Abstract

The CASTEP approach, based on density functional theory, has been used to determine the structural, optoelectronic, and mechanical properties of undoped, Ca-doped, Mg-doped, and Be-doped $SrHfO_3$. $SrHfO_3$'s structure is unaltered at 1.40% Ca, Mg, and Be doping concentration but is transformed into pseudo-cubic tetragonal at 4.22% and 7.04% doping concentration. The electrical band gap is decreased across the board as doping increases. Partial density of states (DOS) and elemental partial DOS have also been calculated to provide a more in-depth description of the narrowing of the electronic band gap. DOS is crucial for understanding the band gap's behavior under different doping circumstances. Increases in pure $SrHfO_3$'s refractive index (n), Loss function (L), absorption (I), and extinction coefficient (k) are all attributed to the introduction of dopants. All Ca, Mg, and Be doping percentages (except for 1.40 percent Mg and Be for cubic shape) in our compound exhibit mechanical stability. We have also calculated many characteristics including bulk modulus (B), shear modulus (G), G/B ratio, Cauchy Pressure (CP), and anisotropic factor (A) to investigate mechanical properties of materials like ductility and brittleness (A). Ca, Mg, and Be may all be doped into the material without affecting its ductility; only at a doping concentration of 1.40 percent Ca does the material become brittle.