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Adsorption of HP Lattice Proteins on Patterned Surfaces[1]
MATTHEW WILSON, GUANGJIE SHI, DAVID P. LANDAU, The University of Georgia, YING WAI LI, Oak Ridge National Laboratory, THOMAS WUEST, Swiss Federal Research Institute WSL — The HP lattice model[2] is a course-grained, yet useful tool for modeling protein sequences where amino acids are treated as either hydrophobic (H) or polar (P) monomers. With the use of Wang-Landau sampling and an efficient set of Monte-Carlo moves[3], HP lattice proteins adsorbed on patterned surfaces are studied. Each substrate is modeled as a periodically bounded pattern of lattice sites that interact with either H or P monomers in the lattice protein, where the energy contributions of the surface are determined by assigned coupling strengths. By analyzing energy degeneracies, along with the thermodynamic and structural quantities of the protein, both the protein folding and surface adsorption can be observed. The adsorption behavior of the lattice proteins on patterned surfaces will be compared to those interacting with uniform surfaces.

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[3]T. Wüst and D. P. Landau, J. Chem. Phys. 137, 064903 (2012).

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