BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA
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"QM/MM simulations of the electrochemical interface"

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Abstract: Understanding the interface between electrolytes and electrified metallic surfaces is essential for many technological applications, but still poses important scientific challenges. Computer simulations could contribute to solve them, but to simulate accurately and realistically the interface is not an easy task. For Density Functional Theory (DFT) simulations, in particular, the complexity of the interface, the presence of the electrode's potential, and the very long time scales involved, represent serious obstacles. In previous work, we have proposed a method, based on Non-Equilibrium Green's Functions (NEGFs), to perform DFT simulations in the presence of externally imposed electrode potentials, and have implemented this NEGF-DFT methodology in the SIESTA code. Although successful in describing the effect of the electrified surface, the method still suffers the drawback of only being able to access times scales of up to tenths of nanometers, too short to fully describe the response of the electrolyte to the applied potential. In this talk, we will describe the ideas behind the use of NEGFs to study the electrochemical interface, and some multiscale approaches to reach larger system sizes and longer time scales in our DFT simulations. One of them is a hybrid QM/MM approach which, linked to the NEGF-DFT methodology, allows to reach longer simulation times. We will describe the application of these methods in different problems, including the use of organic compounds to inhibit corrosion in metals.

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