Modelling of Hydrogen Production and CO_2 Capture by Natural Amphibole Minerals

Keywords: Natural hydrogen; Decarbonization; Molecular modelling (DFT); Energy transition; Geological H_2; Grunerite

Project Overview

This PhD project explores an emerging and potentially transformative pathway for clean energy: the natural production of hydrogen coupled with carbon dioxide capture by iron-rich minerals. Recent discoveries suggest that certain geological systems can generate hydrogen continuously and at low cost, while simultaneously trapping CO_2. Understanding these processes at the molecular level could significantly contribute to the global energy transition.

The project focuses on amphibole minerals—particularly grunerite—as reactive substrates capable of producing H_2 through interactions with CO_2-bearing fluids in the Earth's crust. By combining computational chemistry and experimental geology, the research aims to uncover the mechanisms governing hydrogen formation, transport, and storage in natural environments.

Objectives

The PhD candidate will develop a multiscale model of natural hydrogen systems by i) identifying atomic-scale mechanisms of H_2 production and CO_2 capture at mineral–gas interfaces ii) Linking molecular-level insights to macroscopic geological observations iii) Predicting reactivity in unexplored systems to guide geo-inspired material design

Methodology

The project integrates theoretical modelling and experimental characterization through three main stages

1. Molecular Modelling: Build bulk and surface models of grunerite, use periodic Density Functional Theory (DFT) to study reaction pathways, intermediates, and energy barriers ; Analyze thermodynamics and kinetics of H_2 formation and CO_2 adsorption/desorption

2. Experimental Characterization: Analyze mineral samples from natural hydrogen sites in Brazil, Apply techniques such as XRD, XRF, infrared spectroscopy, and optical microscopy

3. Integrated Modelling: Combine computational and experimental data to construct a comprehensive model of hydrogen generation and storage in geological systems

Candidate Profile

- Master's degree (or equivalent) in Chemistry, Physics, Materials Science, or Geosciences
- Strong background in computational chemistry (DFT) or solid-state physics, previous experience with materials modelling codes (VASP, CRYSTAL) is a plus. Basic programming skills (scripting) is required.
- Interest in interdisciplinary research bridging chemistry and geology
- Good communication skills and willingness to work in an international environment

Research Environment

The PhD project combines expertise in theoretical chemistry and geosciences. The candidate will benefit from access to high-performance computing facilities (local and national), advanced modelling software and scientific databases, experimental facilities in for mineral characterization, in a rich pluridisciplinary scientific environment.

This PhD project will be conducted as a cotutelle between France (Sorbonne Université) and Brazil (Universidade Estadual do Norte Fluminense Darcy Ribeiro). **A mobility period of 1 year in Brazil is mandatory.** A 6-month secondment with IFPEN (France) may be planned depending on the progress of the project.

Supervisors: Prof. Dr. M. Calatayud (MONARIS, Sorbonne Université, Paris, France), Dr. Corinne Arrouvel (IMQ-Universidade Federal do Rio de Janeiro, LENEP-Universidade Estadual do Norte Fluminense Darcy Ribeiro, Macaé, Brazil).

The Thesis will be registered in Ecole Doctorale 388 (Sorbonne Université). A standard, official French contract "contrat doctoral" will be established for 3 years (gross salary 2300 EUR/month, social security, unemployement allowance after completion).

Recruitment process

Before 3rd April 2026: candidates send their CV, motivation letter and academic track record specifying in the subject "application for PhD position in natural hydrogen"to

monica.calatayud@sorbonne-universite.fr and corinne.arrouvel@imq.macae.ufrj.br

6-10 April 2026: interview between pre-selected candidates and supervisors

20-24 April 2026: selected candidate uploads documents in the Sorbonne Universite site

6-26 May 2026: interview between candidate and Sorbonne Université doctoral school