

## Coprecipitation of Cd(II) aqua-ion on calcite surface: a first principles study

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Coprecipitation is the incorporation of metal ions into a mineral structure by substituting for lattice atoms. This complex uptake mechanism occurs during crystal growth mostly in aqueous environment. Calcite, the most stable form of calcium carbonate, has the ability of trapping heavy metals and it is a good candidate to be used in water decontamination. As discussed in a recent document of the Environmental Protection Agency [1], calcite is effective as a natural site-specific remediation, the so called “monitored natural attenuation”. To this end, it is essential to know how the surface of calcite interacts with metals in the presence of water. Despite the large body of experimental and theoretical results the details of the interfacial properties are yet to be fully elucidated. In this work the interaction between an hydrated Cd(II) complex,  $[\text{Cd}(\text{H}_2\text{O})_6]^{2+}$ , known as aqua-ion, and two stepped calcite surfaces, namely the  $\{318\}$  and the  $\{3\bar{1}16\}$ , is investigated by means of ab initio DFT-GGA simulations. Favored adsorption sites are located and the adsorption energy calculated accordingly. Relaxation calculations show the presence of a water layer between the cation and the calcite surface. The detailed electronic structure of the interacting system is described.

- [1] Richard T. Wilkin, *Metal Attenuation Processes at Mining Sites*, EPA, (2007).