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The electronic structure, electronic charge density and optical properties of the diamond-like semiconductor Ag2ZnSiS4

Abstract

The electronic structure, electronic charge density and optical properties of the diamond-like semiconductor Ag_2ZnSiS_4 compound with the monoclinic structure have been investigated using a full-relativistic version of the full-potential augmented plane-wave method based on the density functional theory, within local density approximation (LDA), generalized gradient approximation (GGA), Engel–Vosko GGA (EVGGA) and modified Becke Johnson (mBJ) potential. Band structures divulge that this compound is a direct energy band gap semiconductor. The obtained energy band gap value using mBJ is larger than those obtained within LDA, GGA and EVGGA. There is a strong hybridization between Si-s and S-s/p, Si-p and Zn-s, Ag-s/p and Zn-s, and Ag-s and Ag-p states. The analysis of the site and momentum-projected densities shows that the bonding possesses covalent nature. The dielectric optical properties were also calculated and discussed in detail.

Keywords; Semiconductor, Ag_2ZnSiS_4, Semiconductor Ag_2ZnSiS_4,