Abstract Submitted
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Replica-exchange Wang-Landau simulations of the H0P lattice protein model[1] GUANGJIE SHI, Center for Simulational Physics, The University of Georgia, THOMAS WÜST, ID Scientific IT Services, ETH Zürich, Switzerland, YING WAI LI, National Center for Computational Sciences, Oak Ridge National Laboratory, DAVID P. LANDAU, Center for Simulational Physics, The University of Georgia — The hydrophobic-polar (HP) lattice protein model has been the subject of intensive investigation in an effort to aid our understanding of protein folding. However, the high ground state degeneracies caused by its simplification stands in contrast to the generally unique native states of natural proteins. Here we proposed a simple modification, by introducing a new type of "neutral" monomer, 0, i.e. neither hydrophobic nor polar, thus rendering the model more realistic without increasing the difficulties of sampling significantly[2]. With the replica exchange Wang–Landau (REWL) scheme [3] we investigated several widely studied HP proteins and their H0P counterparts. Dramatic differences in both ground state and thermodynamic properties have been found. For example, the H0P version of Crambin shows more clear two-step folding and 3 order of magnitudes less ground state degeneracy than its HP counterpart.

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[2]G. Shi, T. Wüst, Y. W. Li and D. P. Landau J. Phys.: Conf. Ser. 640, 012017 (2015)
[3]T. Vogel, Y. W. Li, T. Wüst, and D. P. Landau, Phys. Rev. Lett., 110, 210603 (2013)

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