Uptake of selenium oxyanions by hematite

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Performance assessments of nuclear waste disposals evidenced ^{79}Se ($t_{1/2} \sim 3.27 \times 10^5$ years) to be one of the most important contributors to the overall dose in long-time safety assessments. The concentration, the bioavailability, the mobility, the distribution and the oxidation state of selenium in the environment are greatly influenced by the pH, nature of mineral sorbent and temperature. Hematite was studied because it is a ubiquitous iron oxide mineral present in the environment, thus often found in rocks and soils in the vicinity of underground repositories. This work combined batch and spectroscopic studies to characterize the interaction of Se(VI) and Se(IV) with hematite, which was so far not well understood.

At the macroscopic level, sorption of both oxyanions was found to decrease with increasing pH. An increase of the ionic strength (from 0.01 M to 0.1 M) decreased the sorption of Se(VI), while the Se(IV) uptake remained unchanged. Electrophoretic mobility measurements revealed that Se(IV) sorption shifted the isoelectric point (pH_{IEP}) of hematite to lower pH values, while the pH_{IEP} was not significantly modified upon Se(VI) uptake. At the molecular level, *in situ* ATR FT-IR and EXAFS measurements revealed the formation of inner-sphere complexes (IS) during Se(IV) sorption onto hematite. Concerning Se(VI), sorption proceeded predominantly via the formation of outer-sphere complexes, together with a small fraction of IS complexes.

High level and long-lived radioactive wastes are well-known to increase the temperature at the vicinity of the waste disposal site. Such a thermal effect raises the question how the retention of selenium is influenced at elevated temperatures. Therefore, information and insights about mechanisms working at higher temperatures (from 25 °C to 60 °C) are also provided.