Abstract

We have investigated the cubic form of potassium Tantalum Oxide ($KTaO_3$) utilizing CASTEP software, correlation of GGA and PBE, and density functional theory. The effects of the doping concentration of metals (Rb and Cs) on the phase transition, elastic and optical properties, as well as the band structure and electrical features of $KTaO_3$, are examined. At 2.82% and 5.6β% Rb and Cs modification concentration, the structure of $KTaO_3$ is still cubic, but when the doping concentration is raised to 8.45%, it transforms from cubic to tetragonal. Band gap reduced when we doped material with higher concentration. A thorough examination of the partial and total densities of states has been conducted to elucidate the impact of this modification on the band gap. The presence of Rb and Cs affects the refractive index (n) and other optical properties of both pure and doped systems. The elastic constants for cubic and tetragonal symmetry satisfy the mechanical stability criterion for all doping concentrations. Additionally, the evaluation of a number of variables, including the bulk modulus (B), shear (G), Young's modulus €, Poisson's ration, and anisotropic factor (A), is included in the determination of elastic parameters. Additionally, the measurement of the B/G value is utilized to analyze the ductile/brittle properties displayed by both pure and doped compounds. The material would change in terms of its structural, electrical, optical, elastic and mechanical properties if Rb and Cs were added. These adjustments would also be brought about by changes o the material's elasticity. These adjustments offer a workable solution for optimizing UV filters because their absorption spectra occur in the UV area.