Abstract

A detailed theoretical analysis of Lithium (Li) and potassium (K)-doped BaTiO3 is described on the basis of the GGA-PBE density functional theory (DFT). TDOS and PDOS examine and describe the effect of doping on the electronic structure, and consequently on the optical properties. Structural parameters differ separately by partial replacement of the Barium atom with Lithium and K at $BaTiO_3$, and by creating new symmetric states, PDOS is adjusted to increased the electronic band gap. We have found that pure $BaTiO_3$ indirect band gap is converted into direct band gap after doping. Pure and doped BaTiO3's optical characteristics are associated with its electronic determinations. Doping Li and K shows that the doped content is more desirable for many electronic devices compared to pure BaTiO3 due to a major improvement in the band structure and optical properties.