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X-ray Absorption and X-ray Magnetic Circular Dichroism in the soft X-ray range: Experiment and Theoretical Simulations

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X-ray absorption (XA) spectroscopy in the soft X-ray range is a tool widely used in the study of systems with transition metal ions. In this energy range (typically 400-2000eV) lies most of the transition metals $L_{2,3}$ edges, which correspond to a transition from the 2p to *n*d levels. Therefore, the XA spectrum probes directly the density of unoccupied d-states, being very sensitive to the transition metal valence, environment and degree of hybridization with its ligands. In the case the absorbing atom exhibit a net magnetic moment, the X-ray magnetic circular dichroism (XMCD) can also be employed. The XMCD signal is the difference between two XA spectra measured with an applied magnetic field parallel and anti-parallel to the X-ray photon helicity. The XMCD spectrum is often analyzed by the so-called sum-rules, which relate the integrated area of both XA and XMCD spectra to the orbital and spin moments of the absorbing atom. In many cases the interpretation of XA and XMCD spectra passes through theoretical simulations. The ligand-field multiplet theory is one of the most used theoretical models in this energy range. It starts from a purely atomic model and the ion environment in the condensed matter is included through ligand field theory.

In the first part of my talk I will introduce XA in the soft X-ray range and XMCD techniques discussing the applicability of the sum-rules. In the second part I will focus on the ligand-field multiplet, giving an introduction about the model, discussing what are the input parameters and which kind of information one can find from the simulations.