Analysis of X-ray absorption and fluorescence spectroscopy data

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X-ray fluorescence (XRF) and X-ray Absorption Spectroscopy (XAS) are two incredibly popular techniques used to study a wide variety of materials. Requiring little to no sample preparation, they can be employed to study materials at any temperature or pressure, providing chemical and structural information.

XRF is routinely employed to identify and quantify elements down to ppm concentrations. This technique can also be used to evaluate the distributions of the elements on a sample surface: to do so the beam is raster-scanned on the sample and the output data are commonly presented as elemental maps. In the first part of the tutorial, we will explore the basic functions of the most common software for XRF analysis. We will see how to navigate and extract information from a real XRF dataset, working from single-point spectra to 2D elemental images.

The second part of the tutorial will be devoted to XAS analysis, which is commonly employed to extract elemental-specific information such as: oxidation state, coordination, and local structure around the absorbing element. In the tutorial, we will see how to deal with the near-edge structures (XANES) and how to interpret the extended region (EXAFS) of real synchrotron data.