

Nucleation and growth of calcium carbonate: how non-classical is it?

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The interface between calcium carbonate and water is one of the most fascinating “hard-soft” interfaces, being of significance to mineralogy and biomineralization processes. CaCO_3 is known to form an amorphous precursor (ACC) that can subsequently evolve to produce crystalline polymorphs. To add to the complexity, the ACC precursor is not a single well-defined material as it can vary in water content and have polyamorphic characteristics [1]. Furthermore, it has been demonstrated that stable pre-nucleation species also exist [2], but their relationship to ACC remains unknown.

In this presentation we will explore the use of computer simulation methods to try to unravel the complexities of the nucleation and growth processes for calcium carbonate. Central to this is the development of a force field that is accurately calibrated against experimental free energies [3] since failure to do so can result in qualitative errors for interfacial properties. Based on this we have explored the stability of ACC versus crystalline nanoparticles while accounting for the variable water content in the amorphous structure [4]. In the light of this, and new experimental results, we propose a model to explain the non-classical aspects of the nucleation mechanisms of calcium carbonate, the origins for which can be traced back to the interfacial properties.

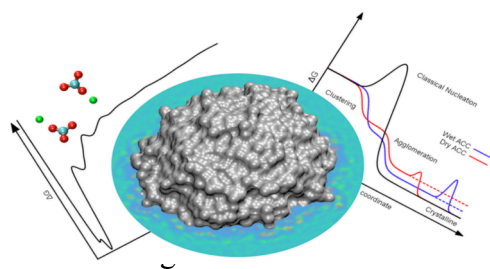


Figure 1: Montage showing from left to right, the free energy of ion pairing, the hydration of ACC and the consequences for nucleation and growth.

[1] D. Gebauer *et al.*, *Angew. Chem. Int. Ed.*, **49**, 8889 (2010)

[2] D. Gebauer *et al.*, *Science*, **322**, 1819 (2008)

[3] P. Raiteri *et al.*, *J. Phys. Chem. C*, **114**, 5997 (2010)

[4] P. Raiteri and J.D. Gale, *J. Am. Chem. Soc.*, **132**, 17623 (2010)