XVII School on Synchrotron Radiation
"Gilberto Vlaic":
Fundamentals, Methods and Applications
Muggia (Trieste), Italy / 16-26 September 2024

X-ray absorption and fluorescence spectroscopy

Andrea Di Cicco
School of Science and Technology, Physics Division, University of Camerino, Camerino, Italy

The basic principles of the x-ray absorption spectroscopy (XAS) and x-ray fuorescence (XRF) techniques 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 simulations of the so-called EXAFS (Extended X-ray Absorption Fine Structure) region of the x-ray absorption spectra.[1,2] Calculation methods of the x-ray absorption cross-section 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.

REFERENCES

[1] P. Fornasini, Chapter 6 in *Synchrotron Radiation: Basics, Methods and Applications*, Eds. S. Mobilio, F. Boscherini, C. Meneghini, Springer-Verlag Berlin Heidelberg, **2015**.
[2] A. Filipponi, A. Di Cicco, C. R. Natoli, *Phys. Rev. B* **1995**, 52, 15122 and 15135.
[3] A. Filipponi, A. Di Cicco, C. R. Natoli, GNXAS I. *Phase shifts and signal calculations*, International Tables for Crystallography (2021). Vol. I. . **https://doi.org/10.1107/S1574870720003286**
[4] A. Filipponi, A. Di Cicco, C. R. Natoli, GNXAS II. *Structural refinement of experimental data*, International Tables for Crystallography (2021). Vol. I. . **https://doi.org/10.1107/S1574870720003390**
photoelectric absorption and scattering.