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Title: Conformational transitions of a confined lattice protein: A Wang-Landau study

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We use Wang-Landau sampling with suitable Monte Carlo trial moves to study a hydrophobic-polar (HP) lattice protein confined between two parallel attractive walls. The density of states is determined iteratively by a random walk in energy space. Thermodynamic and structural properties, such as specific heat, number of surface contacts and radius of gyration, are then calculated. When the surface attraction is comparable to the internal attraction among the hydrophobic monomers in the chain, two conformational "transitions", adsorption at higher temperature and collapse at lower temperature, have been analyzed based on these properties. The transition behaviors are also confirmed by snapshots of typical conformations of the system. Reducing the separation between the two attractive surfaces decreases the vertical degree of freedom of the chain, resulting in a lower adsorption temperature and a smaller peak in the specific heat, while the collapse transition temperature is not affected. It is also observed that the difference in adsorption temperatures determined by the positions of the peaks in the specific heat and the derivative of the number of surface contacts systematically increases with the reduction of surface separation.