# Band Structure Approach to RIXS

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We present formalism for calculating resonant inelastic x-ray spectra (RIXS) within the density functional band structure approach implemented recently in the PY LMTO computer code. The implementation allows studying photon momentum and polarization dependence of RIXS spectra of magnetic as well as non-magnetic compounds.

Ir $L_3$ RIXS spectra calculated for $Na_3Ir_3O_8$ and $Li_3Ir_3O_8$ show good agreements with experimental data and allow to identify transitions from occupied Ir *d* states to unoccupied $j_{\text{eff}}$=1/2 and $e_g$ states.

Band structure RIXS calculations for $SrRu_2O_6$ cannot describe contributions to experimental Ru $L_3$ spectra coming from collective magnon excitations or localized intra-ionic spin-orbital ones. On the other hand, the calculations allow to distinguish these contributions from electron-hole continuum which is reasonably well described using the band structure approach [1].

**References**

[1] - H. Suzuki, *et al*, Nature Materials **18**, 563 (2019).