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Electronic, optical and thermoelectric properties of $SnGa_2GeX_6$ (X= S, Se) compounds

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Abstract

Electronic, optical and thermo-electric properties of two quaternary chalcogenides $SnGa_2GeX_6$ (X= S, Se) have been studied by using density functional theory. Modified Becke-Johnson exchange potential (mBJ-GGA) was used to calculate the band gaps of these compounds. Both compounds show pseudo direct band gap of 1.74 and 1.24 eV for $SnGa_2GeS_6$ and $SnGa_2GeSe_6$, respectively. The band gap decreases when replacing the X cations from S to Se. The optical properties such as dielectric function, energy loss function, extension coefficient, refractive index, and reflectivity of these compounds are discussed in details. The thermo-electric properties are studied using Boltzmann statistics through BoltzTrap code. High absorption peaks and figure of merits (ZT) for both compounds reveal that they are good candidates for the optoelectronics and thermo-electric devices.

Keywords: Semiconductors; Band structure; Optical response; Thermoelectric

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