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Density of State Calculations for *T l3SbS3* and *SbT eI*

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Based on the full-potential linearized augmented plane waves method (FL-LAPW) with local density approximation (LDA), the partials and totals densities of state of *T l*3*SbS*3 and *SbT eI* are calculated in order to find the semiconductor character *via* direct or indirect gap. *T l*3*SbS*3 and *SbT eI* 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 3*s* and I 5*s* states respectively, and a three-peak structure at the top of the valence band from S 3*p* and I 5*p* states hybridized with Sb 5*p* and Te 5*p* 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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