

Topic for Master 2 internship – Academic year 2023-2024

A new approach coupling experiments and *ab initio* calculations to describe the solid-liquid electrochemical interfaces

General Scope :

Electrochemistry describes the properties of the coupling between matter and electricity. It deals with reactions involving transfer of electrical charges at interfaces between an electrode and chemical species in solution.

Electrochemical interfaces play a crucial role in many systems used for clean energy production, conversion and storage as well as for material processing. The structure of the electrode/electrolyte at the interface, as well as the charge transfer mechanisms, are properties and processes which can crucially affect reactivity and performance of electrochemical applications.

While physical characterization with *in situ* surface x-ray diffraction experiments at synchrotron sources has enabled the description of the atomic order at the interface, insight into the charge distribution at the interface is still lacking.

We aim at proposing advances into this direction in order to be able to link atomic scale models and the charge distribution at the electrochemical interface.

We recently developed a new approach, coupling *in situ* surface resonant x-ray diffraction experiments (SRXRD) at synchrotron sources with the home-developed first principle simulation software FDMNES. This approach will be able to give access to the charge distribution at the electrochemical interfaces.

Research topic and facilities available :

Using FDMNES software, the student will work on the theoretical description of *in situ* surface resonant x-ray diffraction experimental data obtained on electrochemical interfaces; she/he will directly compare the *ab initio* calculations against experimental data. A SRXRD experiment is foreseen in spring 2024.

Possible collaboration and networking :

The student will work in SIN team, where all the experimental and theoretical competences are present

Possible extension as a PhD : to be discussed

Required skills:

Condensed matter physics. Taste for numerical simulation

Starting date :

February 2024

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