

Calcium Carbonate Growth and Dissolution: Building an Atomistic Picture via Computer Simulation

MARCO DE LA PIERRE,^{1*} PAOLO RAITERI,¹ BERNHARD REISCHL,¹ ANDREW G. STACK² AND JULIAN D. GALE¹

¹The Institute for Geoscience Research (TIGeR), Curtin Institute for Computation and Department of Chemistry, Curtin University, Perth (Australia) (*correspondence marco.delapierre@curtin.edu.au)

²Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge (TN, USA)

Among the processes that can occur at a mineral-water interface, crystal growth and dissolution are of major interest, not only to geochemists wanting to understand transformations undergone by minerals at the Earth's surface and crust, but also to materials scientists seeking to optimise industrial processes. Whereas accurate investigations of these phenomena at a macroscopic scale are made possible by modern experimental techniques, a convincing description of the underlying (often complex) mechanisms at the atomic scale is often out of reach.

This contribution will focus on calcite, a mineral that is widely found on Earth as a result of biomineralisation [1], and a subject of technological challenges such as scale formation control and CO₂ sequestration [2,3]. State-of-the-art classical molecular dynamics and free energy calculations [4] have been employed to probe the adsorption and desorption of Ca and CO₃ ions along surface steps at the basal plane. Results from this approach will provide insights into the thermodynamics and kinetics of calcite growth and dissolution in aqueous solution, shedding light on the relevant atomistic processes behind experimental observations [5].

[1] Belcher *et al.* (1996) *Nature* **381**, 56–58. [2] Chen *et al.* (2005) *J. Petrol. Sci. Eng.* **46**, 185–194. [3] Matter and Kelemen (2009) *Nat. Geosci.* **2**, 837–841. [4] Raiteri *et al.* (2015) *J. Phys. Chem. C* **119**, 24447–24458. [5] De La Pierre *et al.* (2017) *Angew. Chem. Int. Ed.*, accepted.