Simulations of HERFD XANES of actinide systems

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X-ray Absorption Near-Edge Structure (XANES) is an invaluable tool in material science, allowing to probe the oxidation state and the local electronic structure of a selected atomic species. The theory behind XANES is complex and extracting information from data is not straightforward. Nowadays the availability of *ab initio* codes specifically written for XANES analysis boosted the interpretation of XANES. Moreover, the use of High Energy Resolution Fluorescence Detected (HERFD) XANES, giving better-resolved spectral features, increases the information that can be extracted. HERFD XANES is particularly advantageous to study actinide systems since the gain in resolution is big.

We present two examples where we systematically used the *ab initio* code FDMNES [1] to reproduce the HERFD XANES L_3 edge and obtained valuable information on the local structure of the systems studied: ThO_2 nanoparticles and U adsorbed on graphene oxide.
The analysis of ThO_2 small nanoparticles revealed that a post-feature of the Th L_3 edge is very sensitivity to the more exposed cations at the surface [2].

The simulations of U adsorbed in different local geometries onto graphene oxide reveals that it preferentially occupies holes in the graphene sheet, pointing out to the importance of the defect density in the perspective of maximizing the adsorption capabilities of graphene oxide [3].

The cases presented illustrate that HERFD XANES supported by *ab initio* simulations have great potential for the investigation of actinide-based materials.

References

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