

## Surface speciation of yttrium at the rutile-water interface: Incorporation of structural information and charge distribution within the MUSIC model

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Ion adsorption at metal (hydr)oxide surfaces is dependent on the surface structure and the coordination geometry of adsorption complexes. At the microscopic scale, surface structure and ion sorption have been examined extensively using various X-ray techniques. Additionally, theoretical simulations also provide molecular-scale details of mineral-solution interfaces. The binding configuration of adsorbed ions may change as a function of solution conditions; for example, surface complexes may protonate or deprotonate. Such changes are best investigated at the macroscopic scale as a function of pH. Therefore, to develop an unambiguous understanding of the reactivity of mineral-solution interfaces it is necessary to scale from the molecular to the macroscopic scale. Surface Complexation Models (SCM), specifically the MUSIC model, provides a powerful framework in which microscopic information can be utilized to rationalize bulk experimental adsorption data.

This contribution will concentrate on the adsorption of  $Y^{3+}$  on rutile. The sorption of  $Y^{3+}$  was studied as a function of pH and loading, in NaCl media at 25 and 50°C. The potentiometric titration data were rationalized successfully using the MUSIC model in combination with the charge distribution (CD) model. The CD values for the surface species were evaluated in relation to available structural information from X-ray techniques and MD simulations. Moreover, changes in surface speciation as a function of pH and surface loading, were also evaluated. X-ray studies have shown that on the predominant (110) rutile surface  $Y^{3+}$  adsorbs mainly as an inner-sphere tetradentate complex, comprising two bridged and two terminal rutile surface oxygens. In addition to this tetradentate complex, SCM revealed a bidentate inner-sphere complex (one bridged and one terminal group) with increased surface loading. Furthermore, both inner-sphere  $Y^{3+}$  complexes hydrolyze with increasing pH.

## Dehydration processes in the subducting slab: Seismological observations from the Andean subduction zone

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Subduction zones, the expression of convergent plate boundaries, generate the world's largest and most destructive earthquakes. The Chilean subduction zone is an ideal natural laboratory to study the processes involved in generating these devastating earthquakes. While the upper limit of the seismogenic zone will be soon in reach of scientific drilling projects the lower limit of the seismogenic zones will only be accessible by remote techniques like passive seismological observations. In the last decade several high resolution passive seismic imaging experiments have been carried out to shed light into subduction zone processes, focussing on the lower limit of the seismogenic zone and its transition into intermediate depth seismicity (300 km).

While in the upper depth range (depth < 20 km) seismicity is predominantly related directly to the subduction thrust a more complicated seismicity feature is found at greater depth. At greater depth (~100km) a double seismic zone with a separation distance of about 8 km could be identified at intermediate depth. Additionally, the analysis of guided wave arrivals suggests, that a thin low velocity layer (thickness < 3 km) is present down to a depth of 200 km, preferably located between the upper and lower band of the double seismic zone. At shallower depth (<50 km) a low velocity layer associated with the subducting oceanic crust can be identified in the nucleation area of the 1960 Chile earthquake. Dehydration processes in the subducting slab can explain most of the seismological observations made.