



Contribution ID: 165

Type: Talk

## Multiplet code for X-ray spectroscopy - a new approach for low symmetry

*Friday, 16 September 2011 17:20 (20 minutes)*

The analysis and interpretation of state-of-the-art synchrotron x-ray measurements often have to rely on the theoretical understanding of the splittings of the atomic energy levels relevant to the case, and the simulation of spectra. Besides electron-electron interaction and spin-orbit coupling, the crystal field may contribute to the multiplets in a non-trivial fashion, particularly when the crystal symmetry is low. The existing multiplet codes based on describing the crystal field by its symmetry are therefore not suited to cases where the symmetry is destroyed. We therefore propose a computational approach to calculating the multiplets and XAS/RIXS spectra that does not require a knowledge of the crystal field symmetry, but where the crystal structure is entered as point charges. The Coulomb interactions and the crystal field as point charges are explicitly calculated, while the spin-orbit interaction is obtained from the solution of the atomistic Dirac equation in the density functional theory formalism. Therefore no parameterisation is required in order to calculate the multiplets. Scaling factors aiming at adjusting the screening effects on the radial functions are however available and can be used to fit the spectra. Various XAS and RIXS examples will be discussed, in particular in view of the polarisation dependence and symmetry of the crystal field.

### Please specify the session

RIXS

### Please specify poster or talk

Talk

**Primary author:** Dr ULDRY, A (Condensed Matter Theory, Paul Scherrer Institut, Villigen, Switzerland)

**Co-authors:** Dr DELLEY, B (Condensed Matter Theory, Paul Scherrer Institut, Villigen, Switzerland); Dr VERNAY, F (Condensed Matter Theory, Paul Scherrer Institut, Villigen, Switzerland, present address: Université de Perpignan, France)

**Presenter:** Dr ULDRY, A (Condensed Matter Theory, Paul Scherrer Institut, Villigen, Switzerland)

**Session Classification:** Resonant Inelastic and Elastic X-ray Scattering

**Track Classification:** Resonant Inelastic and Elastic X-ray Scattering