Abstract Submitted
for the OSS11 Meeting of
The American Physical Society

**Protein-like folding and free energy landscape of a homopolymer chain**[1] MARK TAYLOR, Dept. of Physics, Hiram College, WOLFGANG PAUL, Martin-Luther-Universität, Halle, Germany, KURT BINDER, Johannes-Gutenberg-Universität, 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 have recently reported an analogous direct coil-to-crystallite transition for a flexible homopolymer [1]. Wang-Landau sampling was used to construct the 1D density of states for square-well chains up to length 256 and a microcanonical analysis shows that for short-range interactions the usual polymer collapse transition is preempted by a direct freezing transition. A 2D configurational probability landscape, built via multi-canonical sampling, reveals 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 those of two-state protein folding. Homopolymer folding proceeds over a free energy barrier via a transition state folding nucleus, displays a protein-like Chevron plot, and satisfies the van't Hoff two-state criterion.

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

[1] Funding: NSF DMR-0804370 and DFG SFB-625/A3

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Date submitted: 11 Mar 2011

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