Goldschmidt 2022 Abstract
https://doi.org/10.46427/gold2022.11037

Biomineralization at the atomic scale. 2022 Houtermans Award

RAFFAELLA DEMICHELIS

The Institute for Geoscience Research (TIGeR), Curtin Institute for Computation, Curtin University

Presenting Author: raffaella.demichelis@curtin.edu.au

Living organisms have the powerful ability to synthesize minerals with specific crystal structures, textures, shapes, sizes and compositions as part of their functional hard tissues. Despite being relatively well known at a macroscopic level, little or nothing is known about the chemistry underpinning the formation of these biominerals. Indeed, achieving a molecular-level understanding of these processes would be a key to learn how to mimic them, resulting into a major step beyond the current limitations in materials synthesis.

Computer modelling can provide insights into the atomic scale processes that lead to the formation of such specifically designed materials, both *via* helping to interpret experiments and making predictions that can direct experiments (Fig. 1).[1] The main challenge here is developing a realistic, thermodynamically and kinetically predictive model able to access significant size and time scales at an affordable computational cost.[2]

This presentation will show research undertaken in my group, where ab initio, semi-empirical and classical computational methods are used to investigate the fundamental chemistry and physics of complex mineral systems.

[1] Demichelis *et al., Annu. Rev. Mater. Res. 2018 48, 327-352*

[2] Demichelis *et al*. *Nat. Commun.* 2011, 2, 590; Raiteri *et al. J. Phys. Chem. C* 2015, 119, 24447; Schuitemaker *et al. J. Chem. Phys.* 2021, 154, 164504

[3] Jiang et al., Nat. Commun. 2019, 10, 2318

[4] Demichelis *et* al. *J. Phys. Chem. B* 2018, 122, 1471-1483

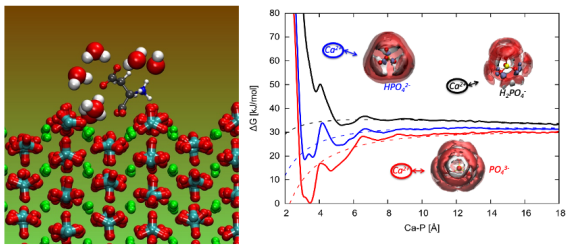

Figure 1. Left: Adsorption of aspartate zwitterion on $CaCO_3$ vaterite in water[3] (only water molecules in the first coordination shell are shown for sake of clarity). Right: Pairing free energy profile between calcium and phosphate species in water.[4]