

# Accepted Manuscript

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PII: S0925-8388(17)34208-1

DOI: [10.1016/j.jallcom.2017.12.033](https://doi.org/10.1016/j.jallcom.2017.12.033)

Reference: JALCOM 44119

To appear in: *Journal of Alloys and Compounds*

Received Date: 21 September 2017

Revised Date: 21 November 2017

Accepted Date: 4 December 2017

Please cite this article as: N. Yousaf, W. Khan, S.H. Khan, M. Yaseen, A. Laref, G. Murtaza, Electronic, optical and thermoelectric properties of  $\text{SnGa}_2\text{GeX}_6$  (X = S, Se) compounds, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2017.12.033.

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**Electronic, optical and thermoelectric properties of  $\text{SnGa}_2\text{GeX}_6$  (X= S, Se) compounds**Naveed Yousaf<sup>1</sup>, Wilayat Khan<sup>2</sup>, Shah Haider Khan<sup>1</sup>, M. Yaseen<sup>3</sup>, A. Laref<sup>4</sup>, G. Murtaza<sup>5,\*</sup><sup>1</sup>*Department of Physics, University of the Peshawar, KP, Pakistan*<sup>2</sup>*New Technologies – Research Center, University of West Bohemia, Univerzitni 8, 306 14  
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King Saudi Arabia*<sup>5</sup>*Materials Modeling Lab, Department of Physics, Islamia College University, Peshawar***Abstract**

Electronic, optical and thermo-electric properties of two quaternary chalcogenides  $\text{SnGa}_2\text{GeX}_6$  (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  $\text{SnGa}_2\text{GeS}_6$  and  $\text{SnGa}_2\text{GeSe}_6$ , 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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