Ab initio simulations to study valence to core XES and HERFD-XANES

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Materials for catalysis and batteries have the complexity of their atomistic structure in common. Moreover, *operando*, the correlated atomic disorder can influence the chemical properties. Its understanding is crucial and X-ray spectroscopies are very good candidates for this purpose.

After a brief introduction to show how these spectroscopies are calculated in the fdmnes code, we present two cases where *ab initio* simulations help to solve the electronic and geometric structures of such materials. The first one concerns nanoparticles of Pt and PtSn adsorbed on alumina. We show that thanks to XANES recorded in High-resolution Fluorescence Detection mode, the *ab initio* determination of their structure and the confrontation to the calculated spectra, it is possible to find the general structure of the particles, with the number of Hydrogen atoms bonded to them. The second one deals with characterization of nano-Li_2MnO_3 where both HERFD-XANES and XES were used to observe the local geometry and some aspects of the associated electronic structure.