ABSTRACT

We have investigated the cubic form of Cesium Germanium Fluoride ($CsGeF_3$) utilizing CASTAP software, correlation of GGA and PBE, and density functional theory. The effects of the doping concentration of metals (Li, Mg, and Sr) on the phase transition, elastic, and optical properties, as well as the band structure and electrical features of $CsGeF_3$, are examined. At 1.40% Mg and Sr-atom modification concentration, the structure of $CsGeF_3$ is still cubic, but when the doping concentration is raised to 7.04%, it transforms from cubic to tetragonal. In a similar manner, doping Li atoms between 1.40 and 7.40% causes an apparent transition to a tetragonal form. A consistent, considerable band gap reduction is observed every time we doped the atoms in our material, and it always has an effect on the G-symmetry point. 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 Li, Mg, and Sr affects the refractive indices (n) and other optical properties of both the clean and doped systems. The elastic constants for cubic and tetragonal symmetry satisfy the mechanical stability criterion for all doping concentrations, with the exception of the 1.4% Li, Mg, 4.22%, and 7.4% Sr levels. Additionally, the evaluation of a number of variables, including the bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio, and anisotropic factor (A), is included in the determination of elastic parameters. Additionally, the measurement of the B/G value is utilized to analyse the ductile/brittle properties displayed by both pure and doped compounds. All compounds exhibit brittle nature, with the exception of doping with 1.40% Mg and 4.22% Sr. Non-homogeneity is also brought on by the doping of 1.04% magnesium and strontium (Mg and Sr), 7.04% lithium and strontium (Li, Sr), and 4.22% lithium (Li). The material would change in terms of its structural, electrical, optical, elastic, and mechanical properties if lithium, magnesium, or strontium were added. These adjustments would also be brought about by changes to the material's elasticity. These adjustments offer a workable solution for optimizing UV filters because their absorption spectra occur in the UV area.