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Structure and chemistry of the calcite-water-interface

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Calcite is the most stable polymorph of $CaCO_3$ at ambient conditions. It is ubiquitous in natural systems and controls to a large degree the geochemistry of terrestrial soils and sediments, but also of lacustrine- and seawater. Due to the reactivity of its surface, calcite has impact on the mobility of nutrients and contaminants in subsurface environments. Electrostatic phenomena at the calcite-water-interface provide a link between surface chemistry on the one hand side and hydrogeophysical methods like streaming potential- or induced polarization measurements on the other hand side.

In this study we present an updated view of the structure of the calcite(104)-water interface on the basis of a new extended crystal truncation rod data set, which allows to resolve previous ambiguities with respect to the coordination sphere around the surface Ca-ions and the relaxation of surface carbonate groups. On the basis of resonant surface diffraction data we investigate the interaction between calcite and weakly / non adsorbing Rb^+ alkali metal cations. The structural aspects will be related to a newly developed electrostatic surface complexation model (SCM), describing the calcite-water-interface chemistry. For the first time, direct information on the inner surface potential of calcite, as measured with a calcite single crystal electrode, is included in the data constraining the calcite SCM, besides zeta potential data.

Potential links between the calcite SCM and hydrogeophysical measurements will be highlighted.