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Modelling the Effect of Magnesium and Cadmium Ions on Calcite Growth and Dissolution

Nora H. de Leeuw (n.h.deleeuw@reading.ac.uk)[1] & **Stephen C. Parker** (s.c.parker@bath.ac.uk)[2]

[1] Department of Chemistry, University of Reading, Whiteknights, Reading, Reading RG6 6AD UK
[2] Dept. of Chemistry, University of Bath, Claverton Down, Bath, Bath BA2 7AY, UK

We modelled the effect of Mg^{2+} and Cd^{2+} ions on crystal growth in aqueous environment from two experimentally found monatomic calcite steps: an acute and an obtuse step on the {104} surface. Using potential parameters which reproduce experimental enthalpies of formation of calcite from its aqueous ions, growth of $CaCO_3$ at the obtuse step was found to occur preferentially, in agreement with experimental findings of calcite growth under aqueous conditions. The simulations suggest that formation of the kink sites on the growing edges of the steps are the rate determining steps for calcite growth at the edges and this formation energy is calculated to be higher for the acute step, possibly due to the greater stability of the surface containing complete acute steps. Growth of magnesium ions onto the growing calcite steps is an exothermic process, indicating that incorporation of magnesium into the calcite crystal is a straightforward process on energetic grounds. These results agree with the fact that large amounts of magnesium are found in calcite crystals. Subsequent growth of calcium ions onto the magnesium terminated edges is calculated to be endothermic which indicates that incorporation of magnesium onto the edges inhibits calcite growth, again in agreement with experimental findings. Once a full layer of $CdCO_3$ or $MgCO_3$ is formed on the main calcite cleavage plane, the cadmium ions will segregate to the bulk crystal unlike the magnesium ions which prefer to remain at the surface, due to the strong interactions between magnesium ions and water. However, segregation energies for both cations in second and further layers of some calcite surfaces are positive, indicating that once a calcium carbonate layer has overgrown the substituted surface layer segregation to the bulk is energetically possible.