Electronic band structure and optical properties of titanium oxyphosphates $Li_{0.50}Co_{0.25}TiO(PO_4)$ single crystals: An ab-initio calculations

Abstract

From the refined atomic positions obtained by Belmal et al. (2004) [1] using X-ray diffraction for $Li_{0.50}Co_{0.25}TiO(PO_4)$, we have performed a structural optimization by minimizing the forces acting on the atoms keeping the lattice parameters fixed at the experimental values. With this relaxed (optimized) geometry we have performed a comprehensive theoretical study of electronic properties and dispersion of the linear optical susceptibilities using the full potential linear augmented plane wave (FP-LAPW) method. The generalized gradient approximation (GGA) exchange-correlation potential was applied. In addition, the Engel-Vosko generalized gradient approximation (EVGGA) was used for comparison with GGA because it is known that EVGGA approach yields better band splitting compared to the GGA. We have calculated the band structure, and the total and partial densities of states. The electron charge densities and the bonding properties were analyzed and discussed. The complex dielectric optical susceptibilities were discussed in detail.