X-ray Absorption Spectroscopy and Multiple Scattering Theory

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X-Ray Absorption spectroscopy (XAS) is a powerful tool to investigate both the electronic and geometrical structure around a well-defined absorbing atom belonging to any type of material, from biological samples to condensed matter. In these lessons I will present a general theoretical scheme, based on Multiple Scattering Theory, to analyze the XAS spectra, which allows a complete recovery of the experimental data from the edge up to very high energy.

The fundamental aspects of the theory will be presented in detail. In particular, I will discuss how the possibility of fitting the low energy part of the XAS spectrum, the so-called XANES energy range, allows a complete three-dimensional determination of the local geometry around the photo-absorber, including bond angles and distortions to which EXAFS is largely insensitive.

Since the analysis starts at the edge, a limited energy range is sufficient to perform a structural fit. This is particularly relevant for time-resolved experiments, where the acquisition time is short, and for the analysis of molecular dynamics simulations, where the differences produced by different interaction potentials appear mainly in the near-edge region.

Some applications on the analysis of the XANES spectra of different systems will be discussed in detail, from biology to coordination chemistry.