ABSTRACT

Our work is based on evaluation of structural, optical, and electronic properties of pure and doped $KCaF_3$ regarding density functional theory by utilizing GGA-PBE functional. The transition of cubic to tetragonal and rhombohedral phase takes place because of different doping concentrations (1.40%, 4.22%, 7.04% and 9.86% Cl and Br). The impact of transition in phase on band structure of component is explained with the help of complete and partial DOS as well as elemental PDOS. With the inspection of blend of various DOS, we can determine electronic bandgap. Initially, the bandgap appears to be 5.550eV for pure $KCaF_3$ and was considered indirect but with doping of Cl and Br the band gap was reduced. The value 4.618 Å was determined as lattice parameter of pure material which has incredible correspondence to 4.482 Å that is previously being reported. Cl as well as Br while behaving as dopant changes electronic as well as influences optical characteristics of $KCaF_3$ in pure state. The determination of genuine and imaginary parts of refraction, dielectric and eradication coefficient for optical properties is examined. The reflectivity and conductivity are also being examined in pure and doped $KCaF_3$. The analysis of bandgap and increased absorption power of the compound is detected that lies in the visible and UV energy range anticipate the functionality of compound in optics, optical gadgets as well as anti-reflection coatings.