Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Generic transition hierarchies of lattice HP protein adsorption: A Wang-Landau study[1] YING WAI LI, D.P. LANDAU, Center for Simulational Physics, University of Georgia, T. WÜST, Swiss Federal Research Institute — We have applied Wang-Landau sampling with appropriate trial moves[2] to investigate the thermodynamics and structural properties of the HP lattice protein model[3] interacting with an attractive substrate. The conformational "phase transitions" of several benchmark HP sequences have been identified by a comprehensive canonical analysis of the specific heat and structural observables, e. g. radius of gyration and thermal derivatives of number of surface contacts. Three major "transitions": adsorption, hydrophobic core formation, and "flattening" of adsorbed structures, are observed. Depending on the surface attractive strength relative to the intra-protein attraction among the H monomers, these processes take place in a different order upon cooling. We identify a small number of generic categories that are sufficient to classify the folding hierarchies for different HP chains consisting of assorted sequences and chain lengths, regardless of the monomer type that the surface attracts. We thus believe that this classification scheme is generally applicable to lattice protein adsorption problems.

[1]Research supported by NSF.
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Date submitted: 14 Nov 2011 Electronic form version 1.4