

Multiple Scattering theory and its application to XAS (X-Ray Absorption Spectroscopy) spectroscopy: state of the art and new applications in material science

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Multiple Scattering (MS) Theory is a very powerful approach to the calculation of the electronic structure (both the bound and the continuum part of the spectrum) of molecules and cluster of atoms of any size and symmetry. This method works in the real space and does not need to any translation symmetry as in the band approaches. In this talk I show how MS can be considered a unitary cluster approach to the calculation of several electron and photon spectroscopy with a particular emphasis to the X-Ray Absorption from core levels (XAS). I also show how MS theory gives a strong theoretical background for the quantitative analysis of the experimental XAS data and allows a complete recovery of the experimental spectra in the whole energy range. In particular, I will discuss in details a new method to get structural quantitative information using the low energy part of the spectrum, starting from the edge. This procedure, that has been recently proposed in the literature, allows a complete three dimensional determination of the local geometry around the photo-absorber in many different systems. Some chemical and biological applications will be also presented in details.