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Atomic Multiplets in X-ray Spectroscopies of Solids[1] BERNARD DELLEY, ANNE-CHRISTINE ULDRY, Paul Scherrer Institut, Villigen, Switzerland — The electronic structures of compounds involving open d- and f- shell are studied frequently by X-ray and electron spectroscopies. For a better understanding of the multiplets arising in spectra involving one or more open shells, we have developed recently an easy to use program multiX,[2] which is available to download.[3] This first step allows the inclusion of the crystal environment as a crystal field entered simply as positions and charges of a cluster of atoms around the core hole site. This often gives valuable insights in the case of x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray spectroscopy (RIXS) measurements. However, in many cases it is desirable to allow for hybridization of the open shell electrons with the orbitals of neighbor atoms. This requires dealing with a significantly larger active Hilbert space. This is addressed with our recent Lanczos-based procedure to calculate spectra. First results will be discussed.

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[2]Systematic computation of crystal field multiplets for x-ray core spectroscopies, A. Uldry, F. Vernay and B. Delley, Phys. Rev. B 85, 125133 (2012).
[3]http://people.web.psi.ch/uldry/multiplets/

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