Abstract

The first principle simulations are employed to manipulate the structural, electrical and optical modifications due to Mg (magnesium) doping in $CaZrO_3$ with concentrations of 4.23%, 2.82% and 1.41%. The calculations are executed in CASTEP code with exchange correlation functional as GGA-PBE (Generalized-Gradient-Approximations-Perdew-Burke-Ernzerhof) besides USP (Ultra-Soft-Pseudo-potential). All the calculations are centered on the DFT (Density-Functional-Theory). A strong matching alliance is found exist in between the calculated lattice constant after optimization and the parameter previously reported in literature. The phase transition is also observed when doped with 4.23% Mg in $CaZrO_3$. It transform from cubic to pseudo-cubic tetragonal phase. This doping concentration also caused to increase the *k*-points in BZ (Brillouin-Zone) with the eventual contraction of band-gap in BS (Band-Spectrum). The analysis of electronic spectrum reveals that transition of band-gap nature from indirect (host) to direct when doped with Mg atoms concentrations (1.41% and 2.82%). The band-gap energy varies with divergence of 3.279-2.189eV as a consequence of doping. The PDOS (Partial-Density-Of-States) and TDOS (Total-Density-Of-States) are oriented to illuminate different phenomena like phase transition, band-gap decrease. This is also observed as stimuli for OP (Optical-Properties) variations. However, process of red-shift (1.9-0.65eV) is identified in absorption spectra in case of doped-$CaZrO_3$. While the static refractive index is found to be same in case of Mg doping like pure. A steady reliability is witnessed in the process of loss functions and absorption curves. The modifications made by substituting with Mg atoms cause the potential changes in electrical and optical properties. These variations have made $CaZrO_3$ a practical applicant for optoelectronic devices.