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Title: Surface adsorption of lattice HP proteins: studies on thermodynamics and structural transitions using Wang-Landau sampling

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We have applied Wang-Landau sampling to investigate the thermodynamics and structural properties of lattice hydrophobic-polar heteropolymers (commonly known as the HP protein model) 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 such as radius of gyration and number of surface contacts. Three major "transitions", namely adsorption-desorption, collapse (formation of hydrophobic core) and "flattening" of adsorbed structures, are observed. Depending on the surface attractive strength relative to the inter-protein attraction among the H monomers, these processes take place in different orders upon cooling, which can be classified into a few categories. Such a connection of folding hierarchy with the surface attraction is found to be generic 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 polymer and protein adsorption problems and may even apply to off-lattice models.