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Simulation Of REXS With FDMNES -II

Monday, 6 October 2025 10:55 (1h 20m)

The tutorial is devoted to the ab initio simulations of resonant X-ray diffraction spectra using the FDMNES code1.
First a little lecture will be given. It will include a brief historical overview, the basics in theory necessary to understand the sensitivity of the technique, and some typical examples. To introduce the practical, an introduction to the FDMNES code and its specificities will also be given.
Then, the participants will start simulations on different examples. They will learn at the same time the use of the FDMNES code and the way to check specific properties as the polarization in and out dependence, the effect of dipole and quadrupole transitions, what can be seen in azimuthal scans, etc⋯
We will also show how the extraction of the spherical components of the scattering tensors can give information on specific projections of the density of states on the absorbing atoms. Relation to the magnetic and spatial symmetries will be evocated. Effects of self-absorption and birefringence will also be simulated.

Examples at K edges in magnetite, V2O3 and L23 in CuO will illustrate all this for non-magnetic and magnetic studies. Eventually on demand, examples from the participants could be addressed.

Participants must have their own laptop. A specific package with documentation, in-data files and the FDMNES executables for Mac OS, Windows 64 and Linux are provided. They must nevertheless have their own software to plot spectra (Origin, Kaleidagraph, ⋯).

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Session Classification: Tutorials + coffee break