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The density functional study of electronic structure, electronic charge density, linear and nonlinear optical properties of single crystal alpha-$LiAlTe_2$

Abstract

Self-consistent calculations is performed using the full potential linear augmented plane wave (FP-LAPW) technique based on density functional theory (DFT) to investigate the electronic band structure, density of states, electronic charge density, linear and non-linear optical properties of α-$LiAlTe_2$ compound having tetragonal symmetry with space group $I\bar{4}2d$. The electronic structure are calculated using the Ceperley Alder local density approach (CA-LDA), Perdew Burke and Ernzerhof generalize gradient approach (PBE-GGA), Engel–Vosko generalize gradient approach (EVGGA) and modified Becke Johnson approach (mBJ). Band structure calculations of (α-$LiAlTe_2$) depict semiconducting nature with direct band gap of 2.35 eV (LDA), 2.48 eV (GGA), 3.05 eV (EVGGA) and 3.13 eV (mBJ), which is comparable to experimental value. The calculated electronic charge density show ionic interaction between Te and Li atoms and polar covalent interaction between Al and Te atoms. Some optical susceptibilities like dielectric constants, refractive index, extension co-efficient, reflectivity and energy loss function have been calculated and analyzed on the basis of electronic structure. The compound α-$LiAlTe_2$ provides a considerable negative value of birefringence of −0.01. Any anisotropy observed in the linear optical properties which are in favor to enhance the nonlinear optical properties. The symbol $\chi^{(2)}_{abc}(\omega)$χabc(2)(ω) represents the second order nonlinear optical susceptibilities, possess six non-zero components in this symmetry (tetragonal), called: 1 2 3, 2 1 3, 2 3 1, 1 3 2, 3 1 2 and 3 2 1 components, in which 1 2 3 is the dominant one having value 26.49 pm/V.

Keywords; Electronic structure, Electronic charge density, Linear optical properties, Nonlinear optical susceptibilities, DFT