

Probing the role of water dynamics in calcium carbonate crystal growth using classical molecular dynamics

MARCO DE LA PIERRE^{1*}, PAOLO RAITERI¹ AND JULIAN D. GALE¹

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

Calcium carbonate is a key material in the context of biomineralisation, occurring with abundance at the Earth's surface in the form of exoskeletons of marine organisms (seashells, coral reefs, ...) [1] as well as in limestone deposits. It is also relevant to several technological challenges, including the control of scale formation in industrial plants and CO₂ sequestration [2,3].

In the above context, state-of-the-art computer simulation is of particular value, with its unique capability to provide insights at the atomic scale for processes such as crystal nucleation and growth that have aspects that are not yet fully understood. In recent years, classical molecular dynamics techniques have been successfully applied to investigate possible pathways toward nucleation for calcium carbonate, thereby clarifying the role played by the water of hydration for the various species [4,5].

In the present contribution we will discuss the structural and dynamical properties of water around surface features of calcite, such as steps and kinks, the most relevant sites for crystal growth in aqueous solution. The properties of the surface water layers will also be discussed in relation with the mechanisms for ion adsorption at these surface features.

[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 and Gale (2010) *J. Am. Chem. Soc.* **132**, 17623–17634. [5] Demichelis *et al.* (2011) *Nature Commun.* **2**, 590.