Abstract

By using first-principles calculations in line with density functional theory, the structural, electronic, optical, elastic, and mechanical properties of pure and substituted $PbHfO_3$ have been investigated. Here the substituted elements are Bi, Sn and Tl. To express the effect of substitution, all computations are determined by a generalized gradient approximation and an ultra-soft pseudopotential. In the current research, Bi, Sn, and Tl are substituted at the Pb-site which is preferable to the Hf-site due to the stability of cubic perovskites. According to the structural properties, cubic to pseudo-cubic transition is obvious. Moreover, the decline in band gap is noticed, when specific concentration of impurities (Bi, Sn) atoms is substituted. However, substitution of Tl increases the gap between conduction/valence bands. It is not just the change in band gap that increases or decreases, the nature is also shifted from indirect to direct. Moreover, this behavior is explained by the different density of states. Since then, a significant alteration in band gap is mainly due to the *p*-states. As a result, our material is a favorable choice for optoelectronic devices. The changes in electronic characteristics also influence the optical properties including the complex dielectric functions, absorption, reflectivity, loss function, and refractive index. We also explored the elastic constants (C_{ij}), stability criteria, and mechanical attributes like Bulk modulus (B), Young's modulus (Y), shear modulus (G), Poisson's ratio (and anisotropic factor (A). Furthermore, we concluded that our material is elastically stable, ductile, and stiff.