

## Distribution of Selenate and Selenite adsorbed on $\alpha$ -Alumina (012) studied by High-Resolution X-Ray Reflectivity

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Selenium (Se) is an essential nutrient but at higher doses also a chemo-toxin. Additionally, the Se-79 isotope is a long-lived, radiotoxic fission product contained in spent nuclear fuel. Therefore, Se is considered a hazardous material, which must be removed efficiently and cost-effectively from contaminated water, e.g., by adsorption to minerals such as  $\alpha$ -alumina. The targeted design of high-performance adsorbents can benefit from knowledge about adsorption processes on specific surface orientation of the substrate. For example, recent computational work suggested that adsorption of selenate on  $\alpha$ -alumina (012) is controlled by changes in the surface H-bonding network. Validation against experimental data was, however, limited because most of the available sorption data were obtained using powder samples.

Here, we probe the impact of Se concentration and pH on adsorption structures of selenate and selenite anions on the  $\alpha$ -alumina (012) surface using high-resolution X-ray reflectivity (XR). Preliminary XR results show that both selenate and selenite form multiple sorption species on alumina (012) in 10 mM Se solutions at pH 3. The selenate species that adsorbs closest to the surface is located at a height of  $\sim 4$  Å (measured from the topmost Al plane), consistent with a monodentate inner-sphere configuration, in which one oxygen of the selenate anion forms a H-bond to a surface Al-OH group. In comparison, selenite species that adsorbs closest to the surface is located at a height of 2–3 Å. These differences in adsorption speciation appear to be related to the adsorption efficiency, which is lower for selenate than selenite, with ion coverages of 0.4 Se/nm<sup>2</sup> vs.  $\sim 1$  Se/nm<sup>2</sup>, respectively. The relationship among sorption speciation, strength, and surface hydration structure will also be investigated using sum frequency generation spectroscopy to provide a comprehensive insight into the ongoing sorption mechanisms.

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