X-ray absorption spectroscopy: experimental aspects and data analysis

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The basic principles of the x-ray absorption spectroscopy (XAS) will be discussed. Basic theoretical background, typical experimental configurations and applications of this technique will be briefly illustrated.[1] The lecture will be mainly devoted to describe methods and examples for performing accurate experiments and data-analysis of the so-called EXAFS (Extended X-ray Absorption Fine Structure) region of the x-ray absorption spectra, that can be measured using various techniques providing information about the local structure in ordered and disordered systems. Suitable theoretical and computational methods for performing accurate simulations of the EXAFS region of the x-ray absorption spectra, based on the multiple-scattering theory, will be discussed using the specific formulations related to the GnXAS method for XAS data-analysis [2-4]. The relationship between the EXAFS spectra measured in typical synchrotron radiation experiments and the local structural properties in molecular and condensed systems will be elucidated in terms of the so-called n-body expansion of the absorption cross-section.[2-4] It will be shown that the x-ray absorption spectroscopy, especially in the EXAFS regime, has the capability to provide precise atom specific information on the average distribution of the nearest neighbors, beyond the pair correlations when combined with suitable data analysis strategies. Methods and examples refer specifically to the application of the GnXAS suite of programs [2-4] for EXAFS data-analysis but can be easily extended to other popular approaches using similar strategies. Specific issues concerning data treatment and normalization, including possible background contributions due to multielectron excitations, will be mentioned. Model-dependent and independent refinement strategies of multiple-edge EXAFS data will be presented introducing the relevant structural parameters and the uncertainty levels associated with the experimental noise on the measured data[3,4]. Examples on the accuracy of structural refinements of molecular and crystalline systems will be discussed in detail using the traditional peak-fitting (coordination shells) technique. Application to amorphous and liquid systems [5] will be discussed, highlighting the potential of the EXAFS technique and its complementarity to x-ray/neutron diffraction. More advanced data-analysis approaches including refining of tridimensional models of the structure, like those obtained using Reverse Monte Carlo [6] RMC-GnXAS simulations will be mentioned with specific examples.

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