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Optoelectronic and thermoelectric properties of KAuX5 (X = S, Se): A first principles study

Abstract

The electronic structure as well as optical and thermoelectric properties of the orthorhombic polychalcogenides of gold $KAuX_5$ (X = S, Se) compounds have been investigated using full-potential linearized augmented plane wave within the framework of the density functional theory (DFT). The local density approximation (LDA), generalized gradient approximation (GGA) by Perdew, Burke and Ernzerhof (PBE), Engel–Vosko generalized gradient approximation (EV-GGA), and the recently modified Becke–Johnson approximation (mBJ) formalism are used for the exchange correlation energy to calculate the total energy. The results show that $KAuX_5$ (X = S, Se) is a direct band gap semiconductor at Γ–Γ point. The total and partial density of states indicate that the states Au-*d*, S-*p*, and Se-*p* of both compounds have strong contributions to valence band in the energy range from −10 up to 0.0 eV. One can notice from electronic charge density that both compounds show greater iconicity and smaller covalency. Optical properties with photon incident energy up to 14.0 eV have been calculated and analyzed. Important transport properties such as Seebeck coefficients as well as thermal and electrical conductivities and effective mass are obtained and discussed in details.

Keywords; Electronic structure, Orthorhombic polychalcogenides, Gold