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Analysis of X-ray absorption spectroscopy data

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This tutorial provides a comprehensive base for the analysis of X-ray Absorption Fine Structure (XAFS) data, including both the X-ray Absorption Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS) regions. The primary objective is to guide students through the intricacies of XAFS data analysis, progressing from initial data pre-treatment and normalization to more advanced data refinement techniques.

The tutorial covers:

- 1. XANES analysis, focusing on Linear Combination Analysis (LCA)
- 2. EXAFS data fitting using multi-shell structural models

To facilitate an efficient learning experience, this tutorial will be conducted online. Students are strongly encouraged to pre-install the following software packages:

- 1. DEMETER (<u>https://bruceravel.github.io/demeter/</u>) *Mandatory* A comprehensive software suite for XAFS data analysis
- 2. VESTA (<u>https://jp-minerals.org/vesta/en/</u>) Recommended Visualization software for structural models and volumetric data
- 3. Fityk (<u>https://fityk.nieto.pl/</u>) *Recommended* Non-linear curve fitting tools

By the conclusion of this tutorial, students will have acquired practical skills in XAFS data manipulation and interpretation, essential for XAFS studies in materials science and related fields. This knowledge base will enable researchers to confidently approach more sophisticated XAFS analytical methods as their research demands evolve.