The role of electrostatics in the protein adsorption process on nanostructured surfaces: a multiscale approach based on the Poisson-Boltzmann equation and molecular dynamics

Speaker

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Protein adsorption on nanostructured surfaces is a critical process in the design and development of biotechnological applications such as biosensors and biocatalytic surfaces. These devices are widely used to detect target molecules through a bioreceptor immobilized on a surface, and their performance is closely related to variables such as orientation of the bioreceptor, the number of adsorbed proteins, and conformational changes during immobilization. Although the adsorption arises due to a competition between different processes, under a specific conditions, mean-field electrostatic plays a dominant role with direct influence on the coverage and orientation of adsorption. In this talk, I will present a multiscale strategy coupling Molecular Dynamics and the Poisson-Boltzmann equation to study the effect of electrostatics and structural rearrangement in protein-surface interaction through an MMPBSA approach[1].

Under this methodology, the structure conformational changes due to adsorption on a surface are predicted with a molecular mechanics model, and the solvation free energy landscape is computed with an implicit solvent model. The computational workflow will be based on Amber24[2] to perform molecular dynamic simulations, PyGBe[3] to solve Poisson-Boltzmann equation, that allows us to evaluate the electrostatic solvation free energy for different orientations; and MDTraj to calculate the molecular surface (SASA) of each of the configuration, variable required to compute the non-polar solvation free energy. We will focus on discussing the role of electrostatics in an experimental/computational application case: the interaction of trypsin with a carbon electrode under external electric fields, and how these polar effects might affect enzyme activity in the context of biosensor design[4].

In addition, I will introduce how conformational changes due to temperature would affect the interaction with nanostructure surfaces, taking as an example L-lysine oxidase interacting with graphene oxide.

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