

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title	Molecular Dynamics of Electrochemical systems
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Internship supervisor

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Laboratory	ICPEES – Equipe Electrochimie et Conversion d’Energie
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : Elena R. Savinova

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	Fundamentals in coding

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 its properties can drastically affect the reaction kinetics. These properties are primarily influenced by the reorganization of the interface when a potential is applied to induce the reaction. 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. This region is defined as the "electrochemical double layer" (EDL). 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 (*e.g.*, water) that can nevertheless alter the electrolyte properties near the interface. In this context, the use of molecular dynamics allows for simulating a realistic representation of the reorganization of molecules in the solution when applying a potential while also accounting 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 1**, along with the cation distribution). 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. This feature of MetalWalls allowed our group to recently demonstrate/put in evidence that the dynamic of the charge is impacted by the cations size on Pt(100) surfaces. Hence, during this internship, the objective is to further investigate the effect of the cation nature (*e.g.*, Li^+) and of the Pt orientation (*e.g.*, Pt(110); Pt(111) – this on Na^+) on the organisation of the EDL as observed previously by MetalWalls. The selected candidate will study the impact of the cation/surface on the charge dynamic and identify solvent orientation trends based on simulation parameters. In this perspective, a solid knowledge of electrochemistry as well as a basic understanding of molecular dynamics and cheminformatics are necessary.

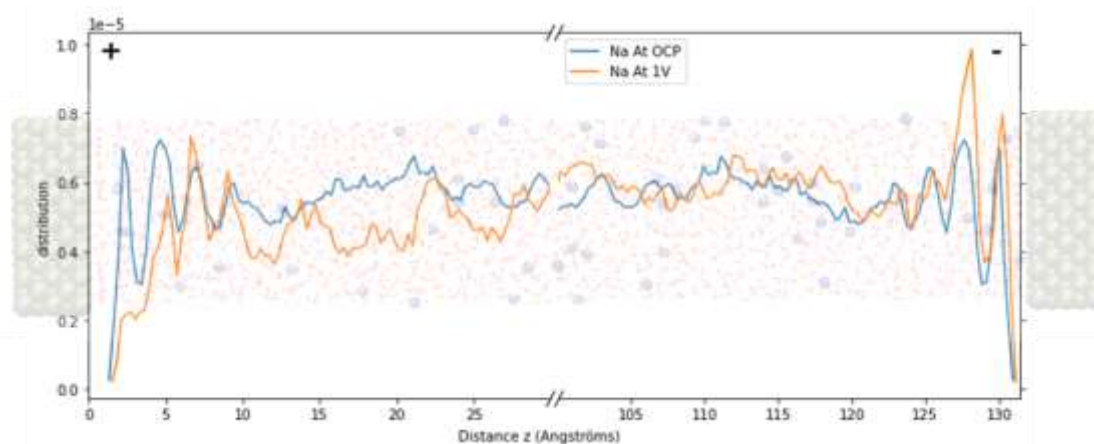


Figure 1. Distribution of the Na^+ cations in 1M NaOH near Pt(100) surfaces, in absence of an applied voltage (*i.e.*, at open circuit potential – OCP) and with a 1V voltage between the two electrodes stacked on a representation of the studied system