Atomistic modelling approach for interpretation of spectroscopic data.

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X-ray Absorption Spectroscopy (XAS) is widely used for the interpretation of surface complexation mechanism and incorporation of ions into the mineral structure. Traditional analysis of XAS data is based on either a qualitative comparison of the measured spectra with the reference ones for the known compounds or shell fits for the structural interpretation of the local coordination environment. The shell fitting provides accurate information about nearest coordination and approximate information about the coordination numbers. One of the main limitations of the traditional approach is the lack of information about the 3D arrangement of atoms in the local coordination environment. If several species are present in the sample the discrimination of individual components is not always feasible.

The interpretation of XAS data can substantially be improved and enriched using structural information from atomistic simulation. The atomistic structures are used to theoretically calculate reference spectra of relevant atomic complexes, which are used for the interpretation of the measured data. Such an approach enables to obtain quantitative information about possible speciation and provides an explicit representation of structural configuration of the studied ions. This approach has successfully been applied for the interpretation of ion uptake by clay minerals and zeolites [1].

[1] Churakov, Dähn, (2012) *ES&T.*, 46(11), 5713-5719; Kéri et al., (2017) *ES&T.*, 51(18), 10585-10594; Kéri et al., (2019) *ES&T.*, subm.; Cametti. et al., (2019) *JPCB*, subm..