Electrostatic modeling of the interaction of [NiFe] hydrogenases with graphite electrodes

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Hydrogenases are a group of enzymes that have caught the interest of researchers in renewable energies in the last years, due their ability of catalyze the redox reaction of hydrogen:

$$2H^+ + 2e^- \leftrightarrow H_2$$

This reaction indicates that hydrogenases could be used to produce hydrogen or electricity whitin electrochemical cells[1]. One of the problems of the implementation of hydrogenases in electrochemical devices is to immobilize the enzyme on the surface of the electrodes. The orientation of the enzyme with respect of the electrode surface is important in order to ensure a good flux of electrons to the catalytic center. In this talk I will discuss a computational approach to determine the possible orientations of a hydrogenase (pdb code: 1e3d) on a graphite electrode, as a function of pH, salinity and electrode potential. The calculations are based on the linearized Poisson-Boltzmann equation using the PyGBe software[2]. The preliminary results at pH 7 suggest that under potentials of 0.05 and 0.0 V, the amino acid Glu 155 is the closest to the surface of the electrode. While under a negative potential of -0.05 V the closest amino acid is His 351. This type of information can be valuable in the development of more efficient bio-electrochemical devices.

1. Bat-Erdene J., Welch J., Kondo-Francois A., and Marquis C. 2013. Fundamentals and electrochemical applications of [Ni–Fe]-uptake hydrogenases. RSC Advances (3) 8142- 8159.

2. Cooper C. and Barba L. 2016. Poisson–Boltzmann model for protein–surface electrostatic interactions and grid-convergence study using the PyGBe code. Computer Physics Communications 202, 23–32.