



Investigation of thermoelectric properties of novel cubic phase SnSe: A promising material for thermoelectric applications



Faheem K. Butt ^{a, b, *, 1}, Bakhtiar Ul Haq ^{c, **, 1}, Sajid ur Rehman ^a, R. Ahmed ^{d, e}, Chuanbao Cao ^f, S. AlFaifi ^c

^a Department of Physics, The University of Lahore, 1-Km Raiwind Road, Lahore, 53700, Pakistan

^b Energy Conversion and Storage – ECS, Physik-Department, Technische Universität München, James-Frank-Straße 1, 85748, Garching, Germany

^c Advanced Functional Materials & Optoelectronics Laboratory (AFMOL), Department of Physics, Faculty of Science, King Khalid University, P.O. Box 9004, Abha, Saudi Arabia

^d Department of Physics, Faculty of Science, Universiti Teknologi Malaysia, UTM, Skudai, 81310, Johor, Malaysia

^e Centre for High Energy Physics, University of the Punjab, Lahore, Pakistan

^f Research Centre of Materials Science, Beijing Institute of Technology, Beijing, 100081, People's Republic of China

ARTICLE INFO

Article history:

Received 9 February 2017

Received in revised form

10 April 2017

Accepted 1 May 2017

Available online 3 May 2017

Keywords:

Semiconductors

Cubic SnSe

Thermoelectric properties

Electronic properties

Energy materials

ABSTRACT

The novel cubic structured SnSe (π -SnSe), with narrow band-gap and substantial phonon restraining effect, is considered a perspective energy storage material for futuristic applications. In this study, we explore the thermoelectric properties of π -SnSe in the framework of density functional theory and is therefore believed to be the first report of its kind. As a prerequisite for the calculations of thermoelectric properties, the electronic structure of π -SnSe was determined at the level of modified Becke-Johnson potential. The calculated bandgap of magnitude 0.97 eV is found to be in good agreement with recently reported experimental results of energy band-gap. Our calculations for electrical conductivity (σ/τ) show that the highest values occur at modest doping level magnitude to $3.6 \times 10^{19}/\Omega\text{ms}$ for p -type doping and $1.54 \times 10^{20}/\Omega\text{ms}$ for n -type doping and was found to be decreasing linearly with increasing temperature. Similarly, it is found that π -SnSe exhibit high Seebeck coefficient at low temperature, observing a drastic degradation in the span of 2292 $\mu\text{K}/\text{V}$ to 444.3 $\mu\text{K}/\text{V}$ with increasing temperature ranging from 200 to 900 K, respectively. In consequence, a notable reduction in the values of thermoelectric power factor (PF) and figure of merit (ZT) has also been observed with increase in temperature. The maximum value of PF was documented to be $8.77 \times 10^{10} \text{ W}/\text{mK}^2\text{s}$ at 200 K. An exceptionally high and record ZT value of ~ 1 was obtained at 200 K which is superior to orthorhombic structure SnSe (polycrystalline and bulk). Thus our study point to cubic phase SnSe as an avenue for the next generation thermoelectric materials for a wide range of operational temperature devices.

© 2017 Elsevier B.V. All rights reserved.

1. Introduction

The advancements and downsizing effects in technological gadgets have escalated the demand of energy manifolds [1–8]. The upsurge in the consumption of energy is giving rise to the concerns

* Corresponding author. Department of Physics, The University of Lahore, 1-Km Raiwind Road, Lahore, 53700, Pakistan.

** Corresponding author. Advanced Functional Materials & Optoelectronics Laboratory (AFMOL), Department of Physics, Faculty of Science, King Khalid University, P.O. Box 9004, Abha, Saudi Arabia

E-mail addresses: faheem.khurshid@gmail.com (F.K. Butt), bakhtiarjaddon@gmail.com (B. Ul Haq).

¹ These authors contributed equally.

which are coupled with environmental issues and sustainability. This demands alternative energy sources to reduce the use of fossil fuels and provide environmental harmony with the provision to realize the dream of green energy. In this regard lithium ion batteries (LIB), supercapacitors, hydrogen storage, fuel cells and thermoelectric materials etc are considered the most resourceful renewable energy systems [8,9]. However, all these systems need potential materials to make it viable. Thermoelectric materials provide an innovative pathway of converting the heat energy into electric power, thus enabling waste heat into useful energy. The exploitation of thermoelectric materials in practical applications can considerably improve the way energy is used and can spare a lot of energy resources.

The performance of a thermoelectric material is identified by the “figure of merit” ZT which is described as $ZT = S\sigma^2T/\kappa$. Here S represents the Seebeck coefficient, σ is known as electrical conductivity and the thermal conductivity is represented by κ . Many efforts have been devoted to increasing the figure of merit in the light of above formula. In order to expedite the process of thermoelectric, more economical and realistic materials with the higher value of ZT are proposed [10].

Tin-selenide has exhibited promising results for many energy storages and conversion applications including lithium ion battery, supercapacitors, solar cells, infrared optoelectronics and so on [11–24]. It is also pointed out as an alternative for the Lead-Cadmium based chalcogenides and ternary I-III-VI group semiconductors such as CuInS_2 , CuInSe_2 , and $\text{CuIn}_x\text{Ga}_{1-x}\text{Se}_2$ because of the economic and environmental concerns [24]. However, the recently discovered cubic phase of SnSe has garnered the particular attention [25–27]. Ran E. Abutbulab et al. reported nanocrystalline cubic phase π -SnSe [25]. The calculated lattice parameters were $a^0 = 11.9702 \text{ \AA}$ with an indirect bandgap of 1.28 eV. Sajid et al. reported under pressure investigation of cubic phase π -SnSe and its effect on the optical properties [28]. Recently, Zhao et al. have probed the anisotropic orthorhombic SnSe single crystal for thermoelectric performance along the b axis at 923 K and found a ZT value of ~ 2.6 and noted that the enhanced value was ascribed to the low lattice thermal conductivity which is stimulated by the strong anharmonic bonding [29]. Lately, Zhang et al. also performed the pressure induced thermoelectric studies of orthorhombic phase SnSe and concluded that the ZT values along b and c directions can reach to 2.5 and 1.7 at 6 GPa and 700 K [30]. But, the reported studies of thermoelectric properties are concerning orthorhombic SnSe phase, and mostly are at high temperatures. The stability of the orthorhombic SnSe phase is another issue because of changing from $Pnma$ to $Cmcm$ symmetry. Moreover, obtained results at a very high temperature and increased pressure might create a hindrance for the practical and widespread use of SnSe as a thermoelectric material.

In this manuscript, we investigate the electronic structure and thermoelectric properties of novel cubic π -SnSe from a low-temperature range of 200 K until 900 K. The ZT value at 200 K was found to be 0.998 which is exceptionally high value at relatively lower temperatures ever reported as compared to the orthorhombic phase of SnSe (polycrystalline and bulk). To the best of our knowledge, there exist no studies on the thermoelectric performance of cubic phase SnSe. This study provides an opportunity for the use of the novel phase of π -SnSe as prosperous thermoelectric material.

2. Computational method

The present electronic structure results needed for thermoelectric calculations are based on the full potential linearized-augmented-plus-local-orbital (FP-L(APW + lo)) method as implemented in WIEN2k code [31]. In this approach, the simulated unit cell is partitioned into two regions. To treat the exchange-correlation energy, the generalized-gradient-approximations (GGA)-type of exchange-correlation functional proposed by Perdew–Burke–Ernzerhof (PBE) [32] with additional Tran–Blaha modified Becke–Johnson (mBJ) potential has been used. The later flavor of exchange potential has been proved effective in overcoming the inherent problem of band-gap underestimation in DFT with common exchange-correlation functionals [33–37]. For the expansion of wave functions inside MT spheres, $l_{\text{max}} = 10$ has been chosen whereas in the interstitial region the energy cutoff $K_{\text{max}} = 8.0/R_{\text{MT}}(\text{Ryd})^{1/2}$ was taken into account for reproducing sound results. The R_{MT} values for Sn and Se were chosen as 2.50 a.u.

2.44 a.u. and 2.30 a.u., respectively. The Fourier-expanded charge density was truncated at $G_{\text{max}} = 16 \text{ au}^{-1}$. The Monkhorst–Pack special k-points approach [38] has been adopted for performing the integration over the Brillion Zone (BZ). For good convergence of energy, the integrals over the special BZ are performed up to 119 ($13 \times 13 \times 13$) k-points. The total energy was converged to 10^{-5} Ryd/unit cell in our present self-consistent computations for sound results.

For determining the thermoelectric properties of SnSe, the electronic-structure results obtained with the above mentioned computational details were used within a semiclassical Boltzmann theory under a constant scattering time approximation as implemented in the BoltzTraP code [39]. A brief summary of the methodology for obtaining the thermoelectric coefficients has been described in following, where a comprehensive explanation of the Boltzmann transport theory can be found elsewhere [40,41]. The thermoelectric coefficients such as electrical conductivity ($\sigma_{\alpha\beta}$) and Seebeck coefficient ($S_{\alpha\beta}$) are determined as a function of chemical potential (μ) and temperature using the following equations.

$$\sigma_{\alpha\beta}(T, \mu) = \frac{1}{\Omega} \int \sum_{\alpha\beta}(\epsilon) \left[-\frac{\partial f_0(T, \epsilon, \mu)}{\partial \epsilon} \right] d\epsilon, \quad (1)$$

$$S_{\alpha\beta}(T, \mu) = \frac{1}{eT\Omega\sigma_{\alpha\beta}(T, \mu)} \int (\epsilon - \mu) \sum_{\alpha\beta}(\epsilon) \left[-\frac{\partial f_0(T, \epsilon, \mu)}{\partial \epsilon} \right] d\epsilon, \quad (2)$$

where α and β are Cartesian indices of the tensor quantities. Symbols e , Ω and f_0 represent the electronic charge, volume of the unit cell and the Fermi–Dirac distribution function of the carriers respectively.

The energy projected transport distribution function represented by $\sum_{\alpha\beta}$ is central term in equations (1) and (2) and can be defined as

$$\sum_{\alpha\beta}(\epsilon) = \frac{e^2}{N} \sum_{i,k} \tau v_{\alpha}(i, k) v_{\beta}(i, k) \delta(\epsilon - \epsilon_{i,k}), \quad (3)$$

where $v_{\alpha}(i, k) = \frac{1}{\hbar} \frac{\partial \epsilon_{i,k}}{\partial k_{\alpha}}$ represents the group velocity, and i, k, N , and τ mentioned in Eq. (3) are used for the band index, wave vector, the total number of k-points used for the BZ sampling and relaxation time, respectively. Since the wave-vector-dependent relaxation time is an undetermined quantity in the present DFT-based first-principles calculations, the τ -dependent quantities such as electrical conductivity and power factor ($S^2\sigma$) are reported with respect to τ i.e. σ/τ and $S^2\sigma/\tau$.

3. Results and discussion

The π -SnSe belongs to a class of non-centrosymmetric crystals. It has 64 atoms per unit cell containing 32 Sn atoms and 32 Se atoms in a unit cell as shown in Fig. 1 and is distinctive from the SnSe-RS which have 8 atoms per unit cell [25]. In cubic SnSe structure (space group No. 198) tin and selenide ions having 3-fold symmetry in which each ion is surrounded by three ions of the opposite valence and Sn and Se ions are located in “4a” and “12b” Wyckoff sites respectively [26].

Fig. 2 demonstrates the energy band structure of cubic-SnSe in form of graphical representation. The electronic band structure of π -SnSe has been calculated in the first Brillouin zone (BZ) along with high symmetry directions. High-symmetry points G(0,0,0), R(1/2,1/2,1/2), X(0,1/2,0) and M (1/2, 1/2,0) were used to calculate

Download English Version:

<https://daneshyari.com/en/article/5459211>

Download Persian Version:

<https://daneshyari.com/article/5459211>

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