Simulation Of XANES Using The FDMNES Code

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ABSTRACT

The goal of this tutorial is to understand the basic principles of X-ray absorption; this will be achieved through *ab initio* simulations using the FDMNES code. Participants will simultaneously learn to use this code, which is designed to be user-friendly.

After a short introduction, we will begin with a very simple case: a metal atom in an octahedral environment. We will examine the dipole and quadrupole contributions and test for anisotropy. We will then introduce distortions to observe their quantitative impact on the signal and on dichroism. Next, we will move on to crystalline materials, such as magnetite. We will look at the influence of the calculation radius on the results and the effect of the two iron sites. Subsequently, we will examine magnetic cases by performing XMCD calculations.

Given the limited duration of the tutorial, it will be difficult to carry out full calculations achieving optimal agreement between experiment and theory, but the methodology for doing so will be explained.

Depending on participant requests, we will look at how to calculate the absorption signal for dopants or cases where multiple chemical elements occupy the same site. We may also explore calculations for X-ray Raman scattering, X-ray emission, or resonant diffraction. Finally, if participants have specific examples, these can be addressed—at least to provide the right direction for analysis.

MATERIAL

The participants must have their own laptop (Windows, Mac or Linux) with a software to plot spectra (Origin, Kaleidagraph, or any other simple to use… (not Excel !). It is also possible to plot using Larix.

A special package containing the FDMNES executable for the different operating system will have to be first downloaded (web site address will be given in September). It is not the standard package but a more complete one containing special documentation and indata files necessary for the tutorial.

Note that the Mac users could test first if the executable is working. If not, instructions are given in the “doc” directory of the package.