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THE ASYMMETRIC SHAPE IN PHOTOEMISSION SPECTRA: THE EXPERIMENTAL POINT OF VIEW

The main peak of most of the *p*, *d*, and *f* X-ray photoemission spectra from transition metals exhibit an asymmetry that extends towards the high binding energy side. This asymmetry is observed also in some oxides. The asymmetry in peaks of photoemission spectra arises from a non-symmetric distribution of the final states of the core hole. These states can be related to multiplet components or to transitions of Fermi-level electrons. We analyzed the 3*d* photoemission spectra of the 5th -period elements (from Rb to In), modeling the asymmetries with a Double-Lorentzian (DL) line shape. The DL line shape closely reproduces the asymmetries, and the asymmetry parameter exhibits a clear trend across the 5th period elements. For instance, there is a significant difference in the DL parameter between the two 3d branches for elements with an empty 4d band (Rb and Sr). In contrast, for elements with a partially or completely filled 4d band, this difference is smaller. Additionally, the DL parameter is lower for elements with a half-filled (Mo [Kr]5s1 4d5), almost filled (Ru [Kr]5s1 4d7 and Rh [Kr]5s1 4d8) or completely filled 4d band (Ag [Kr]5s1 4d10, Cd [Kr]5s2 4d10, and In [Kr]5s1 5p1) compared to those with an empty (Rb [Kr]5s1 and Sr [Kr]5s2), less than half-filled (from Y [Kr]5s2 4d1, Zr [Kr]5s2 4d2, and Nb [Kr]5s1 4d4), or completely filled 4d band (Pd [Kr]4d10). These results also suggest a possible relation between the d valence electrons and the physical origin of the asymmetric shape.

Keywords

asymmetry, 3d photoemission spectra, metals, valence electrons

Reference

A. Herrera-Gomez, et al., Double Lorentzian lineshape for asymmetric peaks in photoelectron spectroscopy, J. Vac. Sci. Technol. A 41 (2023). https://doi.org/10.1116/6.0002602.

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