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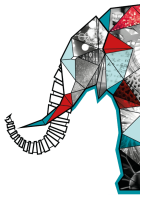

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STRUCTURAL ELECTRONIC AND OPTICAL PROPERTIES OF KESTERITE CU2ZnSnS4 (CZTS), USING (FP–LAPW) METHOD

The structural, electronic and optical properties of Kesterite CZTS, have been studied using the full potential linearized augmented plane wave (FP–LAPW) method within the density functional theory (DFT) and showed good agreement with our experimental results. The calculations were carried out using the Wien2K code, for the potential of exchange and correlation we used two approximations; local density approximation (LDA), and modified Becke-Johnson potential (mbj).
This study allowed us to determine the values of the crystalline parameters (a = 5.36 Å and c = 10.74 Å) at equilibrium that are close to those we obtained experimentally. The analysis of the electronic structure of the CZTS confirms its character of band structure with a direct gap equal to 1.3eV, nevertheless its value remains underestimated compared to the experimental value (1.4-1.6) eV. The analysis of the total (T DOS) and partial (P DOS) state densities obtained by the LDA-mbj for the CZTS compound allowed us to study the hybridization of atomic states and their contributions in the band structure of KS-CZTS. According to the spectrum of the total density (T DOS) we note that the maximum of the conduction band is dominated mainly by the d states of copper (d-Cu), whereas the minimum of the valence band is dominated by the contribution of the states s/p of tin and p of sulfur. The comparison between the experimental study and the theoretical study shows a good agreement between these two aspects.

Choix de session parallèle

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