Full potential study of the elastic, electronic, and optical properties of spinels $MgIn_2S_4$ and $CdIn_2S_4$ under pressure effect

Abstract

The structural, elastic, electronic, and optical properties of cubic spinel $MgIn_2S_4$ and $CdIn_2S_4$ compounds have been calculated using a full relativistic version of the full-potential linearized-augmented plane wave with the mixed basis FP/APW+lo method. The exchange and correlation potential is treated by the generalized-gradient approximation (GGA). Moreover, the EngelVosko GGA formalism is also applied to optimize the corresponding potential for band structure calculations. The ground state properties, including the lattice constants, the internal parameter, the bulk modulus, and the pressure derivative of the bulk modulus are in reasonable agreement with the available data. Using the total energy-strain technique, we have determined the full set of first-order elastic constants C_{ij} and their pressure dependence, which have not been calculated or measured yet. The shear modulus, Young's modulus, and Poisson's ratio are calculated for polycrystalline XIn_2S_4 aggregates. The Debye temperature is estimated from the average sound velocity. Electronic band structures show a direct band gap () for $MgIn_2S_4$ and an indirect band gap (K) for $CdIn_2S_4$. The calculated band gaps with EVGGA show a significant improvement over the GGA. The optical constants, including the dielectric function $\varepsilon(\omega)$, the refractive index $n(\omega)$, the reflectivity $R(\omega)$, and the energy loss function $L(\omega)$ were calculated for radiation up to 30 eV.