ABSTRACT

Our work is based on evaluation of structural, optical, elastic and electronic capabilities of pureand doped $CsPbF_3$ with regard to density functional theory by utilizing GGA-PBE functional. The transition of cubic to pseudo-cubic tetragonal phase takes place as a result of different doping concentrations (4.22% and 7.04% Sr and Mg). The impact of transition in phase on band structure of component is explained with the help of complete and partial DOS as well aselemental PDOS. With the inspection of blend of various DOS, we are able to determine electronic bandgap. Initially, the bandgap appears to be 3.031eV for pure $CsPbF_3$ and was considered direct but with doping of Sr and Mg the band gap was reduced. The elastic parameters like shear, bulk or Young's modulus, Poisson's ratio, and anisotropic components are determined for cubic and tetragonal symmetry by utilizing elastic parameters. The Cauchypressure, Pugh and Poisson's ratio were also determined to assess the brittle (ductile) characterof this compound. The value 5.066 Å was determined as lattice parameter of pure material which has incredible correspondence to 4.774 Å that is previously being reported. Mg as wellas Sr while behaving as dopant changes electronic as well as influences optical characteristicsof $CsPbF_3$ in pure state. The determination of genuine and imaginary parts of refraction, dielectric and eradication coefficient for optical properties are examined. The reflectivity and conductivity are also being examined in pure and doped $CsPbF_3$. The analysis of bandgap andincreased absorption power of the compound is detected that lies in the visible and UV energyrange anticipate the functionality of compound in optics, optical gadgets as well as anti- reflection coatings.