K. Hamaida et al., Int J Mater Sci Res. 2017
http://dx.doi.org/10.18689/2638-1559.a1.002

Valence Band Distribution Studied by GGA and mBJ Approximation in a Comparison with AES and EELS Spectroscopy

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Information on electronic distribution of the valence band and deep levels on In_2O_3 is very necessary to predict its applications in technological fields. We adopt the computational simulation based on GGA (Generalized Gradient Approximation) and mBJ (modified Becke Johnson) approximations using the Wien2K program to obtain the electron distribution. The valence band involves the hybridization of the s and p states of the indium chemical species and the oxygen in the range 6eV to 0eV. The characteristics related to these states s and p are very discriminated from other characteristics located at low energies linked to the d states of indium in the range 13 eV to 11eV. The calculation results allow us to predict the interband transition. Moreover, the distribution of electrons around the cation (indium) and the anion (oxygen) allows us to determine the ionic character of the chemical bond in the compound In2o3. We confirm these results using AES (Auger Electron Spectroscopy) and EELS (Electron Energy Loss Spectroscopy) electronic spectroscopy characterization methods.

Keywords: GGA and mBJ approximations; In_2O_3; AES and EELS spectroscopy.