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Exploring Non-Centrosymmetric TlSb3Te2O12 Layered Compound for Renewable Energy Applications: A Density Functional Theory Study

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Abstract

In the pursuit of environmentally friendly and energy-efficient materials, thermoelectric compounds have become a focal point of research. The structural, electronic, and thermoelectric properties of the non-centrosymmetric layered selenite $TlSb_3Te_2O_{12}$ are explored through theoretical analysis. Utilizing Density Functional Theory with the Local Density Approximation in the WIEN2k software, geometry optimization was conducted, yielding lattice parameters that closely align with experimental values. The electronic structure analysis revealed a wide indirect bandgap of 2.71 eV, indicating the semiconducting nature of $TlSb_3Te_2O_{12}$. The BoltzTraP code, based on Boltzmann transport theory, was utilized to evaluate the thermoelectric properties. The results show that the Seebeck coefficient is positive (p-type) and ZT reaches a peak value of 1.56 at 300 K, and approaches unity in the temperature range of 200 K to 600 K. This high ZT value suggests excellent thermoelectric performance, making $TlSb_3Te_2O_{12}$ a promising material for energy conversion applications, particularly in waste heat recovery. The findings highlight its potential for developing cost-effective and sustainable thermoelectric devices, contributing to advancements in energy-efficient technologies.

Categories: Advanced Materials, Materials Engineering, Energy Efficiency and Conservation
Keywords: optical band gap, zt, dft, wide bandgap, lda, non-centrosymmetric

Introduction

Non-centrosymmetric oxides have garnered significant interest due to their distinctive symmetry-dependent properties, such as piezoelectricity, ferroelectricity, superconductivity, topological phase transitions, multiferroic behavior, and second harmonic generation (SHG). Compounds like $Cs_2Mo_3TeO_{12}$ and $CsV_3Te_2O_{12}$ exhibit non-centrosymmetric hexagonal tungsten oxide (HTO)-type layered structures, showing a pronounced SHG response [1-9]. Although extensive research has been conducted on non-centrosymmetric oxides for various applications, their potential in sustainable and renewable energy solutions remains underexplored. This work aims to investigate a non-centrosymmetric layered selenite using first-principles methods, focusing on its potential for energy-related applications. Thermoelectric energy conversion, which directly transforms heat into electricity, relies on the interaction between temperature gradients and the electrical properties of specific materials. This mechanism is a promising avenue for waste heat recovery and sustainable energy use, characterized by the dimensionless figure of merit (ZT). The ZT value is influenced by the Seebeck coefficient, electrical conductivity, and thermal conductivity. The origins of thermoelectric research trace back to the 1780s when Aloisio Galvani's experiments on galvanism suggested "animal electricity," sparking interest in the interactions between thermal and electrical energies [10,11].

In 1821, Thomas Johann Seebeck discovered the Seebeck effect, where an electric current is generated in a closed loop of two different conductors subjected to a temperature gradient. This discovery laid the foundation for thermoelectric power generation, and is now widely used in thermoelectric generators. Following this, the discovery by Jean Charles Athanase Peltier in 1834, the Peltier effect revealed that an electric current flowing through the junction of two different metals could either absorb or emit heat. This phenomenon forms the foundational principle behind thermoelectric coolers used for precise temperature control. William Thomson (Lord Kelvin) later unified these thermoelectric effects with the Thomson effect in 1851, providing a theoretical framework for the heating or cooling of conductors under a temperature gradient when electric currents flow through them. Although practical applications were limited in the early 20th century due to the low performance of metal-based materials, significant advancements occurred in the mid-20th century with the exploration of semiconductors like bismuth telluride (Bi_2Te_3), which offered higher Seebeck coefficients and lower thermal conductivities, thus enhancing efficiency.

In the 1950s and 1960s, the advancement of thermoelectric modules using Bi_2Te_3 facilitated practical applications, including portable power sources for space missions. Notable examples include the use of radioisotope thermoelectric generators in NASA's Voyager spacecraft, which converted heat from

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radioactive decay into electricity, allowing operations in deep space environments, where solar power is not viable [12,13]. Recent research has focused on improving the ZT value, crucial for efficient thermoelectric materials. Strategies such as nanostructuring and quantum confinement have been employed to reduce lattice thermal conductivity and enhance electronic properties. Techniques like incorporating nanoinclusions or designing low-dimensional materials (thin films, quantum dots) have proven effective in scattering phonons, thereby decreasing heat flow and boosting efficiency [14].

Novel thermoelectric materials, including quaternary compounds, half-Heusler alloys, skutterudites, and layered oxides, are being explored for their ability to convert waste heat from industrial processes, automotive exhausts, and electronics into electricity. Current advancements are aimed at optimizing material properties to achieve higher performance, reduce the costs of rare elements, and enhance scalability for practical applications. With ongoing progress in nanotechnology and material engineering, thermoelectrics show great promise for sustainable energy solutions and improved waste heat utilization [15-19]. Among the emerging materials, perovskite compounds stand out for their low thermal conductivity and high Seebeck coefficient, making them attractive candidates for thermoelectric applications. They offer potential solutions for harnessing waste heat from industrial processes, contributing to the sustainable use of energy resources. In this study, we present a comprehensive analysis of the band structure and thermoelectric properties of $TlSb_3Te_2O_{12}$ using Density Functional Theory (DFT). Notably, these properties have not been previously investigated for this specific compound.

Materials And Methods

The full-potential linearized augmented plane wave (FP-LAPW) method, implemented in WIEN2k [13], was used for first-principles calculations based on DFT. The exchange-correlation interactions were described using the Local Density Approximation (LDA) method [20]. Experimental data provided the initial lattice parameters [12]. The Muffin-tin radii (RMT) were set to 2.5, 1.93, 1.81, and 1.56 for Tl, Sb, Te, and O, respectively. The product of the smallest RMT and the maximum k-point value (KMAX) was set as RMT × KMAX = 9. We fixed the angular momentum cutoff (LMAX) to 10 and the Fourier expansion cutoff (GMAX) to 12. An energy threshold of -9 Ry was used to distinguish core and valence electrons. The Self-Consistent Field calculations were performed with an energy convergence criterion of (10^{-4}) Ry, using a Monkhorst-Pack grid of (6 × 6 × 4) k-points for Brillouin zone sampling. For transport properties, the BoltzTraP code [21], interfaced with WIEN2k, was employed for calculations. This code was chosen for its ability to efficiently handle large datasets and its accurate predictions of thermoelectric properties based on the Boltzmann transport equation. Based on the literature, we assume a constant relaxation time (τ) as 10^{-14} s across the temperature range. The temperature range for the analysis was chosen from 50 K to 800 K, which is typical for thermoelectric applications such as waste heat recovery. This range ensures that the material's performance is evaluated under both low and high-temperature conditions, making it suitable for various practical applications. While this simplification makes the calculations tractable, it may not capture temperature-dependent changes in scattering mechanisms, which could slightly affect the accuracy of the results, especially at higher temperatures. Future studies could refine this assumption by incorporating temperature-dependent scattering rates for more precise predictions.

Results

As stated in the Introduction section, the compound $TlSb_3Te_2O_{12}$ exhibits a hexagonal structure and falls within the P63mc (186) space group [19]. We employed DFT with the LDA method. Based on the optical band gap, we fixed LDA to calculate all the properties because LDA optical band gap is closely related to the experimental optical band gap. Although the LDA functional is known to slightly underestimate bandgaps, it provides an accurate description of the electronic properties for $TlSb_3Te_2O_{12}$, aligning with experimental observations. This choice was made to ensure consistency with experimental data, particularly for electronic properties. We probed the structural characteristics of this non-centrosymmetric layered selenite, $TlSb_3Te_2O_{12}$. To find the optimal lattice constant, we repeatedly modified the lattice parameters following the Murnaghan equation of state, as illustrated in Figure *1*. This method minimizes the total energy of the material by iterating over various lattice parameters to achieve the most stable configuration. The resulting optimized lattice constants were in good agreement with experimental data, confirming the validity of our approach. The resultant lattice constants and total energy, obtained via the LDA approach are outlined in Table *1*. Encouragingly, the computed values closely matched experimental observations.

$TlSb_3Te_2O_{12}$ (LDA)	a (Å)	c (Å)	E (Ry)
Experimental [19]	7.2312	11.9844	-
Theoretical	7.2801	11.8241	-216767.891

TABLE 1: The estimated experimental and theoretical lattice constants and total energy of TlSb3Te2O12 compound

LDA, Local Density Approximation

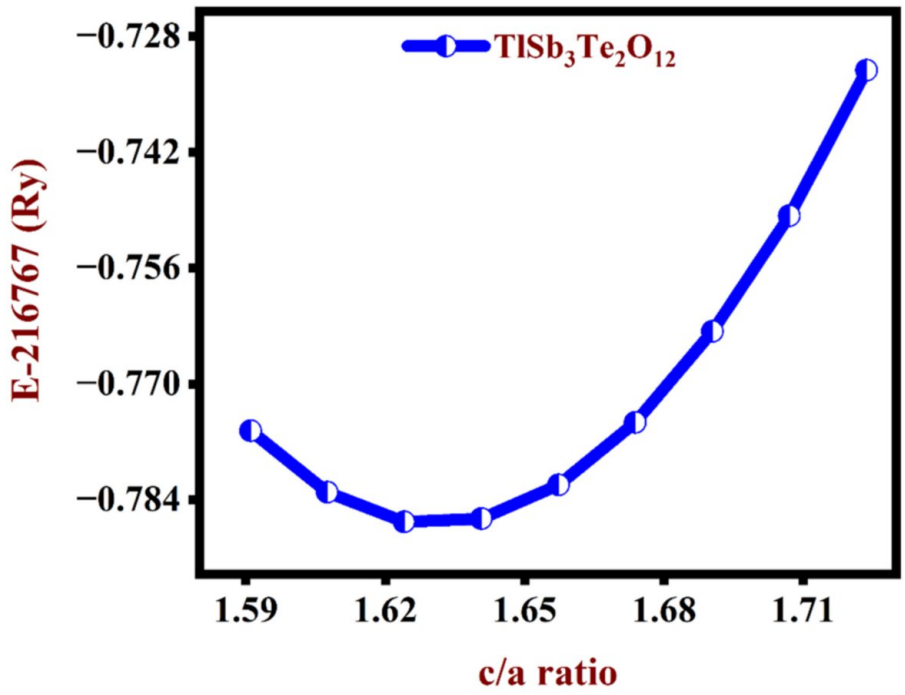

FIGURE 1: The elucidated total energy versus c/a

Using WIEN2k software, a well-established tool for DFT calculations, we generated the electronic band structure of $TlSb_3Te_2O_{12}$. As shown in Figure *2*, $TlSb_3Te_2O_{12}$ exhibits a significant indirect bandgap of 2.71 eV. This is characterized by the highest point of the valence bands being located at the K point, while the minimum point of the conduction bands is at the Γ point, indicating an indirect transition. The Fermi level (EF), set at zero, serves as a critical reference point for evaluating the electronic properties. Furthermore, the optical band gap, which represents the direct transition at the same k-point, was also calculated and the values are provided in Table *2*. For accurate band structure determination, we employed a 6 × 6 × 4 k-point grid, which ensures precise sampling across the Brillouin zone.

The choice of the LDA functional in this study was particularly advantageous. Unlike other exchange-correlation functionals, LDA provided an optical band gap that closely aligns with experimental values, making it a more reliable approximation for this compound. The consistency of LDA in accurately predicting the band gap enhances the credibility of the electronic structure analysis and supports its use in evaluating the thermoelectric properties of $TlSb_3Te_2O_{12}$.

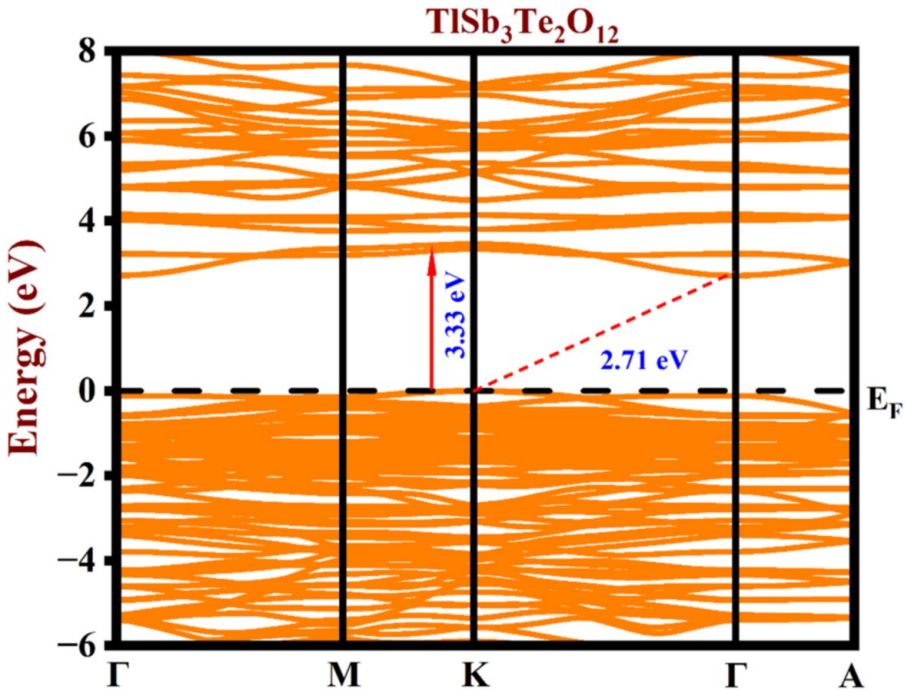

FIGURE 2: The band structure of TlSb3Te2O12

Compound	Experimental optical band gap (eV) [12]	Theoretical optical band gap (eV)
$TlSb_3Te_2O_{12}$	3.00	3.33

TABLE 2: The experimental and theoretical optical band gap of TlSb3Te2O12 compound

Using the semiclassical Boltzmann theory implemented via the BoltzTraP code, we have analyzed the thermoelectric properties of $TlSb_3Te_2O_{12}$. The study focused on key parameters such as the Seebeck coefficient (S), electrical conductivity (σ/τ), electronic thermal conductivity (κe/τ), and the dimensionless ZT. Thermoelectric materials are critical in developing energy-efficient devices, primarily due to their ability to convert dissipated heat energy into electrical power during device operation. Enhancing device efficiency often requires optimizing the balance between electrical and thermal conductivity. Thermoelectric technologies find wide-ranging applications in electronic devices, temperature sensors, aerospace, automotive industries, industrial processes, and medical equipment.

The Seebeck coefficient, S, a vital parameter for evaluating thermoelectric performance, is shown in Figure *3a* for $TlSb_3Te_2O_{12}$ across a temperature of 0 K to 800 K. The coefficient initially increases with temperature, reaching 280 μV/K at 300 K before decreasing, ultimately peaking at 188 μV/K at 800 K. Effective thermoelectric materials also require high electrical conductivity to reduce Joule heating, as indicated in Figure *3b*. The electrical conductivity of $TlSb_3Te_2O_{12}$ increases from 9.36×10^{17} Ωcm^{-1} at 50 K to a maximum value at 800 K, reflecting semiconductor behavior. The overall electrical conductivity lies between 9.36×10^{17} and 9.44×10^{18} Ωcm^{-1}.

For optimal thermoelectric performance, low thermal conductivity is crucial, particularly when operating under fluctuating temperature conditions. As shown in Figure *3c*, the electronic thermal conductivity rises with temperature, driven by increased electron excitation. The trend aligns with that of electrical conductivity, starting at 2.53×10^{12} W/mKs at 50 K and peaking at 2.90×10^{14} W/mKs at 800 K. The power factor (PF), defined as S2σ/τ, measures a material's capability to generate high voltages and currents. As depicted in Figure *3d*, the PF increases from 2.30×10^{10} $Wcm^{-1}K^{-2}s^{-1}$ at 50 K to 4.00×10^{11} $Wcm^{-1}K^{-2}s^{-1}$ at 350 K before decreasing toward 800 K. The ZT, a key indicator of thermoelectric performance, is influenced by the interplay between electrical and thermal conductivities as well as thermopower. $TlSb_3Te_2O_{12}$ indicates a high ZT value of 1.56 at 300 K, attributed to its low thermal conductivity and high

Seebeck coefficient (Figure 4). The material maintains effective performance over a broad temperature range of 50 K to 800 K. Although ZT decreases from 0.45 to 1.56 between 350 K and 800 K, it still indicates considerable potential for waste heat recovery.

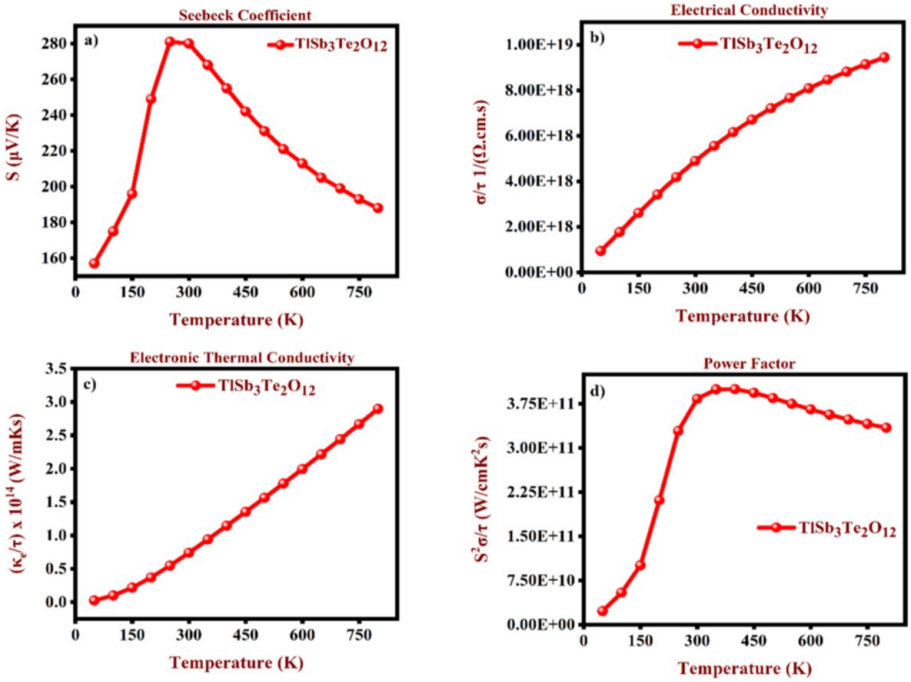

FIGURE 3: The thermoelectric parameters (a) Seebeck coefficient, (b) electric conductivity, (c) thermal conductivity, and (d) power factor

Discussion

The wide bandgap of $TlSb_3Te_2O_{12}$, combined with its high ZT, plays a crucial role in its thermoelectric performance and suitability for specific applications. A wide bandgap is beneficial for thermoelectric materials as it enhances their thermal stability and allows them to maintain performance at elevated temperatures. Wide bandgap semiconductors typically exhibit lower intrinsic carrier concentrations at high temperatures, which reduces the detrimental effects of intrinsic conduction, a common issue in narrow bandgap thermoelectric materials. This characteristic makes $TlSb_3Te_2O_{12}$ particularly effective for high-temperature applications where thermal excitation can compromise the performance of materials with narrower bandgaps. When compared to conventional thermoelectric materials such as Bi_2Te_3 [22], PbTe [23, 24], and SnSe [25, 26], which generally operate effectively in the low to mid-temperature range (up to ~500 K), $TlSb_3Te_2O_{12}$ exhibits a distinct advantage due to its high ZT values across a broader temperature range (50 K to 800 K). The peak ZT value of 1.56 at 300 K indicates superior performance compared to many existing materials. For instance, typical ZT values for Bi_2Te_3 are around 1.0 at room temperature, and for PbTe, range between 1.2 and 1.5 at elevated temperatures (~600 K). The ability of $TlSb_3Te_2O_{12}$ to sustain a high ZT value over a wide temperature range makes it a versatile candidate for applications that require stable performance across varying thermal conditions, such as waste heat recovery in industrial processes and automotive exhaust systems. The combination of a wide bandgap and high ZT values makes $TlSb_3Te_2O_{12}$ particularly suited for thermoelectric applications that demand materials with good performance at both low and high temperatures. Its thermal and electrical properties reduce the risk of thermal degradation and enhance efficiency, positioning it as a promising material for sustainable energy solutions, including power generation from waste heat and cooling in high-temperature environments.

The promising thermoelectric properties of $TlSb_3Te_2O_{12}$, as revealed by our analysis, suggest its suitability for enhancing the efficiency of energy conversion devices. The material's high Seebeck coefficient, low thermal conductivity, and favorable electrical conductivity contribute to its high ZT value, which peaks at 300 K. This efficient conversion makes $TlSb_3Te_2O_{12}$ a strong candidate for waste heat recovery applications. In practical scenarios, such characteristics are instrumental in improving the

performance of thermoelectric devices. In electronic systems and industrial processes, substantial heat is often dissipated as waste. Utilizing thermoelectric materials like $TlSb_3Te_2O_{12}$ enables the harvesting of this waste heat and its conversion into usable electrical energy, enhancing overall system efficiency and contributing to energy conservation. The high ZT value in the temperature 50 K to 800 K indicates that $TlSb_3Te_2O_{12}$ can perform effectively in diverse environments, including both low and high-temperature applications. This adaptability is particularly valuable in aerospace, automotive, and industrial sectors, where temperature variations are common. The ability to maintain stable performance across different temperatures supports ongoing efforts to develop sustainable energy solutions, reduce dependence on conventional power sources, and lower carbon emissions.

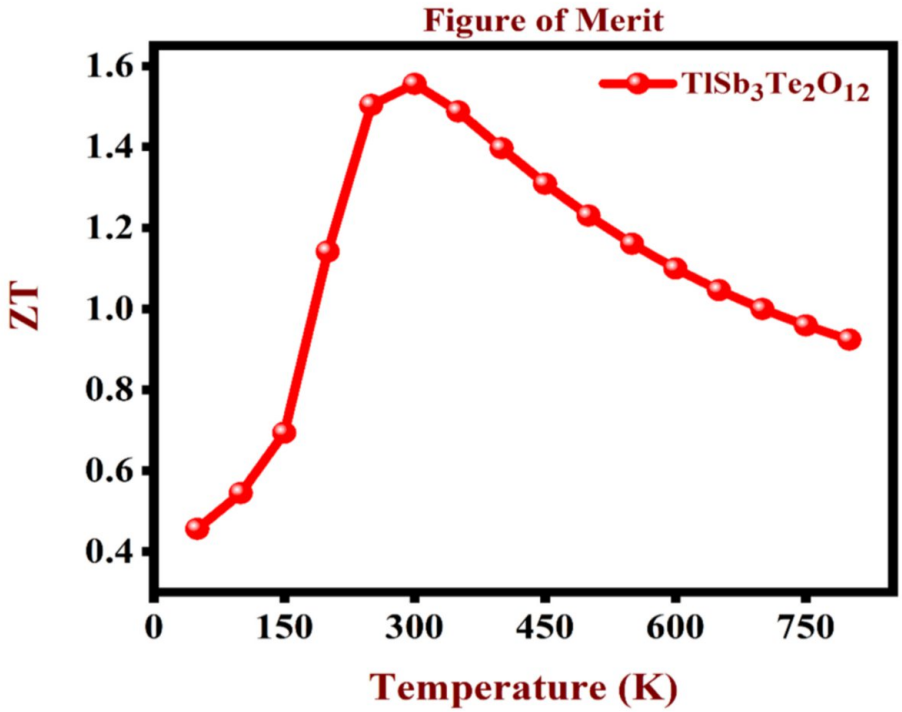

FIGURE 4: The figure of merit (ZT) of TlSb3Se2O12

Conclusions

A thorough examination of the structural, electronic, and thermoelectric properties of the non-centrosymmetric layered selenite $TlSb_3Te_2O_{12}$ was conducted using DFT combined with Boltzmann transport theory. Our findings suggest that $TlSb_3Te_2O_{12}$ is a highly promising material for energy conversion applications, specifically in the area of waste heat recovery. The geometry optimization performed using the FP-LAPW method yielded lattice constants that closely matched experimental data, confirming the accuracy and reliability of our computational model. This structural stability is critical for its potential use in real-world applications. The electronic analysis identified $TlSb_3Te_2O_{12}$ as an indirect bandgap semiconductor with a substantial bandgap of 2.71 eV, which minimizes intrinsic carrier excitation at high temperatures. This property is crucial for maintaining thermal stability, especially in applications involving fluctuating thermal conditions, such as automotive exhaust and industrial heat recovery systems. The evaluation of thermoelectric properties revealed a high ZT of 1.56 at 300 K, which is notably superior compared to traditional thermoelectric materials like Bi_2Te_3 and PbTe under similar conditions. Such a high ZT value indicates exceptional thermoelectric performance, making it suitable for efficient energy conversion processes. The study highlighted the critical interplay between electrical and thermal conductivities, essential for optimizing thermoelectric performance. The high Seebeck coefficient of 280 μV/K at 300 K, combined with increasing electrical conductivity at high temperatures, significantly contributes to a high PF. This interplay ensures effective energy conversion by minimizing heat loss, thus enhancing the overall thermoelectric efficiency. Furthermore, $TlSb_3Te_2O_{12}$ demonstrated a consistent thermoelectric response over a wide temperature range (50 K to 800 K), broadening its applicability to various industries such as automotive, aerospace, and industrial sectors. In summary, our theoretical investigation establishes $TlSb_3Te_2O_{12}$ as a promising material for thermoelectric applications, particularly in waste heat recovery and sustainable energy systems. The results provide a strong foundation for future

experimental validation and suggest further exploration of non-centrosymmetric layered compounds for advanced energy conversion technologies.

Additional Information

Author Contributions

All authors have reviewed the final version to be published and agreed to be accountable for all aspects of the work.

Concept and design: Eithiraj R. D., Hariharan M.

Acquisition, analysis, or interpretation of data: Eithiraj R. D., Hariharan M.

Drafting of the manuscript: Eithiraj R. D.

Critical review of the manuscript for important intellectual content: Eithiraj R. D., Hariharan M.

Supervision: Eithiraj R. D., Hariharan M.

Disclosures

Human subjects: All authors have confirmed that this study did not involve human participants or tissue. **Animal subjects:** All authors have confirmed that this study did not involve animal subjects or tissue. **Conflicts of interest:** In compliance with the ICMJE uniform disclosure form, all authors declare the following: **Payment/services info:** All authors have declared that no financial support was received from any organization for the submitted work. **Financial relationships:** All authors have declared that they have no financial relationships at present or within the previous three years with any organizations that might have an interest in the submitted work. **Other relationships:** All authors have declared that there are no other relationships or activities that could appear to have influenced the submitted work.

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