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The XAFS data treatment software "FASTOSH": main & latest functionalities, including tools to visualize and intrepret Wavelet Transform of the EXAFS

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Since the first release of FASTOSH [1], a number of functionalities have been added to this XAFS data treatment freeware, available on SAMBA beamline's website (Synchrotron SOLEIL). This presentation will showcase its main functionalities, and demonstrate why this program is particularly well suited to investigate systems of environmental/geochemical relevances, and those studied at the XAFS beamline in *operando* conditions. A first focus will be on the latest updates of the program's chemometric functionalities, including MCR-ALS, which can help identify the nature of the principal components present in a complex mixture. Additionnally, the tools to visualize and intrepret the Cauchy or Morlet Wavelet Transform (WT) of the EXAFS, which have been recently added to the program, will be presented. Wavelet Transform may reveal some information that can be less obvious to notice from a simple observation of the Fourier Transform/Reverse Fourier Transform spectra. For instance, it can reveal the presence of two overlapping atomic shells occurring at similar distances and featuring neighboring atoms whose weights are significantly different from each other. Yet, only a few algorithms to perform such operation have been released since the initial development of WT on EXAFS many years ago [2,3]. Multiple approaches are available in Fastosh to display the WT results. One of them consists in stacking, on top of the WT map of the sample chi, the WT maps corresponding to theoritical single-scattering chi spectra, generated in Fastosh with FEFF8L using a user-friendly interface. The structural parameters associated to the theoritical chi, corresponding to the sum of the single-scattering shells modelled, can be refined using a least-square fitting procedure. The later consists in minimizing the difference between the WT maps corresponding to the theoritical and experimental EXAFS spectra. This can be useful as a simple, pre- shell-by-shell fitting procedure to elucidate the local neighboring atomic environment of an absorber present in a sample.

[1] Landrot, *Goldschmidt Abstracts*, 2018 1402 (2018)

[2] Muñoz, P. Argoul and F. Farges, *American Mineralogist* **88,** Issue 4 694-700 (2003)

[3] Funke, A. C. Scheinost and M. Chukalina *Physical Review* B **71** Issue 9 094110 (2005)