Benchmarking the interaction of amino acids with calcite

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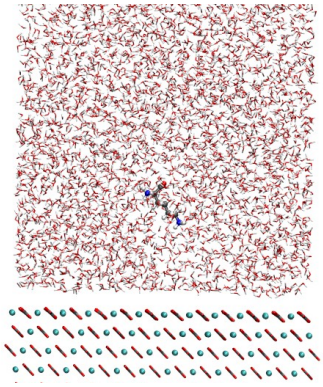

Calcium carbonate or calcite is one of the most widespread minerals found on earth. It interacts favourably with a number of biomolecules, including peptides and proteins. If this interaction takes place during calcite crystal growth, biominerals of remarkable mechanical properties may be formed [1]. These types of minerals have a wide variety of applications in drug delivery systems, oil reservoirs and CO2 storage.

In this study we benchmark the interactions of protected and zwitterionic amino acids with the stable (104) surface of calcite using two different classical force fields [2,3]. Our methodology encompasses fully atomistic molecular dynamics simulations in combination with umbrella sampling. We find that the zwitterionic forms of amino acids generally bind better to the surface. Presence of polar groups or charged groups in side chains and compactness of amino acids also leads to more significant binding.

We apply the same methodology to the unstable (001) surface of calcite exhibited during the nucleation process, description of which is less unique. In the representation of our choice we show that the presence of either negative or positive charged group in the peptide is necessary for binding to this surface.

These results provide a force field benchmark and reference data on binding energies and conformations of specific amino acids which could help interpret the experimental data on peptide and protein mediated calcite functionalization and growth.

[1] J. H. Harding, D. M. Duffy, M. L. Sushko, P. M. Rodger, D. Quigley, J. A. Elliot, *Chem Rev*, **2008**, 108, 4823-54.
[2] C. L. Freeman, J. H. Harding, D. J. Cooke, J. A. Elliot, J. S. Lardge, D. M. Duffy, *J Phys Chem C*, **2007**, 111, 11943-11951
[3] P. Raiteri, J. D. Gale, D. Quigley, P. M. Rodger, *J Phys Chem C*, **2010**, 114, 5997-6010