Electronic structure and magneto-optic Kerr effect in ferromagnetic titanium oxyphosphates $Li_{0.50}Co_{0.25}TiO(PO_4)$: An ab-initio study

Abstract

The X-ray diffraction for $Li_{0.50}Co_{0.25}TiO(PO_4)$, was used as a starting point to perform structural optimization by minimizing the forces acting on the atoms. We have performed a comprehensive theoretical study of electronic properties, including magneto-optic Kerr effect, of titanium oxyphosphates $Li_{0.50}Co_{0.25}TiO(PO_4)$ in the ferromagnetic phase. The generalized gradient approximation (GGA) exchange-correlation potential was applied within the full potential linear augmented plane wave (FP-LAPW) method. The total energy of the ferromagnetic state is 0.72 eV less than that of the paramagnetic state. The total moment is found to be $2.99\mu_B$ with a major contribution of $2.47\mu_B$ coming from the Co atoms. In addition, we have calculated the total and partial densities of states. The electron charge densities and the bonding properties are analyzed and discussed. As a remarkable finding we note that the ferromagnetic $Li_{0.50}Co_{0.25}TiO(PO_4)$, is semiconducting with energy gap of about 1.2 eV for the minority spin and as semi-metallic for the majority spin, in contrast to the paramagnetic $Li_{0.50}Co_{0.25}TiO(PO_4)$ which shows metallic behavior. From the calculated results of band structure and density of states, the half-metallic character and stability of ferromagnetic state for $Li_{0.50}Co_{0.25}TiO(PO_4)$ is determined. The bonding properties of the ferromagnatic $Li_{0.50}Co_{0.25}TiO(PO_4)$ have been analyzed through the electronic spin charge density contours in the (1 0 0) and (1 1 0) planes. The Kerr rotation spectrum is controlled by $\sigma 2xy(\omega)$ at low energies (1.5-3.0 eV) because $\sigma 1xx(\omega)$ is almost constant. The value of the Kerr rotation is close to 0.1 degree at low energies.