

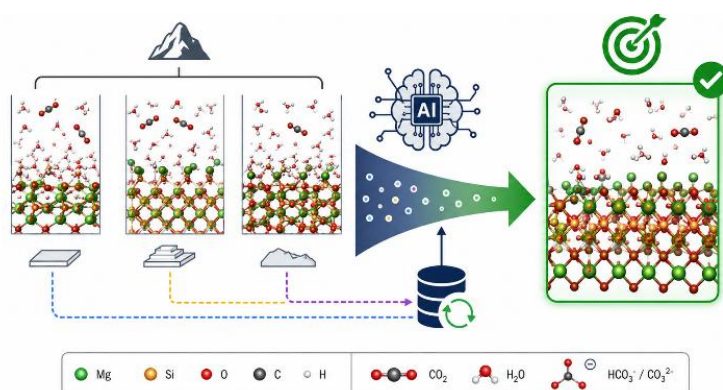
Master thesis

AI-guided exploration of mineral interfaces for CO₂ sequestration

Keywords: Machine learning, CO₂ sequestration, interfacial physics, atomistic simulations, active learning, free-energy landscapes, materials discovery

This Master M2 thesis has been **selected and funded by the DIADEM ACADEMY** for AI-driven accelerated discovery of materials.

SCIENTIFIC DESCRIPTION:



CO₂ sequestration in Mg- and Ca-rich minerals is a promising route for long-term carbon storage, but the atomistic mechanisms and interfacial free-energy landscape controlling this process remain poorly understood. This limits our ability to identify the microscopic parameters governing efficient CO₂ sequestration and to design mineral interfaces with optimized properties.

Recent collaborative work between CPCV and LPENS at ENS has shown, using a fine-tuned MACE machine-learning potential, that at the forsterite–H₂O–CO₂ interface, changes in surface protonation

strongly modify the local interfacial environment and promote Mg²⁺ dissolution, a key precursor to long-term CO₂ sequestration. These results point to surface structure, protonation state and hydroxylation as microscopic control parameters coupling interfacial structure, dynamics and reactivity.

The Master M2 candidate will extend this approach toward an AI-guided exploration of the configurational and free-energy landscapes of reactive mineral interfaces. Starting from the existing forsterite model, the student will combine foundation machine-learning potentials, targeted ab initio calculations and active learning to investigate different surface structures, hydroxylation states and acidities and, where feasible, related Mg- or Ca-bearing minerals. Reactive molecular dynamics and enhanced-sampling calculations will be used to characterize structural fluctuations, relevant collective variables, free-energy barriers and dynamical pathways associated with CO₂ speciation, surface protonation, cation dissolution and ion-pair formation. The objective is to identify physically meaningful descriptors connecting atomic-scale structure and dynamics to CO₂ sequestration efficiency, and ultimately establish design principles for mineral interfaces.

Techniques/methods in use: DFT and ab initio molecular dynamics; MACE machine-learning potentials; fine-tuning and active learning; large-scale atomistic simulations; enhanced sampling and free-energy calculations; Python data analysis.

Applicant skills: solid formation in quantum and statistical physics, familiarity with python and computer skills

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Internship location & environment: CPCV – Campus Ulm – Ecole Normale Supérieure – 24 rue Lhomond 75005 Paris. The CPCV laboratory offers a dynamic and collaborative environment, with researchers from different backgrounds and scientific disciplines working together on a wide range of topics. We value diversity, open discussion, and a friendly atmosphere, with plenty of opportunities for students to interact with researchers across the laboratory.

Possibility for a Doctoral thesis: Yes

