

## Towards an accurate characterization of local coordination environments of trace impurities in Fe (oxyhydr)oxides

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The ease with which a metal impurity substitutes for Fe(III) in regular structural sites in Fe (oxyhydr)oxides depends on a number of factors including size mismatch, charge balance requirements, and symmetry preferences. It follows that the more flexible the host phase structure the greater its ability to accommodate a seemingly incompatible impurity. Such flexibility might be intrinsic to the structure or imposed by defects. Consequently, the local structure surrounding a less compatible impurity could be very distorted and difficult to characterize. In this regard, extended X-ray absorption fine structure spectroscopy (EXAFS) is commonly used to determine the local coordination environment of impurities in a host phase; nonetheless, using traditional shell by shell fitting to resolve the local bonding environment of seemingly incompatible dopants is a difficult task due to a lack of appropriate standard structures and a priori knowledge concerning thermal disorder, coordination numbers, and potential defect associations. These limitations become manifest in very large Debye-Waller factors that convolute thermal and configurational disorder. In order to resolve these uncertainties relating to the incorporation of uranium in Fe (oxyhydr)oxides, we used ab initio molecular dynamics (AIMD) to derive synthetic EXAFS spectra as a function of different potential configurations [1]. These results highlight the need to couple AIMD and EXAFS to understand the complicated bonding environment of incompatible impurities in Fe (oxyhydr)oxides or any host phase.

[1] McBriarty et al. (2017) *Env. Sci. Tech.* **51**, 4970-4977.