TUTORIAL

Use of the Fastosh software for the XAS data treatment

Fastosh is a free standalone program that provides unique functionalities to process X-ray Absorption Fine Structure (XAFS) spectroscopy data. This program was created for Users of SAMBA beamline, SOLEIL Synchrotron, but can be employed to process data generated at any XAFS beamline since it can open data files in ASCII format. The program indeed allows users to easily and rapidly perform a number of operations such as chunking and averaging a large number of scans, auto-deglitching, 2D filtering, 3D plotting, data processing using chemometric methods, and assessing the progress in data acquisition using a fully automatic data viewer tool. Additionally, functions specifically compatible with SAMBA data notably allow to average HDF files and extract new fluorescence spectra from MCA patterns processed to minimize acquisitions artefacts, such as diffraction peaks.

Location : SOLEIL

Organizers : Gautier LANDROT (SAMBA), Amélie BORDAGE (ORGUES)

Number of participants : No limit

Part I : January 18th 14:00 – 17:00

The fundamentals of XAS data treatment will be presented: calibration & alignment, merging, normalization, background subtraction, Fourier Transform & Reverse Fourier Transform. Basic functionalities will be covered in this session, with an emphasis on those that are unique to the program, such as 3D data visualization, merging by sub-groups, 2D filtering, & auto deglitching.

All the users who want to discover XAS data treatment and / or the software developed by the SAMBA beamline can attend this part.

Part II : January 20th 14:00-17:00

The chemometric functionalities of the software will be presented: PCA, Target Transformation (TT), & Multivariate Curve Resolution Alternating Least Squares (MCR-ALS) method. The first part of this session will be dedicated to review the Singular Value Decomposition step of the PCA analysis, including the effects of data centering and scaling, which may subsequently affect the results obtained by TT and MCR-ALS methods that are employed after PCA. The basic functionalities of the Jaumot et al.'s MCR-ALS toolbox included in Fastosh will be covered during a step-by-step tutorial. By the end of this session, any attendee should be able to apply the TT or MCA-ALS procedure using personal computer and XAFS datasets generated at SAMBA or elsewhere.

All users (beginners as well as confirmed) can attend this session. For the beginners who want to attend this part, it is highly recommended to attend also the first part on Wednesday.

Requirement : It is mandatory to download the software prior to the tutorial, and check if it is starting properly on your laptop : https://www.synchrotron-soleil.fr/fr/lignes-de-lumiere/samba

The software can be installed on Linux, Mac and Windows machines.