

Density of State Calculations for Tl_3SbS_3 and $SbTe$

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Based on the full-potential linearized augmented plane waves method (FL-LAPW) with local density approximation (LDA), the partials and total densities of state of Tl_3SbS_3 and $SbTe$ are calculated in order to find the semiconductor character *via* direct or indirect gap. Tl_3SbS_3 and $SbTe$ presents the most important candidates of the antimony chalcogenides family. Their densities of states curves bring out characteristic features in the valence band a core like peak, at environ 13.00 eV below the valence band maximum, originating mainly from S 3s and I 5s states respectively, and a three-peak structure at the top of the valence band from S 3p and I 5p states hybridized with Sb 5p and Te 5p states. Our results give a good agreement with other theoretical calculations and experimental data.

Keywords: The full linearized augmented plane wave method (FL-LAPW); Density functional theory (DFT); The local density approximation (LDA); Kohn Sham orbitals (KSO).

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