ABSTRACT

The study of suitable compounds for photovoltaic applications is one of the most fascinating research areas in the world. One of the less studied materials is KGeCl3 and its potential is yet to be fully determined. Investigations of the structural, electronic, optical and mechanical properties of cubic, tetragonal and trigonal structures of pure inorganic KGeCl3 perovskite have been done. All calculations have been performed using first-principle calculations based on density functional theory (DFT) in generalized gradient approximation with Perdew-Burke-Ernzerhof, PBE-GGA as the exchange correlation functional, as implemented in the Quantum ESPRESSO code. Further calculations using GW approximation have been performed on electronic band structures of the three phases of KGeCl3 in order to validate the accuracy of GGA-PBE functional. The structural properties of the materials have been found to be consistent with previous observations in literature. All compounds have been found to display direct band gaps, with the top of the valence band (VB) dominated by Cl 2p orbitals and the conduction band (CB) dominated by the Ge 2p orbitals. The trigonal perovskite has been observed to have the largest band gap of 2.7 eV, with the cubic and tetragonal counterparts having 0.8 eV and 1.2 eV respectively. Calculated elastic constants, bulk and shear moduli have shown that the trigonal structure is mechanically unstable and brittle at ground state. Generally, the three phases of KGeCl3 have been observed to possess a broad absorption spectrum covering the UV–Vis region and therefore making them suitable candidates for photovoltaic applications.