Laboratoire de Physique des Interactions Ioniques et Moléculaires - UMR 7345

Multi-Scale Modeling of the Interaction between Hydrogen and Nuclear Materials

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Three-year PhD funding will be available in September 2025 at the “Physique des Interactions Atomiques et Moléculaires” Laboratory (PIIM).

We are studying the behavior of hydrogen in the first wall materials of the International Thermonuclear Experimental Reactor (ITER). This subject is part of a strongly structured European framework provided by the EUROfusion Horizon Europe consortium, which offers access to a large collaborative network and European EURATOM funding.

To model the behavior of hydrogen in materials, we use electronic structure calculations based on DFT implemented in Plane-Waves. We determine electronic and vibrational properties, solution energies, diffusion barrier for hydrogen in materials. We model defect creation, adsorption phenomenon, surface reconstruction and more. On top of these properties determined at zero temperature, we build thermodynamic models to provide macroscopic properties depending on external parameters like the temperature, pressure or chemical potential. Kinetic models are also developed in collaboration with the “Institut de Recherche sur la Fusion Magnétique” (IRFM) at CEA Cadarache. To complete this multi-scale approach, we have more recently been integrating the dynamics of the system.

The aim of this project is to build a machine-learning ternary interatomic potential for the W-Cu-H system, based on DFT calculations. This work, which has already begun, is being carried out in collaboration with Julien Tranchida, IRESNE, CEA Cadarache. We will build several models of W/Cu interfaces and determine the defects induced by the connection of two crystal lattices of different geometry and orientation. We will then study the interaction of these defects with hydrogen, and their impact on hydrogen diffusion properties at the copper-tungsten interface.

The candidate will benefit from structured supervision and access to a wide range of scientific skills, with each supervisor covering a specific area of expertise (DFT and Thermodynamics, Kinetics, Molecular Dynamics and ML potentials). The candiadte will contribute to a subject developed within an international framework, benefiting from European funding and computational resources.

The interested candidate will ideally have good knowledge of the following methods: electronic structure calculations (plane wave DFT if possible), statistical thermodynamics, molecular dynamics. Skills in Python, bash scripting, Fortran 90 and machine-learning would be appreciated.

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