Abstract

A comprehensive theoretical analysis exploring influence with doping of Ca, Sr, as well as Rb on phase transition, electronic band structure alongwith their repercussions on optical, elastic, as well as mechanical properties of $CsPbI_3$ has been presented. This analysis was carried out in order to learn more about these properties. The structure of $CsPbI_3$ stays cubic even when doped with 1.40 % of Ca, Sr, and Rb-atoms; however, when the doping concentration is increased to 4.22% or 7.04%, the structure transitions from cubic to a pseudo-cubic tetragonal phase is noted. While every instance of doping, variation in band gap is observed and nature of this phenomenon is shown to be directly related to the G- and sometimes at Z-symmetry point. The total density of states, also known as TDOS, alongwith partial density of states or PDOS, as well as elemental partial density of states (EPDOS) are in line to understand the reduction of the band gap. The optical response of the doped material displays a red shift in the absorption edge, whilst the refractive index rises from 2.1814 to 2.8026 with Ca and Sr doping and marginally lowers after the doping of Rb. The estimated elastic constants for cubic and tetragonal symmetry follow the mechanical stability criterion for each doping concentration, with the exception of 7.04% Rb doping, which deviates from this rule. In addition, when elastic parameters are used, the bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio, and anisotropic anisotropy (A) are computed as estimates. In order to evaluate the brittleness or ductility of a pure or doped compound, the G/B value must first be calculated. In addition, non-homogeneity is shown when doping levels is 7.04%Ca. This is because of the negative stiffness and Poisson ratio. Doping a compound with calcium, strontium, or rubidium would cause changes in its electronic structure, optical, and mechanical properties. The changes, due to doping, would make it a good candidate for better optimization as solar cells as well as in various optoelectronic devices.