

Mesosopic modeling of transport & chemical reactions for energy storage applications

Master internship at [IFP Energies nouvelles](#) (IFPEN)

The proposed Master internship takes place in the general context of suitable options for Underground Hydrogen-Storage (UHS) applications in natural reservoirs. This long-term application requires the understanding of hydrogen transport and interaction with porous and permeable media using multi-scale approaches. In particular, the length and time scales involved in the H₂ reactive-transport process hydrogen over different mineral surfaces under confinement required an adapted technique. The proposed work will focus more specifically on the methodological aspects of reactive-transport at the mesoscopic scale using constant energy Dissipative Particle Dynamics (e-DPD) simulations.

The scientific approach that will be pursued is built around three main steps. The first step is to test the reactive functionalities of the e-DPD as implemented in the Lammmps molecular dynamics code, which is an open-source code and widely used and proven in the scientific community. In a second step, a set of bulk phase decomposition reactions will be incorporated to the system using interaction parameters extracted from the literature. If possible, we will try to extend simulations to consider heterogeneous samples where the effect of confinement on the reactive transport will be analysed.

Required background: Applicants are expected to be in a master's (level 2) program in a STEM (science, technology, engineering, and mathematics) discipline with a substantial research component, have a background in physical chemistry, chemical physics, chemical engineer, or a related field. Basic concepts of thermophysical properties of fluids, computational, programming, and molecular simulation skills would be a significant advantage.

Internship Period: 6-month

Monthly fellowship: between 638€ to 1081€ based on educational levels and experience. Foreign students will receive a single additional compensation of 515€ at arrival.

Localisation: The Master internship will be held at IFP energies Nouvelles in [Rueil-Malmaison](#) (near Paris).

If you have any question about the project, please contact [Dr. Carlos Nieto-Draghi](#) (carlos.nieto@ifpen.fr) or [Dr. Theo de Bruin](#) (theodorus.de-bruin@ifpen.fr).

The complete application should include: (i) a motivation letter; ii) a detailed CV, iii) the name and email address of two references. All documents and information should be sent to the supervisors indicated above.