Valence Band Hard X-Ray Photoelectron Spectroscopy on 3d Transition-Metal Oxides Containing Rare-Earth Element

Ján Minár [1, a)], Laurent Nicolai[1], Daisuke Takegami[2], and Liu Hao Tjeng[2]

[1]*New Technologies-Research Center, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech Republic*
[2]*Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany*

[a)]Corresponding author: jminar@ntc.zcu.cz

Abstract. Here we report on our study to quantitatively describe the intensities of the valence band hard x-ray photoemission spectra (HAXPES) of a rare earth element containing 3d transition metal oxides. Using LaCoO3 as a representative model compound, we compared the experimental data to the results of ab initio one-step photoemission band structure calculations as well as to the sum of the partial density of states of the atomic constituents weighted by their tabulated photoionization cross sections. We discovered that the semicore La 5p density of states surprisingly contributes in a significant manner to the valence band spectrum: Although the La 5p partial density of states in the valence band region is negligible compared to that of the O 2p or the Co 3d, the La 5p cross section in the hard x-ray range is found to be orders of magnitude larger than that of the other subshells. This explains the long-standing issue of why the hard x-ray valence band spectra of a rare-earth element containing materials have line shapes that are very different from those taken at lower photon energies and why they cannot be described in terms of partial density of states of the subshells usually considered for the lower photon energy spectra. We infer that the contribution of the rare-earth 5p must be taken into account and cannot be ignored. [1]

References.

[1] D. Takegami et al., Physical Review B **99**, 165101 (2019)