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HiFunMat
The Interdisciplinary thematic institutes
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funded under the Excellence Initiative program

ITI HiFunMat Master Internship Proposal

☒ M 1   ☒ M 2

Title : <u>Molecular Dynamics of electrochemical systems</u>

Internship supervisor

Name, first name	Asset, Tristan; Wolff, Jules
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Laboratory	ICPEES, CNRS
Collaboration with a HiFunMat member (*please indicate their name*)	☐ No ☒ Yes : SAVINOVA Elena

Student profile looked for

Master program (*more than one box can be ticked*)	☒ Material science and engineering ☒ Chemistry ☒ Physics
Other indications if necessary	

Internship description

Whereas chemical reactions frequently occur in homogeneous environments, electrochemical reactions take place exclusively at the interface between an electrode and an electrolyte. Due to the localized nature of this reaction, understanding this interface is critical, as even the slightest of its properties (*e.g.,* local pH, arrangement of cations in the electrolyte, etc.) can drastically affect the kinetics and thermodynamics of the said reaction. The properties in question are primarily influenced by (i) local variations of reactants and products inherent to the reaction itself and (ii) the reorganization of the interface induced by the application of a potential. Understanding this interface is, in fact, crucial in order to better design future electrochemical systems.

Currently, the Guy-Chapman-Stern model is widely used to predict the distribution of charges as a function of distance from the electrode, within the first nanometers between the electrode and the core of the solution (defined as the "electrochemical double layer"). However, this model has limitations. Firstly, it treats ions as point charges, i.e., completely neglecting their volume and mass. Secondly, it does not account for neutral molecules that can nevertheless affect interactions near the electrode. In this context, the use of molecular dynamics allows for simulating a realistic representation of the reorganization of molecules in the solution and also accounts for uncharged molecules.

Recently, a simulation tool called MetalWalls has been developed, offering the possibility to rigorously simulate electrodes and the applied potential (an illustration of an interface constructed through MetalWalls is presented in **Figure 2**). In classical models, the electrode is approximated to a charged wall, but with MetalWalls, it is possible to dynamically represent the charge distribution in the electrode according to associated physical models. The initial simulations conducted with MetalWalls have highlighted divergences from the Guy-Chapman-Stern model. Indeed, the electrochemical double layer is influenced by a much

broader set of variables than those used in the latter (with an example of profile provided in **Figure 1**). Furthermore, the electrode material plays a crucial role in the distribution and orientation of molecules, including those of the solvent, which is also affected by the nature and concentration of charges near the electrode. This information is essential and contributes to explaining phenomena observed experimentally, in terms of reactivity for various electrochemical systems.

During this internship, the objective is to undertake an in-depth study of the different parameters that influence the concentration distribution near the electrode-electrolyte interface. The selected candidate will have three main tasks: firstly, to study the impact of temperature and concentration on the structure of the electrochemical double layer; secondly, to identify solvent orientation trends based on simulation parameters (*e.g.,* potential, temperature, types of ions in solution); finally, to develop an analysis method for the conducted simulations. In this perspective, a solid knowledge of electrochemistry as well as a basic understanding of molecular dynamics and cheminformatics are necessary.
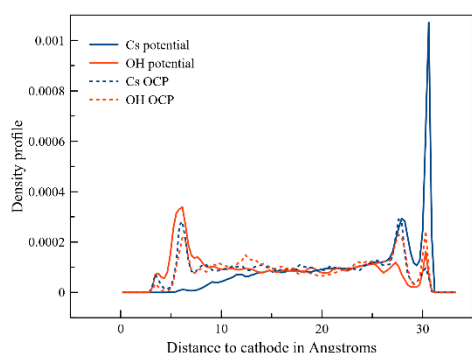

Figure 1 : Concentration distribution of Cs and OH ions in water with graphene electrode as a function of potential (OCP = open circuit potential, potential = 1V difference between the electrodes).
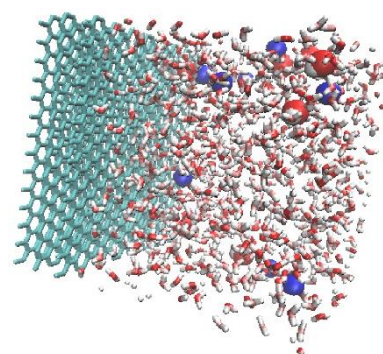

Figure 2 : NaOH 1M in water with graphene electrode (green = graphene, red/white = H_2O, red/white (big) = OH^-, blue = Na^+).