

Iron phases in soils and softwater lakes as determined by EXAFS spectroscopy

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Iron (III) can determine the speciation of other trace metals, due to its ability to bind to dissolved organic matter (DOM) and to form (hydr)oxides. However, the phases of iron are uncertain and need to be investigated, preferably by using several different techniques. In this study, water samples were taken from the surface of one softwater lake in Tyresta (Stockholm, Sweden) and soil samples from Spodosol O horizons were taken around the lake. The water was filtered using 0.45 μm in-line filtration and 1000 Da cross-flow ultrafiltration. The particles on the filter, the colloidal phases of iron and the soil samples were investigated by extended X-ray absorption fine structure (EXAFS) spectroscopy. Flow field-flow fractionation (FIFFF) was used to study the colloidal composition of iron and other trace metals.

The EXAFS results from the particles of the lake water showed that iron was present as ferrihydrite. In the colloidal fraction iron was present as iron (III) monomerically bound to organic material. Similarly, the soil samples showed that iron was mainly bound as monomeric organic complexes. These results are consistent with other results showing that iron (III) formed monomeric complexes with soil fulvic acid [1] or with humic acid [2] under conditions similar to the ones at the Tyresta site. Moreover FIFFF provided further insights into the size fractionation and iron speciation in the lake water.

[1] van Schaik *et al.* (2008) *Environ. Sci. Technol.* **42**, 2367–2373. [2] Karlsson & Persson (2010) *Geochim. Cosmochim. Acta* **74**, 30–40.

A combined computational/experimental approach to understanding the quartz/water interface

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The interaction of quartz with water is a complicated one involving dissolution and surface charging and as a result there is a need to understand the quartz/water and quartz/aqueous electrolyte interfaces at the molecular level. The first step to achieving this is to understand the water structure using a range of different computational and experimental methods. Classical molecular dynamics of the 10 \AA surface of quartz interacting with water using three different force fields, Lopes *et al.* [1], ClayFF [2] and Charmm water contact angle [3], a new, state of the art reactive force field ReaxFF [4], and *ab-initio* molecular dynamics (AIMD) simulations are performed and compared with X-ray reflectivity (XR) data [5]. The axial density of the water and surface atoms are calculated showing favorable agreement for all methods. More sensitive measures of interface water structure such as hydroxide-water radial distribution functions (RDFs) and the angular distribution of water with respect to the surface show significant differences using different computational methods. ClayFF shows the best agreement with AIMD for the hydroxide water RDFs indicating the most accurate description of water/surface hydrogen bonding. Simulations using ReaxFF have the potential to enable the study of hydroxylation and surface charging of quartz, and their viability and accuracy will be discussed.

[1] Lopes *et al.* (2006) *J. Phys. Chem. B* **110**, 2782 [2] Cygan *et al.* (2004) *J. Phys. Chem. B*, **108**, 1255 [3] Cruz-Chu *et al.* (2006) *J. Phys. Chem. B*, **110**, 21497 [4] Van Duin *et al.* (2003) *J. Phys. Chem. A* **107**(19) 3803–3811 [5] Schlegel *et al.* (2002) *Geochim. Cosmochim. Acta* **66**, 3037.