Early and late stages of $CaCO_3$ growth from aqueous solution

PAOLO RAITERI[1], MARCO DE LA PIERRE[1], RAFFAELLA DEMICHELIS[1] AND JULIAN D. GALE[1]

[1]Nanochemistry Research Institute, Curtin Institute for Computation, and Department of Chemistry, Curtin University, Perth, Western Australia

Carbonates are ubiquitous materials that play a crucial role in many geological, biological and industrial processes, and are the focus of a huge body of literature. However, despite this extensive research there is still no unanimous consensus on the fundamental molecular mechanisms and pathway that takes the dissolved ions to the formation of macroscopic crystals. The length-, time-scales and concentrations involved in the early stages of nucleation and growth of these materials lay in the gap between what can be probed with conventional experimental and theoretical techniques. This is driving experimentalists to invent new approaches that can push the boundary of what can be detected to smaller and smaller sizes. On the other hand the advances in supercomputers and the constant development of faster and more accurate algorithms are trying to bridge the gap with experiment from the opposite direction.

In this presentation, I will review the recent progress we have made in developing new forcefields to study the dissolution and growth of carbonates from aqueous solution. I will focus on their use to study ion pairs and the formation of pre-nucleation clusters, and on the molecular processes that control the macroscopic growth of the crystals at the surface. Particular emphasis will be given to the thermodynamic aspects of these events and a direct connection to the available experimental data will be made.