X-ray absorption and fluorescence spectroscopy: the EXAFS technique

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The basic principles of the x-ray absorption spectroscopy (XAS) and x-ray fuorescence (XRF) technique will be discussed. Basic theoretical background, typical experimental configurations and applications of the two techniques will be briefly illustrated [1]. In particular, I shall discuss more deeply suitable theoretical and computational methods for performing accurate data-analysis of the so-called EXAFS (Extended X-ray Absorption Fine Structure) region of the x-ray absorption spectra [1,2]. 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 [2,3]. Standard data-analysis approaches and more advanced methods based on multiple-scattering and Reverse Monte Carlo simulations will be illustrated, with specific examples [3]. It will be shown that the x-ray absorption spectroscopy, expecially in the EXAFS regime, has the capability to provide precise atom specific information on the average distribution of the nearest neighbours, and beyond the pair correlations when combined with suitable data analysis strategies.

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[2] A. Filipponi, A. Di Cicco, C. R. Natoli, *Phys. Rev. B* **1995**, 52, 15122.

[3] A. Di Cicco, A. Trapananti, *J. Phys. Condens. Matter* **2005**, 17, S135. A. Di Cicco, *Rad. Phys. Chem.* **2018,** 175, 108077. A. Di Cicco et al. *J. Chem. Phys.* **148,** 094307 (2018).