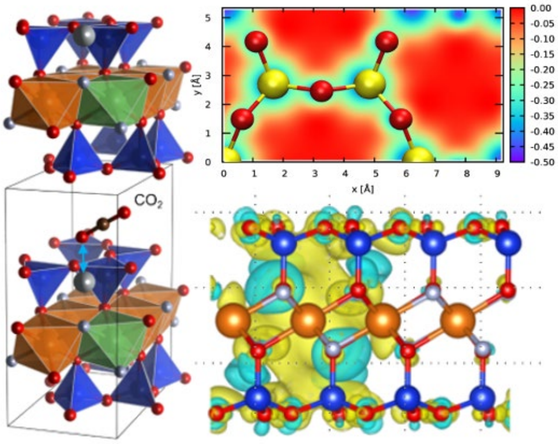
Goldschmidt 2021 Abstract
https://doi.org/10.7185/gold2021.7782




# First principles characterization of the interlayer electrostatic environment influencing the $CO_2$ geochemical trapping in clays

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Carbon capture and storage of greenhouse gases in a safe reservoir is a promising approach within the challenge of global climate mitigation. This strategy involves the gas injection into deep subsurface geological formations exhibiting special features. To have an effective geochemical trapping mechanism, the system should display a large surface area, good adsorption capability. Also, it should not need a lot of energy for it to work, and it must be inexpensive and environmentally friendly. Among the materials, the clays have interesting features for this application, including their layered structure. We address the swelling effect in these systems throughout first principles calculations considering the state-of-art van der walls correction scheme as implemented in the Siesta code. In particular, we investigate interlayer cations' role on the foregein gas molecules' adsorption stability and how they affect the clay basal separation distances. Significant differences in the gas adsorption properties were observed considering Na, Li, and Ni interlayer cations in the Fluorhectoride smectite. We concluded the physisorption of gas molecules in the interlayer space is an ion-depended process. In particular, the relatively higher adsorption energy observed for the Ni-$CO_2$ interaction may result in ionic compounds. Besides, the clay surface charge and interlayer molecules influence the cohesion energy, impacting the swelling phenomena. We expect to guide the exploration of future reservoirs for carbon capture and storage into deep subsurfaces with these results. By unraveling the role of interlayer cations, it may be possible to optimize the choice of geological formation in the context of the trapping mechanism or even for the long-term overall efficiency of the process occurring in artificial devices. The authors gratefully acknowledge Prof. Jon O. Fossum and Kristoffer Hunvik and the Research Centre for Gas Innovation and FAPESP for financial support.