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Multiplets and Crystal Fields: Systematics for X-Ray Spectroscopies FRANCOIS VERNAY, BERNARD DELLEY, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland — Recently Soft X-ray spectroscopies such as XAS and RIXS, became tools of choice to investigate transition metal oxides. The current resolving power is such that it is nowadays possible to investigate multiparticle excitations like, for instance, bi-magnon dispersion throughout the entire Brillouin zone. Yet, these spectroscopies are strongly linked to local physics: the absorption of a photon and creation of a localized core-hole opens up a shell and therefore a multiplet structure becomes apparent in the spectra. From here we see that it becomes crucial, while interpreting the experimental data, to have a systematic, user-friendly and transparent way of computing the multiplet spectra in order to disentangle in the experiment the information arising from single-particle excitations from the information relevant to collective excitations. We present our approach for arbitrary core-valence multiplets arising from a single configuration. The method covers the full range LS-intermediate-jj and allows to introduce splitting by an arbitrary crystal field easily.

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