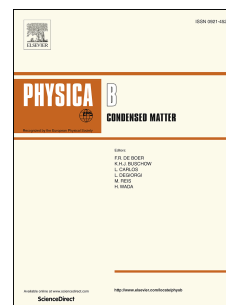


Accepted Manuscript

Structural, electronic and thermoelectric properties of bulk and monolayer of Sb_2Se_3 under high pressure: By GGA and mBJ approaches

H.A. Rahnamaye Aliabad, F. Asadi Rad



PII: S0921-4526(18)30430-7

DOI: [10.1016/j.physb.2018.06.030](https://doi.org/10.1016/j.physb.2018.06.030)

Reference: PHYSB 310938

To appear in: *Physica B: Physics of Condensed Matter*

Received Date: 10 February 2018

Revised Date: 24 June 2018

Accepted Date: 25 June 2018

Please cite this article as: H.A. Rahnamaye Aliabad, F. Asadi Rad, Structural, electronic and thermoelectric properties of bulk and monolayer of Sb_2Se_3 under high pressure: By GGA and mBJ approaches, *Physica B: Physics of Condensed Matter* (2018), doi: 10.1016/j.physb.2018.06.030.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Structural, electronic and thermoelectric properties of bulk and monolayer of Sb_2Se_3 under high pressure: by GGA and mBJ approaches

H. A. Rahnamaye Aliabad*, F. Asadi Rad

Department of Physics, Hakim Sabzevari University, Sabzevar, 96179-76487, Iran

*Corresponding author at: Department of Physics, Hakim Sabzevari University, Sabzevar, Iran, Postal code: 96179-76487; Tel.: +98-5144013155; Fax: +98-5144013170; E-mail address: Rahnama@hsu.ac.ir; Rahnamaye@gmail.com

Abstract

The effects of high pressure on the structural, electronic and thermoelectric properties of Sb_2Se_3 have been studied by using FP-LAPW method combined with Boltzmann transport theory. The variation of lattice constants, band structure, density of states, seebeck coefficient, electrical conductivity, electronic part of thermal conductivity and figure of merit (ZT) with pressure (up to 45.2 GPa) are calculated. Our results show that Sb_2Se_3 has a direct band gap of 1.43 eV in the bulk structure and it has an indirect band gap of 0.4 eV in the monolayer structure, at zero pressure. Increasing pressure led to a decrease in the band gap value and the nature of the band gap shifts from direct to the indirect. With the increase in pressure, the seebeck coefficient, electrical conductivity and electronic part of thermal conductivity increase and ZT decreases. The maximum ZT of 1.12 was achieved at 800 K, $n=10^{19}$ per cm^{-3} for n -type doping. Hence, Sb_2Se_3 is a good candidate for thermoelectric applications. The obtained results are in close agreement with the experimental results.

Keywords: Electronic; thermoelectric; pressure; bulk and monolayer; Sb_2Se_3

PACS: 71.15.Mb; 72.15.Jf

Download English Version:

<https://daneshyari.com/en/article/8160295>

Download Persian Version:

<https://daneshyari.com/article/8160295>

[Daneshyari.com](https://daneshyari.com)