Theoretical investigations of thermoelectric phenomena in binary semiconducting skutterudites

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In this study, we explored the thermoelectric properties of the host thermoelectric materials (TM), namely, binary skutterudites, using a combination of simulations based on density functional theory and post-DFT Boltzmann's semiclassical theory. The calculations were performed close to the Fermi surface for the Seebeck coefficient and other thermoelectric parameters. Our results demonstrated that CoSb 3 exhibited the highest Seebeck value at room temperature among all the compounds (CoP 3, CoAs 3, CoSb 3, IrP 3, IrAs 3, IrSb 3, RhAs 3, and RhSb 3), which confirmed that this compound is an ideal host material for thermoelectric applications. Furthermore, the calculated electrical conductivity values show that RhAs 3 has the largest value of $3.736 \times 10^5 \ \Omega^{-1} \ m^{-1}$. However, at high temperatures, the Seebeck values for all of these compounds are almost constant due to the activation of the minority charge carriers.

**Introduction**

The demand for energy has caused a remarkable unrest across the globe and climate change due to the combustion of fossil fuels is increasing and creating a drastic impact on the social and economic life of human civilization. In this context, the conversion of waste heat from various sources to useful electrical energy can play a key role in the energy crisis as well as growing environmental problem. The heating process of buildings, heat from the automobile exhausts as well as industries, all generate a huge amount of waste heat that could be converted to electricity using thermoelectric (TE) generators. Thermoelectric generators are solid devices having no moving parts, make no noise, reliable and scalable, which make them ideal for small amounts of electric power generation. It is estimated that two-third of used energy is lost as waste heat, so there is a need for good TE materials that can be used to convert heat to electrical energy and vice versa.

Certain materials are identified for their high efficiency of energy conversion from heat to electricity with a high TE figure of merit above unity. These materials have good electrical conductivity, and ultimately maintain a low thermal conductivity. Their interesting results have attracted considerable attention and research is still in progress to further improve their TE properties. High-temperature bulk materials, such as skutterudites, clathrates, half-heusler alloys and complex chalcogenides, have been extensively studied for their TE applications. These materials usually have complex crystal structures and physical properties that are required for a good TE material. For example, the skutterudite-structured compounds and clathrates have cage-like structures that have empty spaces where filler atoms are inserted, which significantly lower the thermal conductivity of these compounds due to the filling atoms' ability to scatter phonons. These materials possess some unusual phenomena, such as heavy fermion superconductivity, an exciton-mediated superconducting state and Weyl fermions.

Skutterudites have attracted significant attention as high temperature TE materials due to their high figure of merit ($zT$) in the temperature range from $300 \ ^\circ C$ to $550 \ ^\circ C$. The experimental observations show that skutterudite semiconductors possess attractive transport properties and have good potential for achieving $zT$ values. For p-type skutterudites, low hole effective mass, high carrier mobility, low electrical resistivity and moderate Seebeck coefficient were obtained; however, the larger electron effective mass and Seebeck coefficients make the n-type skutterudites more attractive candidates for TE applications. The Seebeck coefficient values of all skutterudites are high and therefore can be used as thermoelectric materials. However, CoSb 3 has attracted enormous attention for its conversion applications of waste heat to electricity due to its reasonable band gap, high carrier mobility and the fact that it is...
composed of inexpensive and environmentally friendly elements as compared to other skutterudite materials. The thermal conductivity of pure CoSb$_3$ is, however, very high, which leads to a low $zT$ and poor conversion efficiency for TE applications.$^{10}$

The thermoelectric properties of the binary skutterudite have been studied extensively via experiments. However, some theoretical studies are available on the filled ones, but no detailed theoretical studies are available on the comparison of the binary skutterudites. The motivation of the present study is an attempt to understand the theory of TE properties of the binary skutterudite compounds.

### Theory and calculations

The Boltzmann theory discusses a variation in the charge carriers’ distribution function due to external fields, lattice phonon scattering, or various kinds of defect scattering. For the situation of an electric and magnetic fields and a thermal gradient, the electric current $j$ can be written in terms of the tensor form as

$$j_i = \sigma_{ij} E_j + \sigma_{ijk} E_i B_k + v_i \nabla_j T \tag{1}$$

However, the complexity of various carrier scattering mechanisms causes difficulty in obtaining an exact solution of the Boltzmann transport equation.$^{11,12}$ Mathematically, the relaxation time is given by

$$\frac{\partial f}{\partial t} + \nabla \cdot \left( \frac{\partial f}{\partial \epsilon} \right) = \frac{f - f_0}{\tau} \tag{2}$$

where $f_0$ and $f$ are the equilibrium and perturbed carrier distribution functions, respectively, and $\tau$ is the relaxation time. eqn (2) describes the process of restoring $f_0$ from $f$ via various scattering processes. The net effect is to restore $f$ to $f_0$ exponentially with a relaxation time $\tau$. Basically, $\tau$ is very complicated; however, in this study, $\tau$ has been approximated.$^{13-20}$

Using this approximation, the thermoelectric parameters in the tensor form for a material can be written as

$$\sigma_{\alpha\beta}(T, \mu) = \frac{1}{\Omega} \int \sigma_{\alpha\beta}(\epsilon) \left[ - \frac{\sigma_{0}(T, \alpha, \mu)}{\delta \epsilon} \right] d\epsilon \tag{3}$$

$$S_{\alpha\beta}(T, \mu) = \frac{1}{eT \Omega \sigma_{\alpha\beta}(T, \mu)} \int \sigma_{\alpha\beta}(\epsilon)(\epsilon - \mu) \left[ - \frac{\sigma_{0}(T, \alpha, \mu)}{\delta \epsilon} \right] d\epsilon \tag{4}$$

where $\alpha$ and $\beta$ are the tensor indices, and $\Omega$, $\mu$ and $f_0$ are the volume of the unit cell, Fermi level of carriers, and the carrier Fermi–Dirac distribution function, respectively, and $e$ is the electronic charge. The transport distribution function tensor given in $\sigma$ and $S$ is defined as:

$$\sigma_{\alpha\beta}(\epsilon) = \frac{e}{N} \sum_{i,k} \tau_{\alpha\beta}(i,k) v_{\alpha}(i,k) \frac{\delta(\epsilon - \epsilon_{i,k})}{\delta \epsilon} \tag{5}$$

where $k$ and $i$ are the wave vector and band index, respectively, and $N$ represents the number of $k$ points. In the three-dimensional tensor, $v_{\alpha}(i,k)$ ($\alpha = x, y, z$) is the $\alpha$-th component of the group velocity $v(i,k)$ of carriers, where it can be derived directly from the band structure by

$$v(i,k) = \frac{1}{h} \mathbf{\mathbf{\nabla}}_{k} \epsilon_{i,k} \tag{6}$$

The so-called band-crossing$^{27}$ may introduce problems in calculating $v(i,k)$ from band structures. In these calculations, the band structures of these binary skutterudites were calculated in comparison to the optical band gaps obtained by experimental measurements, as given in Fig. 1. The electronic band structure calculations were performed using the improved Tran–Blaha modified Becke–Johnson potential [improved TB-mBJ].$^{21}$ This newly developed technique yields very accurate electronic band structures and band gaps for various types of semiconductors and insulators in comparison to the well-known Green’s function method (GW) and Tran–Blaha modified Becke–Johnson (TB-mBJ) technique. Furthermore, the details about the electronic structure of the binary skutterudites and improved TB-mBJ can be found in our previous study.$^{22}$ To calculate the thermoelectric parameters, a dense $k$ mesh of 56 000 $k$ points was used in this study as per the method proposed by Madsen and Singh.$^{23}$ By using eqn (2)–(5), the Seebeck coefficient and electrical conductivity of a compound can be estimated based on its band structure. The carrier relaxation time $\tau$ is taken to be a constant with the value approximated to 10–13 s.$^{24}$ The electrical conductivity and power factor were calculated with respect to $\tau$; the Seebeck coefficient is independent of $\tau$. This approach has been employed successfully in evaluating the electrical transport properties of thermoelectric compounds.$^{14-18,24}$ Following similar procedures, we have interfaced this methodology with the Wien2k code.$^{25}$

### Results and discussions

#### Seebeck coefficient

Thermoelectric phenomenon in materials can be quantified by different parameters, one of which is the Seebeck coefficient, which has a unique importance because of its voltage capability for a given temperature gradient. A high Seebeck coefficient value usually leads to a good thermoelectric material. The Seebeck coefficient is a tool that provides a sensitive test of the

Fig. 1 Calculated band structures of (a) RhAs$_3$, (b) RhSb$_3$ and. (c) IrSb$_3$ by the improved TB-mBJ.
The electrical conductivity is the passage of the charge carriers through a material. In a semiconductor, both the electrons and holes are responsible for the electrical conductivity. In these compounds, the electrical conductivity almost linearly increased with temperature, which was due to the increase in the number of carriers and potential, as shown in Fig. 3. The electrical conductivity of these compounds was of the order $10^4 \ \Omega^{-1} \ m^{-1}$.

The calculated and experimental values of the electrical conductivity at room temperature are listed in Table 1 and our comparative study shows that the calculated values of the electrical conductivity agreed with the experimental values. The maximum value of the electrical conductivity in the binary skutterudites was obtained for RhAs$_3$ for all calculated temperatures in the range from 50 to 800 K. The calculated electrical conductivity of CoP$_3$ at 50 K was $0.6645 \times 10^4 \ \Omega^{-1} \ m^{-1}$, and then linearly increased to $2.06379 \times 10^4 \ \Omega^{-1} \ m^{-1}$ at room temperature. Subsequently, the electrical conductivity increased gradually and reached a peak value of $9.9643 \times 10^4 \ \Omega^{-1} \ m^{-1}$ at 800 K. For CoSb$_3$, at 50 K, the electrical conductivity was $0.001592 \times 10^4 \ \Omega^{-1} \ m^{-1}$ and reached $0.32 \times 10^4 \ \Omega^{-1} \ m^{-1}$ at 300 K. This increase in the electrical conductivity was continuous up to $4.643 \times 10^4 \ \Omega^{-1} \ m^{-1}$ at 800 K. The calculated conductivity for CoSb$_3$ at 50 K was $0.2385 \times 10^4 \ \Omega^{-1} \ m^{-1}$ and increased linearly with temperature to a value of $2.05247 \times 10^4 \ \Omega^{-1} \ m^{-1}$ at 300 K. This increase continued until the electrical conductivity reached $9.53315 \times 10^4 \ \Omega^{-1} \ m^{-1}$ at 800 K. The obtained results for IrP$_3$ at 50 K for the electrical conductivity was $1.58836 \times 10^4 \ \Omega^{-1} \ m^{-1}$, and the increase in temperature of IrP$_3$ led to an electrical conductivity value of $3.8848 \times 10^4 \ \Omega^{-1} \ m^{-1}$ at 300 K and $11.83157 \times 10^4 \ \Omega^{-1} \ m^{-1}$ at 800 K. The electrical conductivity of IrAs$_3$ at 50 K was $1.4595 \times 10^4 \ \Omega^{-1} \ m^{-1}$, and then increased to $3.23611 \times 10^4 \ \Omega^{-1} \ m^{-1}$. The increase in temperature caused a further increase in the electrical conductivity to a value of $8.88461 \times 10^4 \ \Omega^{-1} \ m^{-1}$ at 800 K. The calculated value of the electrical conductivity for IrSb$_3$ at 50 K was $2.363589 \times 10^5 \ \Omega^{-1} \ m^{-1}$ and became $2.291882 \times 10^5 \ \Omega^{-1} \ m^{-1}$ at 300 K, which was close to the experimental value at this temperature with the value of $2.33 \times 5 \ \Omega^{-1} \ m^{-1}$. A further increase in the temperature increased the electrical conductivity and reached $2.8827 \times 10^5 \ \Omega^{-1} \ m^{-1}$ at 800 K. A calculation for the electrical conductivity of RhAs$_3$ gave the value of $3.5667 \times 10^5 \ \Omega^{-1} \ m^{-1}$ at 50 K, which changed by increasing the temperature and became $3.7361 \times 10^5 \ \Omega^{-1} \ m^{-1}$ at a temperature of 300 K. Finally, the curve reached $4.2289 \times 10^5 \ \Omega^{-1} \ m^{-1}$ at 800 K. The electrical conductivity values for RhSb$_3$ showed the
The calculated values of the thermoelectric parameters in comparison with experimental values at room temperature are tabulated in Table 1. The electronic thermal conductivity for the RhSb₃ material had an electronic thermal conductivity value of 2.9087 W K⁻¹, respectively. The calculations performed for IrAs₃ determined that the electronic thermal conductivity at 50 K was 0.02376 W K⁻¹ and increased with the increase in temperature, by which the resultant values at 300 and 800 K were 0.5256 and 4.8096 W K⁻¹, respectively. The electronic thermal conductivity findings for IrSb₃ showed a similar behavior as discussed for the previous skutterudite materials, and showed a continuous increase with temperature. The calculated values at the temperatures 0, 300 and 800 K were 0.29456, 2.01718 and 10.00149 W K⁻¹, respectively. The RhAs₃ material had an electronic thermal conductivity value of 0.44776 W K⁻¹ at 50 K, and then became 2.90874 W K⁻¹ at 300 K and finally 11.8569 W K⁻¹ at 800 K. Our calculations for RhSb₃ at 50 K estimated the electronic thermal conductivity value at 0.03378 W K⁻¹. Increasing the temperature to 300 K, the electronic thermal conductivity value showed an increase to the value 0.68953 W K⁻¹. At 800 K, the thermal conductivity became 5.87658 W K⁻¹.

## Electronic thermal conductivity

Thermal conductivity is the flow of heat in materials and it arises from both the electronic and lattice parts of the compound, as shown by \( k = ke + kl \). However, the BoltzTraP code can only estimate the electronic part of the thermal conductivity \( ke \). The electronic thermal conductivity for the semiconductor binary skutterudites is tabulated in Table 1 as well as depicted in Fig. 4. The electronic thermal conductivity variation with temperature was prominent and changed abruptly with temperature. It was found for CoP₃ that the electronic thermal conductivity \( K \) at 50 K was 0.23945 W K⁻¹ m⁻¹, which then increased with temperature and became 1.86913 W K⁻¹ m⁻¹ at 300 K. The value was increased to 10.81445 W K⁻¹ m⁻¹ at 800 K. The CoAs₃ calculated electronic thermal conductivity at a temperature of 50 K was 0.1218 W K⁻¹ m⁻¹ and was 0.1624 W K⁻¹ m⁻¹ at room temperature (300 K). With a further increase in the temperature to 800 K, the electronic thermal conductivity then became 5.4099 W K⁻¹ m⁻¹. The CoSb₃ electronic thermal conductivity obtained in our calculations at 50 K was 0.00646 W K⁻¹ m⁻¹. At a temperature of 300 K, the thermal conductivity of CoSb₃ became 0.44515 W K⁻¹ m⁻¹, and then the electronic thermal conductivity further increased to a value of 9.71322 W K⁻¹ m⁻¹. The calculated values of the electronic thermal conductivity also showed an increase with temperature for IrP₃. At the temperatures 50, 300 and 800 K, the thermal conductivity values were 0.02381, 0.68928 and 6.56185 W K⁻¹ m⁻¹, respectively. The calculations performed for IrAs₃ determined that the electronic thermal conductivity at 50 K was 0.02376 W K⁻¹ m⁻¹ and increased with the increase in temperature, by which the resultant values at 300 and 800 K were 0.5256 and 4.8096 W K⁻¹ m⁻¹, respectively. The thermal conductivity findings for IrSb₃ showed a similar behavior as discussed for the previous skutterudite materials, and showed a continuous increase with temperature. The calculated values at the temperatures 0, 300 and 800 K were 0.29456, 2.01718 and 10.00149 W K⁻¹ m⁻¹, respectively. The RhAs₃ material had an electronic thermal conductivity value of 0.44776 W K⁻¹ m⁻¹ at 50 K, and then became 2.90874 W K⁻¹ m⁻¹ at 300 K and finally 11.8569 W K⁻¹ m⁻¹ at 800 K. Our calculations for RhSb₃ at 50 K estimated the electronic thermal conductivity value at 0.03378 W K⁻¹. Increasing the temperature to 300 K, the electronic thermal conductivity value showed an increase to the value 0.68953 W K⁻¹. At 800 K, the thermal conductivity became 5.87658 W K⁻¹ m⁻¹.

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**Table 1** Calculated values of the thermoelectric parameters in comparison with experimental values at room temperature

| Comp. | S (μV K⁻¹) | \( \sigma \) (1 Ω⁻¹ m⁻¹) | \( \kappa \) (W m⁻¹ K⁻¹) | PF (W Ω⁻¹ m⁻² K⁻¹) |
|-------|------------|-----------------|-----------------|-----------------|
|       | Cal.       | Exp.            | Cal.            | Exp.            | Cal.        | Cal.        |
| CoP₃  | 40         | 50, 40³         | 2.06 × 10⁴      | 2.1 × 10⁴³       | 1.8691      | 0.4042 × 10⁻⁴|
| CoAs₃ | 145        | 145, 140²       | 0.32 × 10⁴      | 0.41 × 10⁴³, 1.19 × 10⁴³ | 0.1625 | 0.6835 × 10⁻⁴|
| CoSb₃ | 215        | 120, 220²       | 2.05 × 10⁴      | 2.5 × 10⁵², 5.28 × 10⁵³ | 0.4451 | 9.5366 × 10⁻⁴|
| IrP₃  | 199        | 200            | 3.88 × 10⁴      | 3.62 × 10⁶      | 0.6892 | 15.3747 × 10⁻⁴|
| IrAs₃ | 148        | 140³           | 3.62 × 10⁴      | 3.62 × 10⁶      | 0.5256 | 7.3490 × 10⁻⁴|
| IrSb₃ | 73         | 72³, 72³       | 2.29 × 10⁴      | 2.3 × 10⁶, 2.331 × 10⁶² | 1.9087 | 12.2335 × 10⁻⁴|
| RhAs₃ | 71         | 70³           | 3.736 × 10⁵      | 3.81 × 10⁶      | 2.9087 | 18.9600 × 10⁻⁴|
| RhSb₃ | 80         | 60³, 80³       | 2.93 × 10⁵      | 2.94 × 10⁶⁵     | 2.3363 | 19.1806 × 10⁻⁴|

³ Ref. 26. ² Ref. 27. ² Ref. 28. ² Ref. 29. ² Ref. 30. ² Ref. 31. ² Ref. 32. ² Ref. 33. ² Ref. 34. ² Ref. 35. ² Ref. 36. ² Ref. 37.

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**Fig. 3** Electrical conductivity versus the temperature of the binary skutterudites.

**Fig. 4** Variation of electronic thermal conductivity of skutterudites with temperature.
Power factor

The power factor is one of the parameters used to measure the thermoelectric efficiency of a compound. Mathematically, it is given as \( \text{PF} = S^2 \sigma \), where \( S \) is the Seebeck coefficient and \( \sigma \) is the electrical conductivity of the material. The power factor, instead of \( S \) or \( \sigma \), is a comprehensive parameter for the electrical performance of a compound. The calculated values of the power factor for the binary skutterudite compounds are tabulated in Table 1. The maximum power factor in a skutterudite semiconductor system is for RhAs\(_3\), with the peak value of 83.233 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) at 800 K, as shown in Fig. 5. For the compound CoP\(_3\), the power factor at 50 K temperature is very low with a value of 5.1228 \( \times \) 10\(^{-10} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \). With the increase in temperature to 300 K, the power factor becomes 0.4042 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) and finally at 800 K, the power factor of CoP\(_3\) then became 10.5941 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \).

The calculations for CoAs\(_3\) at 50 K gave us a power factor value of 2.66 \( \times \) 10\(^{-11} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \). Then, with an increase in the temperature to 300 K, the power factor increased to a value of 0.68351 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \). Finally, at 800 K, the power factor became 16.6251 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \). The estimated value of the power factor for CoSb\(_3\) at 50 K was 0.3863 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) and increased with temperature to the values 9.5366 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) and 72.9146 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) at 300 and 800 K, respectively. The results of the power factor for IrP\(_3\) at the temperatures 50, 300 and 800 K are 1.2846 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \), 15.3747 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) and 59.5952 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \), respectively. The IrAs\(_3\) values of the power factor showed an increase with temperature, and the values obtained at the temperatures 50, 300 and 800 K are 0.3672 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \), 7.3490 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) and 35.7767 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \), respectively.

Our calculations for IrSb\(_3\) gave a value of 0.0011 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \), 12.2335 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) and 58.8840 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) for the power factor at 50, 300 and 800 K, respectively. The calculations performed for RhAs\(_3\) showed an increase with temperature, and the results obtained at 50, 300 and 800 K are 0.0250 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \), 18.9600 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) and 83.233 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \), respectively. The power factor for RhSb\(_3\) at the temperatures 50, 300 and 800 K was 0.18076 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \), 19.1806 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) and 77.7349 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \), respectively.

![Fig. 5 Power factor at different temperatures for the binary skutterudites.](image)

Conclusions

In conclusion, we theoretically explored the behaviour of the Seebeck coefficient, electrical conductivity, thermal conductivity and power factor of the binary semiconductor skutterudites (CoP\(_3\), CoAs\(_3\), CoSb\(_3\), IrP\(_3\), IrAs\(_3\), IrSb\(_3\), RhAs\(_3\), and RhSb\(_3\)) with respect to the temperature using DFT and post-DFT Boltzmann’s transport theory. The Seebeck value for CoSb\(_3\) as investigated here was the highest (215 \( \mu \text{V} \text{K}^{-1} \)) at room temperature among all the compounds under study and this result was in close agreement with the experimental findings; however, the electrical conductivity results for RhAs\(_3\) showed the highest electrical conductance of 3.736149 \( \times \) 10\(^5 \) \( \Omega^{-1} \) m\(^{-1} \) among all the compounds. However, the maximum Power factor was obtained for RhSb\(_3\) with a value of 19.1806 \( \times \) 10\(^{-4} \) W \( \Omega^{-1} \) m\(^{-2} \) K\(^{-1} \) at room temperature. We calculated the room-temperature properties as well as the thermoelectric properties in the temperature range from 50 to 800 K for these compounds and compared their results.

Conflicts of interest

There are no conflicts to declare.

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