

Adsorption of organic molecules on calcite in water

A. SCHUITEMAKER^{1*}, K. KOZIARA¹, M. DE LA PIERRE¹, R. DEMICHELIS¹, P. RAITERI¹ AND J. D. GALE¹

¹ Curtin Institute for Computation, The Institute for Geoscience Research, Curtin University, Perth, Australia (correspondence*: alicia.schuitemaker@postgrad.curtin.edu.au)

Calcium carbonate (CaCO_3), one of the most abundant biominerals, is utilized by a variety of organisms for different functions (e.g. protective shells and support structures/skeletons [1]). It is also relevant to several current challenges, such as industrial scale formation and CO_2 sequestration [2]. Experimental and computational techniques have been applied in an attempt to comprehend how organics can influence calcium carbonate growth [3]. The presence of biomolecules in aqueous environments has been shown to alter polymorph selection and morphology, as well as influencing growth rates of CaCO_3 [3].

This work used computational methods to further the atomistic understanding of the binding of organic molecules to calcite. Specifically, molecular dynamics simulation has been used to determine the free energy maps for different functional groups at calcite surface features with a particular focus on steps and kinks, since these are believed to be the main growth sites. The small organic molecules studied are found to show limited interaction with the pristine surface. However, surface defects alter the adsorption free energy landscape and create the possibility for organic molecules to bind to the mineral surface and change its morphology or even inhibit its growth. The results from this work provide a foundation for the development of well-calibrated models able to determine the thermodynamics for the adsorption of larger organic molecules with multiple functional groups.

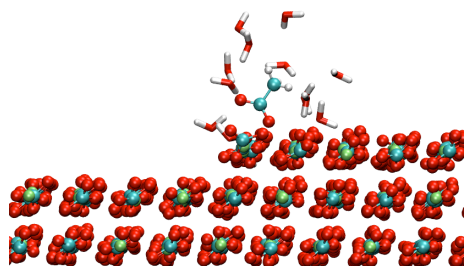


Figure 1: Acetate above the obtuse step on calcite. For clarity only the first solvation shell of acetate is shown.

[1] Dove (2010) *Elements* **6**, 37–42. [2] Matter & Kelemen (2009) *Nature Geoscience* **2**, 837–841. [3] Gebauer *et al.* (2009) *Adv. Mater.* **21**, 435–439.