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Structural, elastic, electronic and optical properties of Cu3TMSe4 (TM = V, Nb and Ta) sulvanite compounds via first-principles calculations

Abstract

The structural and optoelectronic properties of the cubic Cu3TMSe4 (TM = V, Nb and Ta) sulvanite compounds have been calculated using a full-potential augmented plane wave plus local orbitals (FP-APW+lo) method within the density functional theory. The exchange-correlation potential was treated with the generalized gradient approximation of Wu and Cohen (WC-GGA) to calculate the total energy. Moreover, the Engel-Vosko generalized gradient approximation (EV-GGA) and the modified Becke-Johnson potential (TB-mBJ) were also applied for the electronic and optical properties. The ground state properties, including, lattice constants, bulk modulus are in reasonable agreement with the available experimental and theoretical data. The elastic constants Cij are computed using the total energy variation versus strain technique. The polycrystalline elastic moduli, namely; shear modulus, Young's modulus, Poisson's ratio and anisotropic factor were derived from the obtained single-crystal elastic constants. As a result, brittleness behaviour of these compounds is interpreted via the calculated elastic constants Cij. The calculations of the electronic band structure show that these compounds have an indirect energy band gap (R-X) and the TB-mBJ approximation yields larger fundamental band gaps compared to those of WC-GGA and EV-GGA. The dielectric function, refractive index, extinction coefficient, reflectivity, and energy loss function were calculated for radiation up to 45 eV.

Keywords

Ab-initio calculations; Elastic constants; Electronic properties; Optical properties; Sulvanite compounds