

Tunning CO₂ adsorption on feldspar surfaces for geological carbon storage applications

JESSICA SANTO REGO¹, ALVARO TORREZ² AND
CAETANO RODRIGUES MIRANDA³

¹University of São Paulo

²University of Sao Paulo

³University of São Paulo (USP)

Presenting Author: cmiranda@if.usp.br

Concerns over climate change resulting from greenhouse gas emissions, such as carbon dioxide (CO₂), have prompted the search for technologies capable of mitigating their impact. One promising alternative is geological capture and storage through carbonation reactions. The mechanisms responsible for trapping gas within subsurface rock are classified into various processes. Among these, the adsorption process holds significant importance as it directly contributes to two storage mechanisms: residual storage and carbon mineralization. The Rio Bonito formation in the Paraná basin in Brazil appears to be a suitable location for implementing this technology. Molecular-scale simulations are crucial for understanding the mechanisms and processes involved in fluid/mineral interfaces at the geological site reservoir. The most abundant aluminosilicate commonly encountered in both the caprocks and sandstones of these typical reservoirs are the feldspar minerals. Using Density-Functional-Theory (DFT), we evaluated the adsorption behaviour of CO₂ molecules on selected end-member phases of the feldspar solid-solution phase diagram. We focused on preferential feldspar's cleavage plane surfaces, {010} and {001}. We quantified and compared the electronic and thermodynamic properties of different adsorption configurations from an energetic and topological perspective. We also explored the determination of preferential adsorption sites and the influence of the aqueous solvent on adsorption. We found that the alkali-feldspar (K⁺ and Na⁺) surfaces showed a physisorption of carbon dioxide, characterised by small distortion of CO₂ geometry parameters and weak Van der Waals interactions with the mineral surface. Regarding the plagioclase phase (Ca²⁺) strong interactions were found indicating a process of chemisorption with larger distortions in the geometry of the CO₂ molecule. The distinct behaviours observed can be correlated with the aluminium content and the Si/Al ordering in the phase diagram, owing to the disparities between the Si-O-Si and Al-O-Si bonds. Our simulations shed light on significant interactions at complex CO₂-water-mineral interfaces under reservoir minerals. This work was carried out with support from FAPESP (grants 2022/08894-0 and 2020/15230-5)