Abstract Submitted
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Replica-Exchange Wang-Landau Simulations of a Semi-flexible H0P Lattice Protein Model for Crambin ALFRED FARRIS, GUANGJIE SHI, Center for Simulational Physics, The University of Georgia, THOMAS WÜST, Scientific IT Services, ETH Zurich, DAVID P. LANDAU, Center for Simulational Physics, The University of Georgia — The oft studied hydrophobic-polar (HP) lattice protein model has the disadvantage of producing highly degenerate ground states, which is in disagreement with the unique native states found in real proteins. The recently proposed H0P model adds a "neutral" monomer (0), in an attempt to more precisely account for the hydrophobicity of different amino acid residues and has been shown to drastically decrease the ground state degeneracy without significantly increasing sampling difficulty[1]. Here we proposed a further modification to the model by introducing an energetic penalty for "bends" in the protein, effectively accounting for the natural rigidity of real proteins[2]. Using replica-exchange Wang-Landau sampling, we investigated such a semi-flexible H0P model for Crambin, a hydrophobic plant protein consisting of 46 amino acids. With these modifications to the original HP model, we uncovered a new step in the folding process, and obtained a single, non-degenerate (unique) ground state.

[1]G. Shi, T. Wüst, Y. W. Li, and D. P. Landau, J. Phys.: Conf. Ser. 640, 012017 (2015)
[2]G. Shi, A. C.K. Farris, T. Wüst, and D. P. Landau, J. Phys.: Conf. Ser. 686, 012001 (2016)

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