First principles study of the structural, electronic, optical and thermal properties of chalcopyrite semiconductor $LiAlTe_2$

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The structural, electronic, optical and thermal properties of chalcopyrite $LiAlTe_2$ are studied using the full potential linearized augmented plane wave (FP-LAPW) method framed within density functional theory (DFT). The Wu-Cohen generalized gradient approximation (WC-GGA) was used as exchange-correlation potential to calculate the structural properties. Furthermore, the Tran and Blaha modified Becke-Johnson (mBJ) functional was also employed to compute the electronic and optical properties in order to get best values. The structural parameters at equilibrium are in good agreement with previous experimental and theoretical calculations. The band structures and density of states are calculated and it is found that $LiAlTe_2$ compound is a direct band gap (Γ-Γ) semiconductor. In addition, the optical properties such as dielectric function, refractive index, reflectivity and absorption coefficient are calculated for photon energies up to 25 eV. This study on the optical properties has also been enriched by the introduction of the analysis of birefringence and anisotropy for this material. The calculated values of all parameters are compared with the available theoretical data where a reasonable agreement has been obtained. The study of the material properties at high temperatures and pressures is very important to understand the behavior of a material in severe conditions, so the temperature and pressure dependencies of unit cell volume, bulk modulus, Debye temperature and specific heat capacities are obtained at different temperatures ($0-1000$ K) and pressures ($0-8$ GPa) using the quasi-harmonic Debye model. To our knowledge this is the first theoretical prediction of the thermal properties for $LiAlTe_2$ compound and still awaits experimental confirmations. We have included the spin-orbit interaction (SOI) in our calculations which is known to have significant influence on the electronic and optical properties when heavy elements are present. A weak effect is observed for the studied compound.

Keywords: DFT; Wien2k, Chalcopyrite; band gap; dielectric function; thermal properties.

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