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Computational Investigation of Conformational Changes in Proteins upon Adsorption SUMIT SHARMA, Columbia University, GAURAV ANAND, GEORGES BELFORT, Rensselaer Polytechnic Institute, SANAT K. KUMAR, Columbia University — Amyloidogenic diseases, such as, Alzheimer's, are caused by adsorption and aggregation of partially unfolded proteins. Protein adsorption is often accompanied by conformational rearrangements, which are thought to affect many properties such as their adhesion strength to the surface, biological activity, and aggregation tendency. Experiments have shown that many proteins, upon adsorption to hydrophobic surfaces, undergo a helix to sheet or random coil secondary structural rearrangement. To better understand the equilibrium structural complexities of this phenomenon, we have performed Monte Carlo (MC) simulations and Single Chain Mean Field calculations of adsorption of different proteins, modeled as lattice chains, to study the adsorption behavior and equilibrium protein conformations at different temperatures, protein concentration and surface hydrophobicity. Free energy and entropic effects on adsorption have been studied by determining density of states using Weighted Histogram Analysis Method. Conformational transitions of proteins on surfaces will be discussed as a function of surface hydrophobicity.

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