

XANES Spectroscopy

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The X-ray Absorption Near Edge Structure (XANES) region of XAFS spectra provides valuable information on the electronic structure, local coordination geometry, and symmetry around the absorbing atom. Because these features are element-specific and highly sensitive to the local coordination chemistry, XANES spectra can act as fingerprints of distinct chemical environments, enabling the identification and, in many cases, the quantification of different coordination states and crystallographic phases in complicated environments. Such information is often difficult to access using conventional characterization techniques, particularly when long-range structural order is lacking.

In contrast to Extended X-ray Absorption Fine Structure (EXAFS), for which well-established analytical models allow quantitative refinement of local structural parameters, XANES interpretation is more challenging because several structural and electronic parameters simultaneously affect the spectral features and no simple analytical models generally applies.

A variety of quantitative and semi-quantitative approaches have therefore been developed to obtain reliable information from XANES data, contributing to its widespread use across a broad range of scientific disciplines, including physics, chemistry, biology, environmental sciences, and cultural heritage.

This lesson will introduce the main strategies for XANES data analysis and interpretation, discussing their capabilities, limitations, and practical implementation through representative examples.