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# Site-Specific Europium Adsorption on Muscovite (001) Surfaces

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The long-term safety of nuclear waste repositories heavily depends on their potential to prevent the migration of the contained radionuclides. In the host rock, adsorption onto mineral surfaces is a key mechanism to bind radionuclides and inhibit further transport to the biosphere. Several experimental studies have shown that phyllosilicates (e.g., clay minerals or mica) provide surfaces with strong sorption potential. Therefore, clay rock formations such as the Opalinus clay are being investigated as repository sites in several countries. In the natural environment of host rock formations, the mineral surfaces are exposed to a variety of reactions altering the surface nanotopography (e.g., dissolution). These changes can affect radionuclide adsorption processes. A recent study revealed that calcite surfaces show heterogeneous europium sorption due to their nanotopography [1]. The nanotopography leads to a heterogeneous distribution of reactive sites that are available for adsorption reactions.

In this study, we use numerical methods to investigate the adsorption of $Eu(OH)_3$ on muscovite (001) surfaces with varying nanotopography. Density Functional Theory (DFT) is used to calculate adsorption energy barriers of several atomic sites that are present on the muscovite surface. The sites differ in their first and second order coordination environment, which influences their adsorption potential. A series of geometry optimizations with increasing Eu–site distance is computed to obtain the adsorption energy for each site. The site-specific adsorption energy barriers values are then used for the parameterization of a Kinetic Monte Carlo (KMC) model based on a previous study [2]. The KMC model allows for the simulation of adsorption on larger muscovite surfaces. It is separated into: (1) placement of structures (e.g., pits) and subsequent dissolution simulation for nanotopography generation and (2) $Eu(OH)_3$ adsorption based on the available surface sites and their DFT-derived adsorption energy barrier. This combined numerical approach can show the effect of surface site coordination on radionuclide adsorption and predict the resulting adsorption heterogeneity on mineral surfaces.

[1] Yuan et al. (2021) *Environ. Sci. Technol.* 55, 15797–15809.
[2] Schabernack et al. (2021) *Minerals* 11, 468.