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Structure and stability of proteins upon adsorption to hydrophobic surfaces SUMIT SHARMA, Columbia University, GAURAV ANAND, GEORGES BELFORT, Rensselaer Polytechnic Institute, SANAT KUMAR, Columbia University — Experimental evidence suggests that protein molecules adsorbed to hydrophobic surfaces are thermally more stable than in the bulk. To understand this observation, adsorption of a model lattice protein on hydrophobic surfaces was studied using Monte Carlo simulations. It was observed that surfaces with intermediate hydrophobicities can stabilize the secondary structure in adsorbed protein molecules. This happens because an unfolded protein molecule loses conformational freedom upon adsorption, thereby driving the melting point to higher values. However, highly hydrophobic surfaces perturb the secondary structure of the adsorbed proteins. Overall, depending on the magnitude of the surface hydrophobicity, different equilibrium regimes of proteins, namely, aggregated-desorbed; folded-adsorbed; highly aggregated-adsorbed; and weakly aggregated-strongly adsorbed are observed.

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