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Exploring the impact of amines on aluminosilicate weathering: a first principles approach

WANDRILLE GUNDERMANN[1], MARKUS ERLACHER[1], MARTIN P ANDERSSON[2] AND SUSAN LOUISE SVANE STIPP[1]

[1]Technical University of Denmark
[2]King Fahd University of Petroleum and Minerals

The increase of greenhouse gases - and specifically CO_2 - gives rise to genuine concern. One method for decreasing CO_2 in air and water is mineralisation as carbonate phases. A promising approach, that has drawn attention in the past years, is geologic carbon capture and immobilisation in basaltic rocks (www.carbfix.com), leveraging on enhanced weathering processes, one of which is aluminosilicate weathering, that occurs in nature. Modelling weathering rates requires knowledge of several parameters, including the rates of dissolution and release of divalent cations that are needed to react with CO_2 dissolved in water. The resulting carbonates are stable for geologic time.

Organic compounds impact silicate dissolution. Research has been largely focused on the effect of organic acids at low pH, while the impact of organic bases such as amines at high pH has received less attention. To bridge this gap, we studied the impact of amine adsorption on a calcium aluminosilicate glass experimentally and using computational chemistry to explore the molecular level processes. We adopted a (CAS) cluster, used previously (Ramsheh et al., 2023), and investigated the behaviour of amine compounds on local surface thermodynamics using density functional theory (DFT) calculations. The aim was to produce surface complexation equilibrium constants for an existing microkinetic model (Andersson et al., 2025) that describes ligand enhanced dissolution.

Insights from the first principles derived, thermodynamic parameters were linked to the experimental dissolution rates of basaltic glass in aqueous amine solutions so we could define the mechanisms of amine enhanced dissolution. The results of our work contribute to general understanding of solid-water-organic compound interaction and ligand enhanced dissolution. Insights from this study will also help in the search for efficient organic catalysts to enhance CO_2 mineralisation at high pH.

References

Andersson M. P. et al. (2025) *Chemical Geology*, *692*. https://doi.org/10.1016/j.chemgeo.2025.122960

Ramsheh M. et al. (2023) *Journal of Non-Crystalline Solids*, *620*, 122597. https://doi.org/10.1016/j.jnoncrysol.2023.122597