Controlling protein adsorption modes electrostatically

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Protein adsorption on surfaces is ubiquitous in biology and in biotechnology. Here, we introduce an explicit ion coarse-grained molecular dynamics simulation approach for studying the effects of electrostatics on protein adsorption, and 2D protein assembly on charged surfaces. Our analysis suggests that the mode of protein adsorption onto the surface is determined by a local interaction between protein and surface. Moreover, under an increasing salt concentration, we observe that a dense hexagonal structure changes into a sparse structure, which on further increasing the salt concentration dissolves into the bulk solution. This study provides a useful guide for understanding protein adsorption, and the 2D assembly of proteins on surfaces.

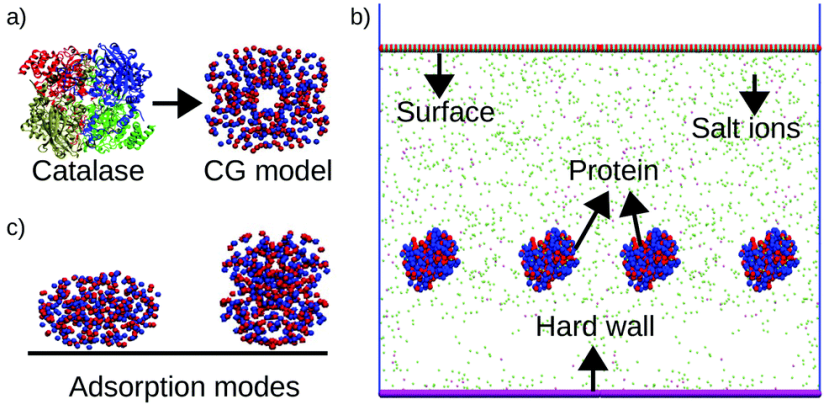

Figure: Schematic of a protein adsorption study. (a) Detail structure of a catalase enzyme (pdb: 1TGU) and its coarse-grained model. (b) Simulation box containing a system of proteins, a charge embedded surface, a hard wall, and explicit salt ions. (c) Two adsorption modes; one via the largest (termed here "flat on") and another via the smallest (termed "standing up") interface contact.

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