K. Hamaida et al., Int J Mater Sci Res. 2017
http://dx.doi.org/10.18689/2638-1559.a1.003

The Calculated Electron Distribution in the In_2O_3 Compound Validated by the Electron Spectroscopy AES and EELS

K. Hamaida[1]*, M. Bouslam[2], M.Ghaffour[2], Z. Lounis[2] and **M. Harmel[1]**
[1]University Center Belhadj Bouchaïb, Algeria
[2]Laboratoire Matériaux (LABMAT) Ecole Nationale Polytechnique (ENP) d'Oran, Algeria

The electron distribution in the valence band and on the core levels in the CTO (Conductive Transparent Oxide) In_2O_3 is very important to predict its applications. We adopt the calculation simulation based on the approximations GGA (Generalized Gradient Approximation) and mBJ (modified Becke Johnson) using the programWien2K to obtain the electron distribution. The valence band involves the hybridation of states s and p of chemical species indium and oxygen in the range -6eV to 0eV. The features related to these states s and p are very discriminated from other features located to low energies related to states d of indium in the range -13 eV to -11eV. The calculation results enable us to predict the interband transition. Furthermore, the electron distribution around the cation (indium) and anion (oxygen) allows us to determine the ionic character of the chemical bond in the In_2O_3 compound.

We confirm such results owing to the characterization methods by the electron spectroscopy AES (Auger Electron Spectroscopy) and EELS (Electron Energy Loss spectroscopy).

Keywords: GGA and mBJ approximations; oxides CTO; AES and EELS spectroscopy.