



Description of the PhD project

“Theoretical Reactivity of MXene-electrolyte interfaces”

The PhD student will participate in the FLUXIONIC Marie Skłodowska-Curie Doctoral Network, an interdisciplinary European network gathering academic and industrial partners in 8 countries on the control of water and ion (and more generally soft matter) transport at the nanoscale.

In this context, the PhD student will study the interfaces between water and a new type of 2D material, titanium-based MXenes, which are metallic and offer many versatile surface terminations depending on their synthesis procedure. The task will first involve simulating the bare MXene termination and studying its reactivity in liquid water and aqueous electrolytes. Then, a single atom of another metal will be incorporated into the metal solid, and we'll vary the nature of the metal to best activate small gaseous molecules. The aim is to understand how the metallic character of the support in which the single metal atom is located plays a role in the adsorption properties of small molecules of interest for the green transition, in order to guide future synthesis and electrochemical measurements by the experimental part of the team.

To this end, using the tools (codes) of condensed-phase density functional theory (DFT), we will study the chemical reactivity of a set of replicas of the solid defining different surface terminations in an aqueous solvent containing the aforementioned ions and/or molecules. The challenge is to advance fundamental knowledge of electron-ion coupling in operando. In order to accelerate screening without losing precision, a collaboration with A. Michaelides' group at Cambridge, involved in the FLUXIONIC network and developing transferable machine learning force fields, will take place during the PhD.

Work Context

The LPENS laboratory (Laboratoire de Physique de l'ENS) is a joint research unit between CNRS and Ecole Normale Supérieure (ENS) and belongs to the Paris Science & Lettres PSL Campus. It is located at the Physics Department of the ENS, in the center of Paris. It consists of more than ~300 people and conducts research in all fields of Physics via more than 20 teams. (<https://www.lpens.ens.psl.eu/>)

The doctoral fellow will be part of the Micromegas team combining experiments, theory and numerical modelling to explore the nano-fluidic transport (<https://www.lpens.ens.psl.eu/flu-int/micromegas-nano-fluidique/?lang=en>). Access will be provided to computational resources at the lab and national level. The doctoral fellow will participate in all FLUXIONIC activities and benefit from their numerous training sessions. The project will be supervised by M.-L. Bocquet and carried out in close collaboration with Lyderic Bocquet, who is heading the Micromegas team .

Constraints and risks

Important: please note that applicants for this position within a MSCA Doctoral Network must not have a doctoral degree at the date of their recruitment and should comply with the mobility rules. In the present case, they must not have resided or carried out their main activity (work or studies) in France **for more than 12 months in the 36 months** immediately before their recruitment date.

Additional Information

Candidates should have a Master in Physical Chemistry or in Physics. Some knowledge in quantum chemistry is preferable as well as some programming skills. Written/oral communication in English is necessary (knowledge of French is not).

Please include in your application the name and contact information of at least one reference who could be contacted during the evaluation process.

More information on the FLUXIONIC Doctoral Network can be found here: www.fluxionic.org