

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**The Anderson-Condon-Shortley Site in X-ray Spectroscopies of Solids**<sup>1</sup> BERNARD DELLEY, ANNE-CHRISTINE ULDRY, Paul Scherrer Inst — Electronic structures of compounds involving open d- and f- shell are studied frequently by X-ray and electron spectroscopies. The excitation, especially core excitation, is localized on a single site makes this the problem of impurity site states interacting with the continuum of bands. on the other hand, the electron-electron interaction within the d- or f- shell leads to a multiplet problem as addressed long ago for isolated atoms. Building on our easy to use program multiX (\*), which treats an atom in a general crystal field environment without symmetry analysis, we now address the interaction of this atomic entity with the band continuum. The crossover from atomic to bandlike spectra is the focus of interest. We discuss experimental examples where available and accessible to our methods.

<sup>1</sup>Swiss SNF grant 200021-129970 is gratefully acknowledged

Bernard Delley  
Paul Scherrer Inst

Date submitted: 12 Nov 2013

Electronic form version 1.4