Abstract

This explanatory article employs the Generalized gradient approximation (GGA) by Perdew Burke Ernzerhoff (PBE) and ultra-soft pseudopotential (USP) in CASTEP code to examine the impacts of doping on the structural, phase transition, optoelectronic, and mechanical features of strontium cerate ($SrCeO_3$). Substantial changes to $SrCeO_3$'s natural behavior result from the addition of impurities at the two distinct places. In this, we add magnesium at the strontium place and thorium at the cerium place. Doping with varying amounts of magnesium (Mg) causes a dramatic shift in the bandgap energy from 2.266 eV to 0.503 eV. Th-doping with different concentrations reduces the bandgap from 2.266 eV to 1.679 eV and a phase transition of structure from cubic to tetragonal. When even a little quantity of dopant is introduced into $SrCeO_3$, new states of the dopant elements develop, changing the band structure and the density of states (DOS). Optical qualities are affected by changes in electronic characteristics, and this effect has been studied and explained. In this study, we estimated the elastic constants for a range of doping concentrations and found that all of them met the stability standards set by Born. All of these crystal forms are, thus, mechanically stable, with the exception of the 7.04% and 9.85% of Mg-doping. To determine whether the material is ductile or brittle, its various mechanical characteristics, including its bulk (B), shear (G), young's moduli (E), Poisson ratio (υ), and Pugh ratio (B/G), have been studied. The anisotropic factor is used to determine whether or not a crystal is isotropic (A).