SSHADE Users Newsletter – November 2024 –

Focus on XAS spectra and the FAME database

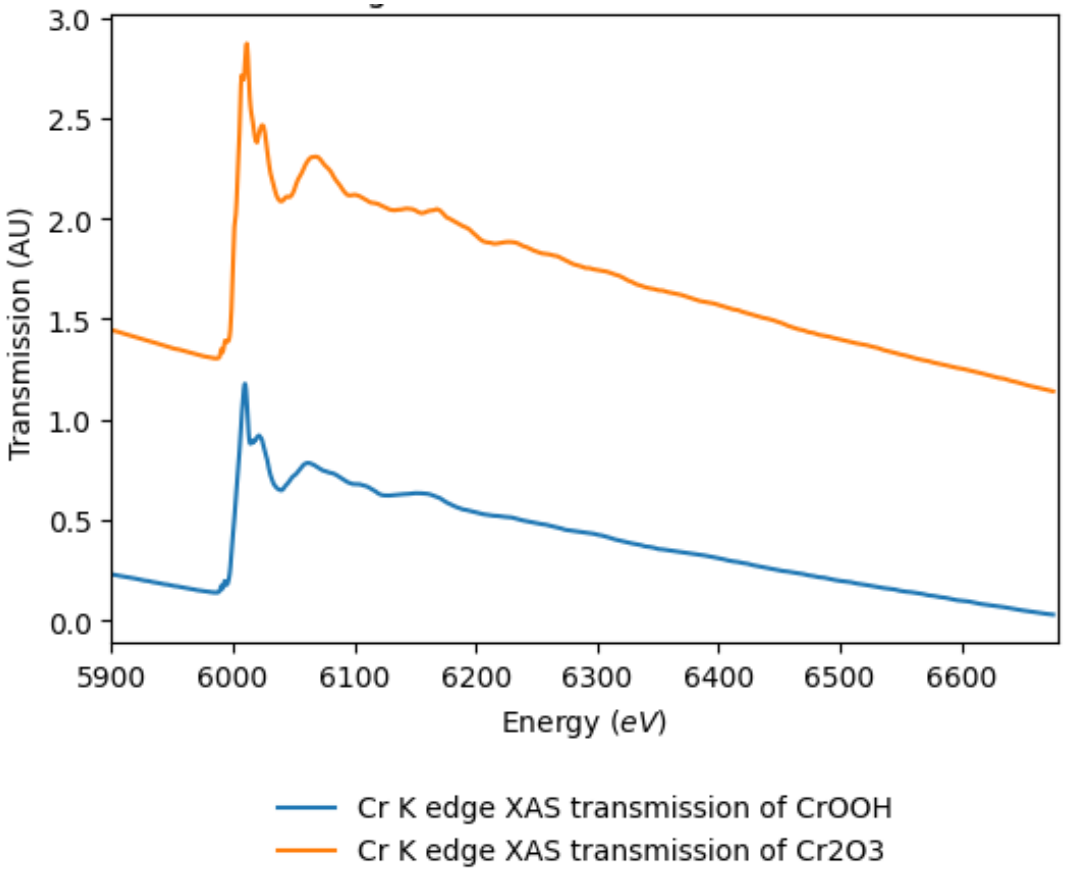
Dear SSHADE users,

This month, we're excited to focus on a specific type of data available in the FAME database @ SSHADE: XAS spectra. XAS (X-ray Absorption Spectroscopy) is a powerful technique used in materials science, chemistry, environmental and planetary science to study the electronic structure and local coordination environment of atoms in a material. By analyzing the absorption of X-rays as they interact with atoms, XAS provides unique insights into the oxidation state, bonding, and geometry of elements.

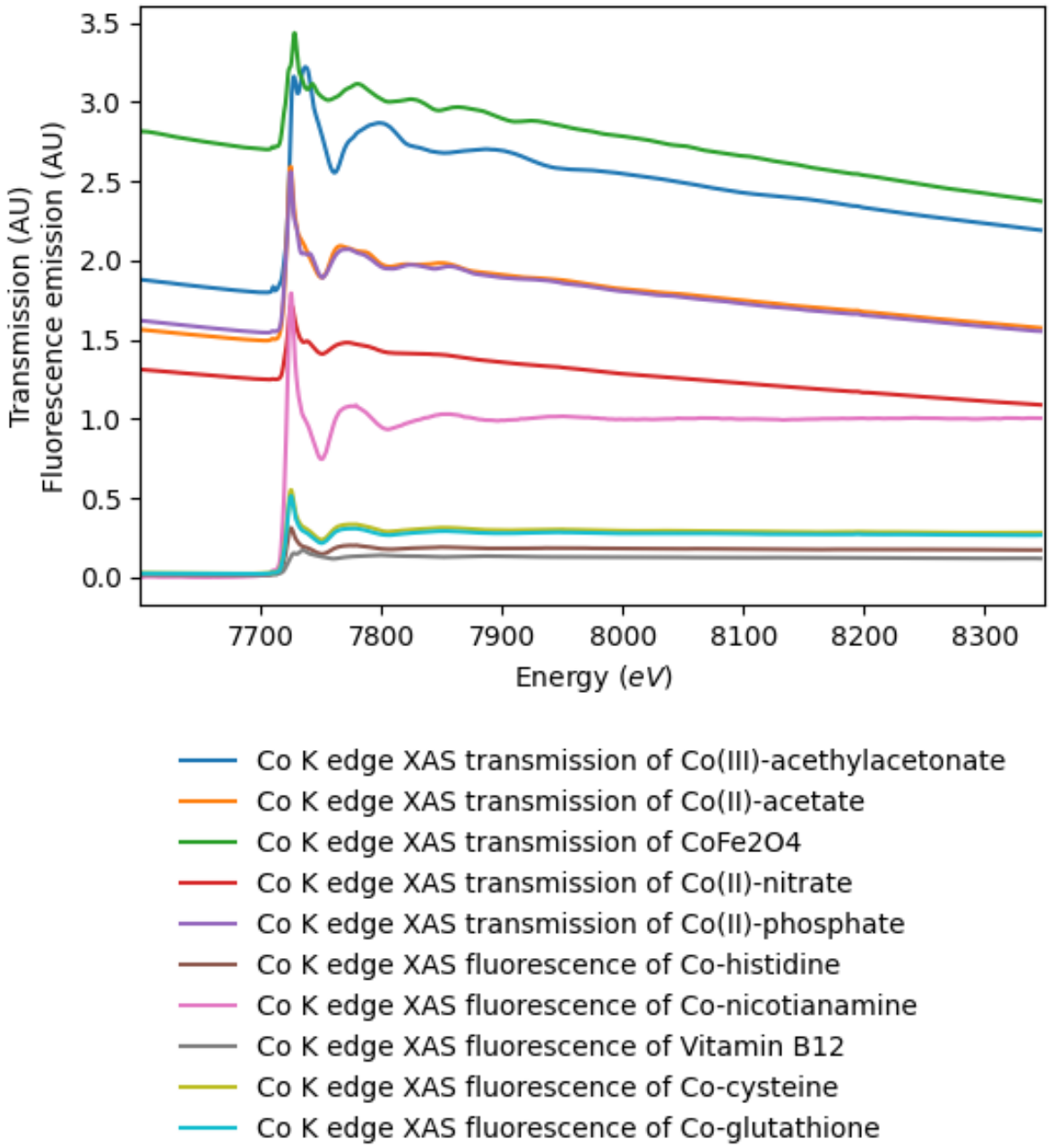
SSHADE hosts a wide variety of XAS spectra in the FAME database for different materials, including minerals, organic compounds, and synthetic samples measured at the FAME beamlines at the European Synchrotron Research Facility (ESRF) in Grenoble, France. Whether you're investigating planetary analogs, exploring interstellar dust composition, or studying terrestrial materials, XAS spectra (in its different measurement variations: XANES, EXAFS and HERFD) can be invaluable for your research.

Here are few examples of what you can find in the FAME database @ SSHADE:

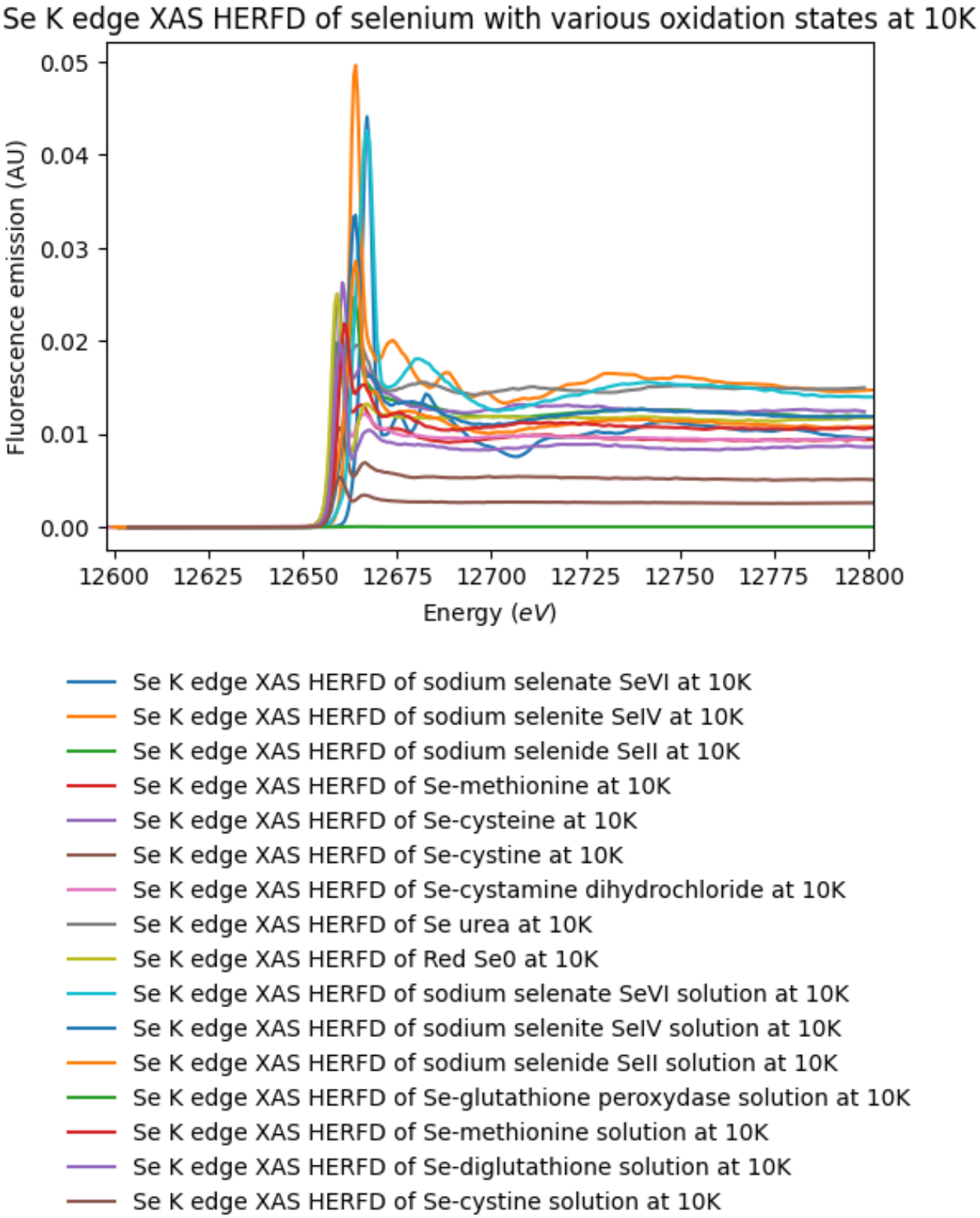
- EXAFS (Extended X-ray Absorption Fine Structure) spectra of synthetic materials like silicates and metal oxides which can give information on the oxidation states and local structures of metal atoms in minerals. For instance, transmission spectra of Cr oxides can be found.



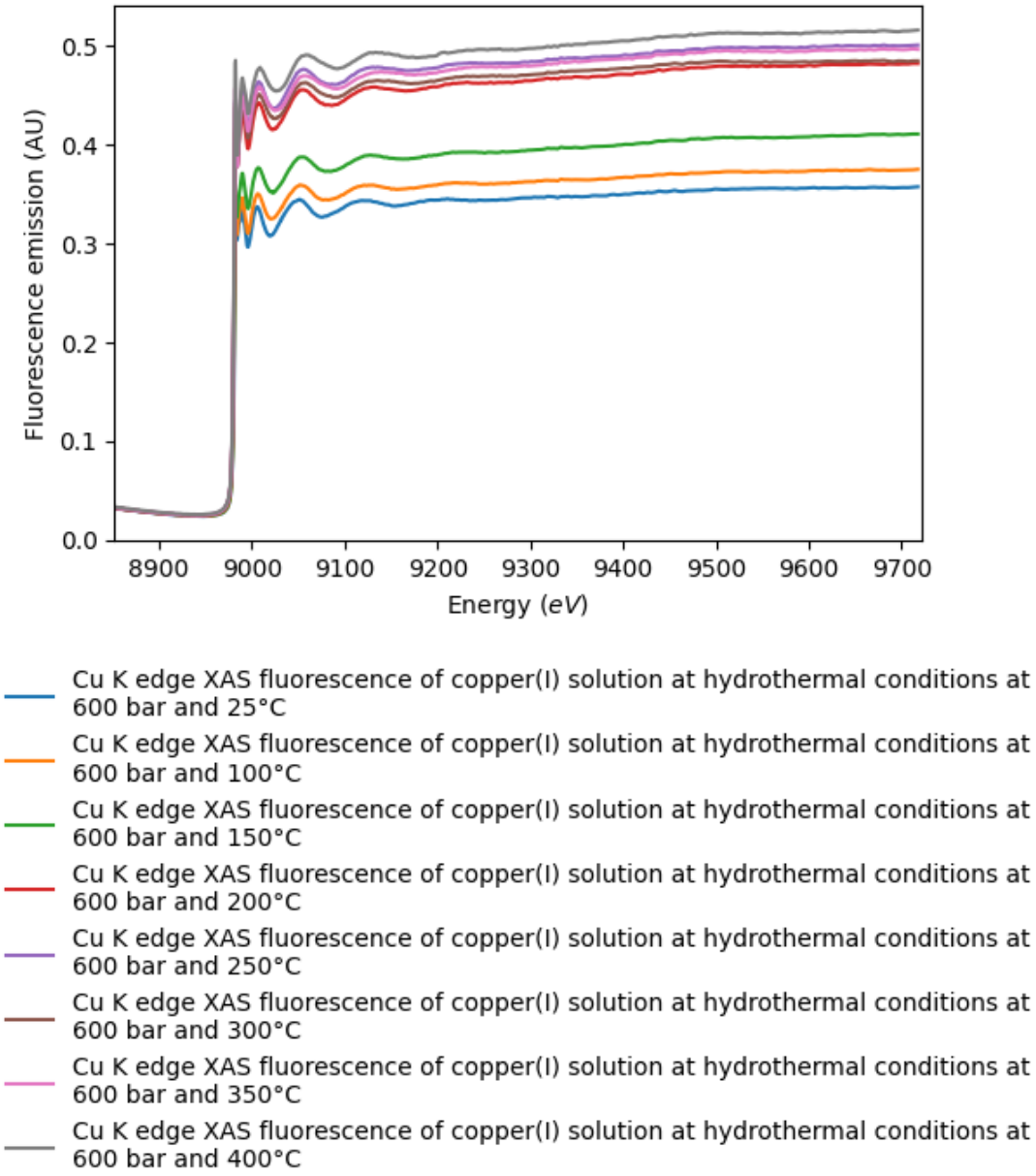
- EXAFS spectra of organic compounds to determine the bonding environments of a metal in complex organic molecules. You can for example find data dealing with Co K edge XAS transmission and XAS fluorescence of organic and inorganic Co(II) and Co(III) reference compounds for the study of Co in bacteria.



- HERFD data for selenium in organic compounds, in the context of cartilage studies. See Se K edge XAS HERFD of selenium with various oxidation states at 10K. HERFD (High Energy Resolution Fluorescence Detection) is a specific detection technique which provides spectra with better spectral resolution: the benefits are more precise information on the metallic structure and better signal-to-noise on very diluted samples (<1ppm), where classical XAS is blinded by matrix contributions.



- SSHADE dataset cover a wide range of experimental conditions, such as varying temperatures and pressures. For instance, SSHADE contains data concerning the Cu K edge XAS fluorescence of copper solution in hydrothermal conditions at 500bars and between 25 and 450°C



The FAME database contains more than 620 XAS spectra on a large set of samples in various conditions. Now it's your turn to explore this diversity.

Stay tuned for future data.

Have fun with SSHADE data!

The SSHADE Team

All previous user newsletters are stored in the dedicated **'News' page** of the SSHADE Wiki