Heavy metal asdorption and transport at clay minerals – water interfaces using atomistic simulations

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The detrimental impact of heavy metal contamination on the environment poses a threat to humans and wildlife. Several strategies promote ex-situ remediation, which aims at removing the mobile ions. However, it is more promising and convenient to perform in-situ immobilization of the mobile heavy metal fraction by increasing the stability of adsorbed species onto minerals surfaces. In those situations where in-situ remediation can be achieved, options include adding natural and synthetic additives. Phyllosilicates display an exemplary sorption capability and can be used to stabilize heavy metals. However, the structures and mechanism behind the processes occurring at the mineral surfaces are unclear and require atom level insights. Atomistic simulations have not been fully exploited to investigate these processes because of the complexity of the systems involved. On the other hand they can provide information on local interactions that could help develop cost effective and green technologies for remediation of heavy metal ions.

We present our recent research to gain atom-level insights into the factors controlling the interaction and reactivity of heavy metal ions at clay mineral – water interfaces. We use a combination of quantum and potential based methods to explore different size and time scales, which enables us to efficiently evaluate structural and dynamical properties of this class of geosorbents. We explore the sorption behaviour of clay minerals not only at the basal plane but also at edge surfaces. Edge surfaces have a greater range of compositions and charges and can provide a more efficient route to heavy metal immobilization.