

Simulation of EXAFS: a live introduction to FITNESS, a new software built-in to Fastosh

Gautier Landrot

Synchrotron SOLEIL, L'Orme des Merisiers, Départementale 128, 91190 Saint-Aubin

ABSTRACT

This tutorial will be mostly dedicated to showcase FITNESS, a new software built-in to Fastosh and dedicated to shell-by-shell fitting of the EXAFS. Since the focus of the tutorial will be on this program rather than on the overall EXAFS fitting methodology, the attendees ideally should have some prior knowledge and experience of the EXAFS shell-by-shell fitting procedure using other FEFF-based EXAFS fitting software. The session will be divided in two parts:

- In the first part, the instructor will provide a “walk-through” live demonstration of the main features of FITNESS. An experimental EXAFS spectrum will be simulated in front of the audience, from start to finish, to showcase:
 - 1) all the specific unique functionalities offered by the program at every step of the fitting procedure (i.e. data importation; preparation of the FEFF input file; management of FEFF results; creation of the theoretical chi ; refinement of the theoretical via least-square fitting minimization.
 - 2) the ability of the program to rapidly fit an EXAFS spectrum on a large R range in Fourier Transform space
- In the second part, an experimental spectrum will be simulated by the attendees. This “hands-on” experience should be help get personally familiar with the program functionalities.

MATERIAL

For the first part, since it will be fully provided by the instructor, no personal computer is required.

For the second part, the attendees should have the latest version of Fastosh installed on their personal computers. **Note:** An oral presentation introducing the program will be given at the conference XAFS50.fr on October 7th, which will represent the official birth of the software. Therefore, the installer (Windows, Mac, Linux) of the latest version of Fastosh, which will feature FITNESS, and data employed in this tutorial, **will be available for free download on SAMBA beamline's website (<https://www.synchrotron-soleil.fr/en/beamlines/samba>) starting from October 7th.**