Proposition de stage M2 pour 2017

Modeling enzymes orientations on electrode surfaces for green energy production

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Sujet :

Enzymes are very efficient biocatalysts that convert a large panel of substrates in a large diversity of environments. Once immobilized on conductive supports, redox enzymes can favorably replace rare and expensive platinum-based catalysts in devices such as fuel cells. Thanks to the current research concerning H_2 production from renewable sources including biomass fermentation or enzymatic splitting of water, H_2/O_2 biofuel cell can thus be considered as a fully "green" device for energy production.

The ENZYMOR ANR project aims to elucidate the molecular mechanisms that control the efficiency of enzymes in the immobilized state which are required to enhance both the stability and performances of the H2/O2 biofuel cell. Although efficient enzymes for H_2 oxidation and O_2 reduction are identified and the catalytic mechanisms in homogeneous and heterogeneous phases are quite well described, a cartography of the enzymes effectively participating to the catalysis in the immobilized state is still not available. The conformation of the immobilized enzymes and the variation of this conformation as a function of parameters such as the electric field, pH, ionic strength, covalent binding are largely unknown. Because they are few nanometers size macromolecular objects, the rate of the interfacial electron transfer relies on the proper structural orientation of the enzymes on the electrode that put the surface electronic relay at a tunneling distance from the electrode. However no tools are available yet to discriminate between the different orientation states and to correlate them with the enzymatic activity.

These are the main objectives of ENZYMOR which unites electrochemists, spectroscopists, and theoretical chemists to develop new required experimental setups and define the molecular basis for efficient enzyme immobilization, including optimized electron transfer rates, reduced biomolecule amount and increased stability with time and under turn-over of immobilized enzymes.

The molecular modeling team in LBT seeks a highly motivated candidate to model the interaction of enzymes with an electrode surface. We develop state-of-the-art computer simulation methods to study the properties of membrane-bound enzymes of the hydrogenase family and their interaction with electrode surfaces. **Using molecular dynamics or coarse grained approaches to drive these simulations, you will explore these systems to guide experiments on innovative fuel-cell prototypes**. The goal is to optimize electron transfer by properly positioning and immobilizing hydrogenases on the electrode support.

This internship might eventually lead to a PhD thesis funded by the ANR.

Compétences souhaitées

We are looking for a student with

- knowledge in molecular modeling or computational chemistry acquired during university course work or internship

- and/or knowledge of the Linux environment and basic skills in programming or computing.