ABSTRACT

In this proposed work, formation energy, the structural, optical, electronic and thermal properties have been studied for pure and (Cu, Zn) doped cuboctahedral $SrTiO_3$ perovskite. Ultra-Soft Pseudo-Potential (USPP) and generalized gradient approximation GGA-PBE function are used by implementation of first-principle computations based on the density function theory (DFT). The results of formation energies revealed that Cu and Zn doping at Sr site in host lattice $SrTiO_3$ were more convenient as compared to Ti site. After Cu or Zn doping in $SrTiO_3$, it was observed that the transformation of density of states to smaller energies results in stronger interactions between (Cu or Zn) atom and its neighboring atoms. It was also observed a significant reduction in unit cell volume upon doping of Zn and enhancement in unit cell volume upon doping of Cu into $SrTiO_3$ was occurred. New states at Gamma/ Brillouin zone symmetry point were introduced by doping of Cu and Zn atoms at Sr site. Electronic band structure of $SrTiO_3$ is affected significantly by the doping of Cu and Zn atoms; consequently transformation of its indirect band gap into the direct one existed. Significant change in the partial density of states of $SrTiO_3$ with doping of (Cu, Zn) at the bottom of conduction band was also occurred. The band gap exhibited a strong bowing/ substantial modification due to the interaction of the all doped p-orbitals. It was explored that Cu doping in host lattice results the optical properties of $SrTiO_3$ to be red shifted. Also thermoelectric properties were investigated of pure and Zn-doped system. Significant changes in physical properties and electronic structure of $SrTiO_3$ by Zn and Cu doping open new areas for appealing applications of these materials in optoelectronics devices.