transitions analogous to the phase transitions exhibited by bulk materials. We have recently studied the conformational transitions of a flexible square-well polymer chain using a Wang-Landau simulation approach in which we directly compute the single-chain partition function [1]. For the case of a tangent-sphere chain, the temperature-interaction range phase diagram includes both a coil-globule and globule-crystal transition as well as an "all-or-none" coil-crystal transition. Despite the non-unique homopolymer ground state, the thermodynamics of this direct freezing transition are identical to the thermodynamics of two-state protein folding. Two-dimensional configurational and free energy landscapes reveal both a dominant "folding" pathway and a "dead-end" pathway resulting in a bimodal distribution of structures at the top of the free energy barrier. A simple AB-heteropolymer variant of this model leads to both rod-like and disk-like ground state structures while a fused sphere version of the model produces helical folded structures.

[1] M.P. Taylor, W. Paul, and K. Binder, Polymer Science Ser. C 55, 23 (2013).

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