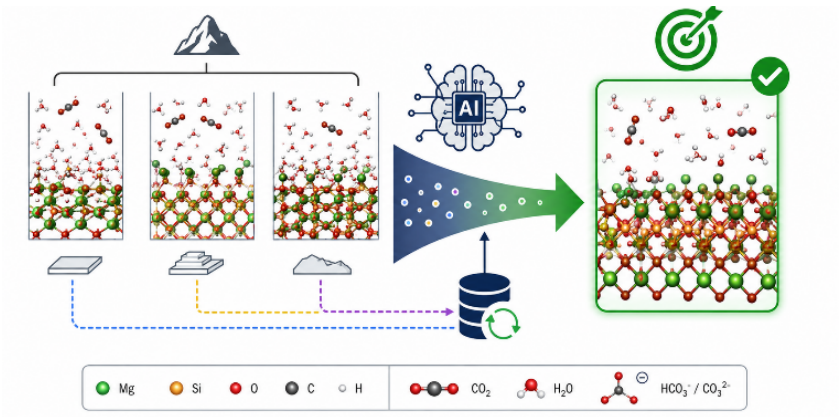
Master thesis proposal

AI-guided exploration of mineral interfaces for CO_2 mineralization

Keywords: Machine learning, CO_2 mineralization, mineral–water interfaces, active learning, reactive molecular dynamics, materials discovery

SCIENTIFIC DESCRIPTION:

CO_2 mineralization in Mg- and Ca-rich minerals is a promising route for long-term carbon storage, but its microscopic mechanisms remain poorly understood. This limits our ability to design and optimize materials for CO_2 capture. Recent work at CPCV has shown, using a fine-tuned MACE machine-learning potential, that at the forsterite–H_2O–CO_2 interface, surface protonation strongly modifies CO_2 speciation and promotes Mg^{2+} dissolution, a key precursor to carbonate formation. This identifies surface acidity and hydroxylation as potential handles for tuning mineralization.



The proposed Master project aims to extend this approach toward an AI-guided exploration 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 terminations, with varying hydroxylation and acidity, and, where feasible, related Mg- or Ca-bearing minerals. Reactive molecular dynamics and free-energy calculations will be used to compare key descriptors of mineralization activity: CO_2 speciation, surface protonation, cation dissolution, and formation of ion pairs. The aim is to establish structure–reactivity relationships and identify mineral structures that are particularly favorable to carbon mineralization.

The project is directly aligned with DIADEM through the use of AI and machine-learning interatomic potentials to accelerate the exploration and selection of materials for a targeted chemical functionality. The knowledge gained from the AI-driven exploration will help to identify relevant surface parameters for controlling the different stages of mineralization, providing guidelines for experimental design of mineral surfaces.

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

Budget description and use: to pay the gratification de stage to the Master2 intern

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

Industrial partnership: None

Internship supervisor(s): Simone PEZZOTTI (CPCV), simone.pezzotti@ens.fr. Marco SAITTA (LPENS), marco.saitta@phys.ens.fr, Rodolphe VUILLEUMIER (CPCV), rodolphe.vuilleumier@ens.fr

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Possibility for a Doctoral thesis: Yes