Abstract Submitted
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Energy landscapes for a homopolymer protein-like folding transition[1] MARK TAYLOR, Dept. of Physics, Hiram College, WOLFGANG PAUL, Martin-Luther-Universitat, Halle, Germany, KURT BINDER, Johannes-Gutenberg-Universitat, Mainz, Germany — Many small proteins fold via a first-order "all-or-none" transition directly from an expanded coil to a compact native state. We recently reported an analogous direct freezing transition from an expanded coil to a compact crystallite for a simple flexible homopolymer [1]. Wang-Landau sampling was used to construct the 1D density of states for square-well chains up to length 256. Analysis within both the micro-canonical and canonical ensembles shows that, for a chain with sufficiently short-range interactions, the usual polymer collapse transition is preempted by a direct freezing transition. A 2D configurational probability landscape, built via subsequent multi-canonical sampling, reveals both a dominant folding pathway and an inherent configurational barrier to folding. Despite the non-unique homopolymer ground state, the thermodynamics of this direct freezing transition are identical to the thermodynamics of two-state protein folding. A free energy barrier separates a high entropy ensemble of unfolded states from a low entropy set of crystallite states and the transition proceeds via the formation of a transition-state folding nucleus.

[1] Phys. Rev. E 79, 050801(R) (2009); J. Chem. Phys. 131, 114907 (2009).

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