ELECTRONIC PROPERTIES OF ORTHORHOMBIC $LIGAS_2$ AND $LIGASE_2$

Abstract

We report theoretical calculations of the band structure and density of states for orthorhombic $LiGaS_2$ (LGS) and $LiGaSe_2$ (LGSe). These calculations are based on the full potential linear augmented plane wave (FP-LAPW) method within a framework of density functional theory. Our calculations show that these crystals have similar band structures. The valence band maximum (VBM) and the conduction band minimum (CBM) are located at Γ, resulting in a direct energy band gap. The VBM is dominated by S/Se-p and Li-p states, while the CBM is dominated by Ga-s, S/Se-p and small contributions of Li-p and Ga-p. From the partial density of states we find that Li-p hybridizes with Li-s below the Fermi energy (E_F), while Li-s/p hybridizes with Ga-p below and above E_F. Also, we note that S/Se-p hybridizes with Ga-s below and above E_F.