

## Chapter

# Advanced Thermoelectric Materials: A Snapshot of Theory, Development, and Applications

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## Abstract

This chapter provides a comprehensive overview of high-performance thermoelectric materials and their transformative role in energy conversion technologies. Beginning with the fundamentals of thermoelectricity, the chapter traces the historical development of materials like bismuth telluride and explores the advancements in organic, hybrid, and nanostructured thermoelectric systems. Special focus is given to cutting-edge materials, including topological insulators, 2D materials, and ionic thermoelectric materials, which exploit ionic conductivity and thermodiffusion for efficient low-grade heat harvesting. Key strategies such as alloying, nanostructuring, and doping are discussed alongside computational methods that drive material innovation. The chapter also highlights diverse applications, from waste heat recovery to wearable devices and green energy systems, emphasizing their role in sustainable energy solutions. Advanced phenomena, including the Soret effect, and state-of-the-art modeling techniques are analyzed to provide insights into optimizing performance. By synthesizing historical perspectives, breakthroughs, and future potentials, this chapter serves as a resource for researchers and engineers aiming to advance thermoelectric materials and systems. It addresses current challenges and outlines future directions to illuminate the path toward more efficient and sustainable energy conversion technologies.

**Keywords:** high-performance materials, ionic thermoelectric, Soret effect, low-grade thermal energy harvesting, Seebeck effect

## 1. Introduction

The search for efficient technologies of energy conversion has become paramount in the quest for sustainable energy solutions. One such avenue can be found in thermoelectric materials, a class of materials possessing the capability to directly transform heat energy into electrical power via the Seebeck effect [1]. Considering global warming, which is an environmental challenge today, devices made of thermoelectric materials can play a role in reducing the harm of global warming by directly converting heat into electrical energy [2, 3]. The conventional sources of energy are per se connected with limited resource supply and environmental impact, making

the satisfaction of the fast-growing demand in power very challenging. Fossil fuel combustion not only causes the release of greenhouse gases but also the consumption of limited reserves; hence, alternative and sustainable energy conversion technologies have to be found. In such a scenario, thermoelectric materials emerge as a very promising solution that will capture waste heat from various sources and convert it into useful electricity [4, 5]. On the other hand, ensuring the sustainability of thermoelectric materials remains a challenge. A sustainable material such as lignin, a complex natural polymer, can be combined with other thermoelectric materials [6, 7]. Recent research has shown that thermoelectric systems can be built using this material. In these systems, positive and negative ions, rather than electrons, serve as electrical carriers in lignin-based microchannels, enabling the observation of the Seebeck effect in this structure [8, 9].

In thermoelectric materials, charge transfer typically requires a medium such as a metal or semiconductor, where the differential potential is governed by the movement of electrons. In contrast, ionic thermoelectric systems rely on the movement of ions (both positively and negatively charged) within an electrolyte or fluid. These fluids exhibit electrical conductivity due to the presence of mobile ions. In such systems, the driving force for ion movement is associated with thermodiffusion phenomena, where a temperature gradient induces ionic motion. Therefore, the movement of particles, such as ions, under the influence of a temperature gradient is referred to as the Soret effect in the context of ionic systems [8, 10]. Qiao et al. introduced a linearized approach to solving the Poisson-Nernst-Planck equations, employing a gradient-flow framework and simplifying the logarithmic function [11]. Fish provided a theoretical model to analyze nanocomposite electrolytes, describing the space charge layer and its influence on the conductivity of insulating spheres within ionically conductive materials [12]. Fleharty examined nanochannels with electric double layers comparable to the channel width, solving the Poisson-Boltzmann equation using charge regulation boundary conditions [13]. Moya et al. investigated cylindrical nanopores containing ternary electrolyte solutions, analyzing the effects of wall charge polarity. They applied the network simulation method to solve the Poisson-Boltzmann equation and used modified Navier-Stokes and Nernst-Planck equations to determine velocity and conductivity [14]. Jing et al. evaluated the electroviscous effect on electric double layers, revealing its insignificance at high  $Z$  potential [15]. Luo and Keh derived expressions for electrophoretic mobility and conductivity in salt-free suspensions, highlighting their dependence on surface charge density [16]. Varner studied dilution effects in ionic liquid supercapacitors to improve performance [17]. Huang explored hydrodynamic slippage and its impact on nanoscale power generation [18]. Levy et al. modeled the dielectric response of ionic liquids, accounting for ion-dipole interactions and deriving a closed-form dielectric constant [19]. Stout et al. summarized ionic transport principles [20], and Qiao et al. further refined numerical schemes for solving ionic transport equations [11].

In other hand, Topological materials, characterized by their distinct band structures, have garnered significant interest in condensed-matter physics, thermoelectrics, spintronics, and other related fields. Thermoelectric technology, which enables the direct conversion of heat to electricity or vice versa, holds considerable promise in addressing the global energy crisis and advancing solid-state cooling solutions. In recent research systematically investigates the magneto-thermoelectric transport properties of a high-quality single-crystalline  $\text{Bi}_{88}\text{Sb}_{12}$  topological insulator. It observes a large magneto-Seebeck effect due to the material's ultrahigh mobility and

linear band dispersion, which results in an enhanced magneto-zT under magnetic fields as low as 1 T. A high zT value of  $\sim 1.7 \pm 0.2$  is achieved at 180 K and 0.7 T, particularly significant below 300 K. The study highlights the importance of magneto-thermoelectric correlations as an effective strategy for optimizing thermoelectric performance. It suggests future exploration of p-type  $\text{Bi}_{1-x}\text{Sb}_x$  with hole doping to further improve the material's response [21].

In conclusion, thermoelectric materials represent a promising avenue for sustainable energy conversion, addressing both global energy demands and environmental concerns. Advances in ionic thermoelectric systems, particularly those utilizing sustainable materials like lignin, offer new pathways for efficient waste heat recovery. Additionally, the exploration of topological materials, such as  $\text{Bi}_{1-x}\text{Sb}_x$ , demonstrates the potential for enhanced thermoelectric performance through magneto-thermoelectric effects. By integrating novel material systems and theoretical models, future research can further optimize thermoelectric technologies for widespread energy applications. Here, we do not categorize thermoelectric materials based on high or low-temperature gradients; instead, we classify them according to material types. Our focus is on sustainable materials and enhancing the performance of thermoelectric materials in light of recent research. Additionally, we aim to identify integrated systems that strive to develop compact electrical or sensor modules.

## 2. Theoretical foundations

Thermoelectric materials represent the research field where the groundbreaking application of the Seebeck effect, a basic concept that permits the direct conversion of temperature gradients into electrical voltage, is put into practice. Such a characteristic makes up the very core of harvesting lost heat and converting it directly into precious electrical output. But before introducing different classes of material and their uses, understanding the principal laws with which the basics of thermoelectricity are embodied would first be appropriate [22]. The very essence of thermoelectricity is dependent upon the behavior of the charge carriers in a material across a temperature gradient. Keeping this view in mind, if two materials with different conductivity to electricity are brought in contact, then electrical charge will start moving from the high-conductivity material, like from the hot side to the low-conductivity material, the cold side. This migration of charge carriers creates the potential difference, hence establishing an electric current. Hence, this would allow conversion of thermal energy into electrical energy on the principle of thermoelectricity [23, 24].

The Seebeck effect is the cornerstone of thermoelectric phenomena. Discovered by Thomas Johann Seebeck in the early nineteenth century, this effect illustrates the generation of an electromotive force (EMF) across a temperature gradient. The magnitude of the generated voltage is proportional to the temperature difference across the material. Harnessing the Seebeck effect allows for the creation of thermoelectric generators capable of converting waste heat from various sources, such as industrial processes or car exhaust, into electricity [25–27]. On the other hand, named after Jean Charles Athanase Peltier, the Peltier effect is the reverse of the Seebeck effect. It describes the absorption or release of heat at an electrical junction, resulting in a temperature gradient. This effect is fundamental in thermoelectric cooling applications, where an electric current is applied to transfer heat from one side of the material to the other. Peltier devices are found to be used in electronic cooling systems

and temperature control applications [28]. Also, the Thomson effect, also known as the Kelvin or Joule-Thomson effect, describes the temperature change that occurs when a current flows through a homogeneous conductor subjected to a thermal gradient. Though less commonly employed in practical applications than the Seebeck and Peltier effects, the Thomson effect plays a role in understanding the overall behavior of thermoelectric materials under varying conditions [29, 30]. To quantify the efficiency of a thermoelectric material, researchers commonly refer to the figure of merit, denoted as  $zT$ . The  $zT$  value amalgamates various material properties, including electrical conductivity, thermal conductivity, and temperature, into a single metric. Higher  $zT$  values signify superior thermoelectric performance. The quest for materials with elevated  $zT$  values is a driving force in the development of high-performance thermoelectric materials, as it directly correlates with their ability to convert heat into electrical power effectively. In subsequent sections, we will explore how different classes of materials strive to optimize  $zT$  values for enhanced energy conversion efficiency [31, 32].

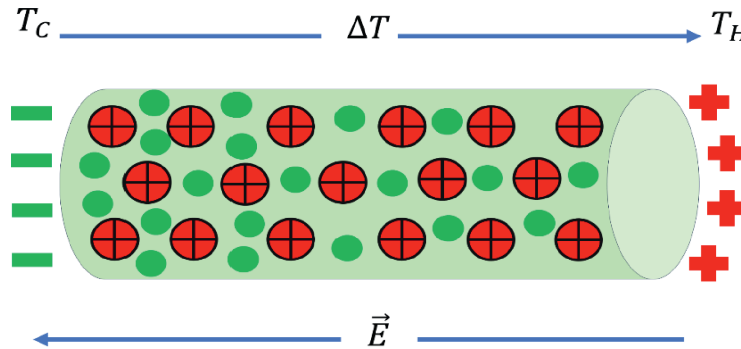
**Figure 1** Considering that the sign of  $\alpha_n$  for electrons is negative, it depicts the production of an electric field that opposes the temperature gradient  $\vec{\nabla}T$  [33]:

$$\vec{E} = \alpha_n \vec{\nabla}T \quad (1)$$

The electronic contribution to the Seebeck coefficient can be expressed generally as

$$S = \frac{k_B}{e} \int \frac{E_F - E}{K_B T} \cdot \frac{\sigma(E)}{\sigma} dE \quad (2)$$

In this equation,  $e$  stands for elementary charge,  $k_B$  for Boltzmann, and constant  $\sigma(E)$  for electric conductivity, which takes energy-dependent scattering mechanisms and density of states into consideration. By integrating electric conductivity over all energies ( $\sigma = \int \sigma(E) d(E)$ ), one may determine the total conductivity, or  $\sigma$ , where  $T$  is the temperature. Furthermore, we take into consideration the mobility edge, where  $E_F - E_v$  denotes the Fermi level location with respect to the valence band edge.



**Figure 1.**

An illustration of the thermoelectric effect in an equilibrium system, when a material is exposed to an external temperature gradient. The mean free path of the more energetic electrons is longer. Green dots represent these higher energetic electrons, which then diffuse to the cool side until an electric field ( $E$ ) is created to prevent any further diffusion, reproduced with permission.

The figure of merit for thermoelectric materials is represented by  $zT$ , according to the expression

$$zT = \frac{\sigma S^2}{\kappa} T \quad (3)$$

In this case,  $T$  is the absolute temperature,  $\sigma$  is the electrical conductivity,  $S$  is the Seebeck coefficient, and  $\kappa$  is the thermal conductivity. As a result,  $zT$  uses in-verse temperature units. The value of  $zT$  is roughly 1 for thermoelectric materials that are efficient. The higher the  $zT$  number, the better thermoelectric generators and refrigerators work. Furthermore, the power factor ( $PF = S^2\sigma$ ) is typically employed to compare materials' thermoelectric efficiencies with similar thermal conductivities. The thermal conductivity can be expressed as  $\kappa = \kappa_L + \kappa_E$ , which is the sum of the lattice contribution ( $\kappa_L$ ) and the electronic contribution ( $\kappa_E$ ). Because charge carriers also contribute to heat transfer, the electronic contribution to thermal conductivity rises with carrier concentration:

$$\kappa_E = L\sigma T = ne\mu_c LT \quad (4)$$

where  $L$  is the Lorenz factor,  $2.44 \times 10^{-8} \text{ (J}^2 \text{ C}^{-2} \text{ K}^{-2})$  for free electrons,  $n$  charge carrier density,  $e$  is Elementary charge,  $\mu_c$  is charge carrier mobility and  $T$  is absolute temperature, and has dimension of K (kelvin).

The efficiency of a thermoelectric device is fundamentally defined

$$\eta = \frac{P_0}{q_h} \quad (5)$$

According to the first law of thermodynamics,  $q_h$  is the rate of heat flow from the hot to the cool section, and  $P_0$  is the electrical power production:

$$\eta_C = \frac{T_H - T_C}{T_H} \quad (6)$$

The efficiency of thermoelectric devices ( $\eta$ ) must be calculated using  $zT$  and the Carnot efficiency ( $\eta_C$ ), which is derived from the temperature differential ( $\Delta T$ ) and the hot-side temperature ( $T_H$ ). The formula for this is  $\eta_C = \Delta T/T_H$ . The word “this relationship” accurately describes

$$\eta = \eta_C \frac{\sqrt{1 + zT} - 1}{\sqrt{1 + zT} + \frac{T_C}{T_H}} \quad (7)$$

On the other hand, the charge on ions plays a crucial role in the mechanism of voltage generation in ionic thermoelectric materials. This process is driven by the interplay between ion transport, electrostatic interactions, and thermal gradients (Soret effect), allowing for the efficient conversion of heat into electricity. Ionic thermoelectric materials leverage the interplay between ion transport, electrostatic

interactions, and thermal gradients to convert heat into electricity efficiently. In lignin-derived ionic membranes infused with KOH electrolyte, the formation of an electric double layer (EDL) plays a crucial role in facilitating selective ion diffusion. Upon immersion in KOH, the lignin surface transforms into negatively charged alkoxide ( $\text{C}-\text{O}^-$ ) groups, attracting  $\text{K}^+$  cations and establishing a structured ionic environment. This arrangement enables efficient charge transport along aligned channels. Under a thermal gradient, ion migration occurs due to the Soret effect, where differences in temperature drive the redistribution of cations and anions. The resulting imbalance in ionic concentration, coupled with electrostatic interactions within the charged channels, enhances thermally driven ionic conductivity and the ionic Seebeck effect. The synergy between selective ion diffusion and thermophoresis highlights the potential of lignin-based membranes for sustainable energy harvesting, offering a pathway toward efficient utilization of low-grade thermal energy [8, 34].

### **3. Material classes**

Thermoelectric Materials encompass diverse categories, with notable examples including inorganic materials like bismuth telluride and lead telluride, organic and organic–inorganic hybrids such as conducting polymers [5] and metal–organic frameworks [35], nanostructured materials like silicon nanowires [36] and quantum dots [37], and advanced materials like topological insulators [38] (e.g., bismuth selenide) and 2D materials like graphene [39]. Ongoing research endeavors aim to optimize the thermoelectric efficiency of these materials by tailoring their properties, exploring novel synthesis methods, and advancing their performance in diverse operating conditions. The collective goal is to harness these materials for converting waste heat into valuable electrical energy, contributing significantly to the development of sustainable energy technologies.

#### **3.1 Inorganic materials**

In the area of thermoelectric materials, inorganic compounds have historically played a very significant role, with typical examples being bismuth telluride and lead telluride. These materials have received a lot of attention due to their favorable thermoelectric properties, making them very basic in thermoelectric device development.

*Development of Traditional Inorganic Thermoelectric Materials:*

Among the inorganic thermoelectric materials, bismuth telluride ( $\text{Bi}_2\text{Te}_3$ ) and lead telluride ( $\text{PbTe}$ ) share significant importance. Known since the middle of the twentieth century, bismuth telluride has a high Seebeck coefficient and low thermal conductivity, so it was considered the material of choice for cooling applications. On the other hand, good electrical properties are hosted by the lead telluride, which makes it particularly effective in power generation.  $\text{Bi}_2\text{Te}_3$  has been under investigation since 1954 and is still one of the most commonly applied TE materials. Nevertheless,  $\text{Bi}_2\text{Te}_3$  remains a material with a high potential of interest and has recently been subject to remarkable improvements. The thermoelectric figure of merit  $zT$  of material limits the efficiency of thermoelectric energy converters. Recent progress in  $zT$ , particularly nanostructure-based approaches aiming to limit phonon heat conduction, is reaching the fundamental limit. The thermal conductivity cannot be reduced below the amorphous limit. Joseph P. Heremans and colleagues explored the enhancement of the Seebeck coefficient by a distortion of the electronic density of states and showed



thallium impurity levels that gave high Seebeck coefficients in lead telluride, PbTe. This engineering of the band structure resulted in an improvement in  $zT$  in p-type PbTe by a factor of two to values above 1.5 at 773 Kelvin. The combination of this new physical principle with nanostructuring for lowering thermal conductivity can further improve  $zT$  and broaden the uses for thermoelectric systems [40]. Another intriguing class of materials is the silver-copper chalcogenide family, which has garnered significant attention for its exceptional thermoelectric properties. Remarkably, studies have reported  $zT$  values ranging from 0.3 to 1.6, showcasing their potential for high-efficiency thermoelectric applications. These materials exhibit a unique combination of high electrical conductivity and low thermal conductivity, which is often attributed to their complex crystal structures and effective phonon scattering mechanisms [41]. Nanostructured  $\text{Bi}_2\text{Te}_3$ -based materials significantly outperform their bulk counterparts in thermoelectric efficiency, as reflected in their higher  $zT \sim 1.4$  values. Bulk  $\text{Bi}_2\text{Te}_3$  typically achieves  $zT \sim 0.8\text{--}1.0$  at room temperature (300 K), which serves as a benchmark for comparison [42]. In contrast, nanostructured variants, such as nanocomposites (e.g.,  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ ) and superlattices [43], achieve  $zT$  values ranging from 1.2 to 2.4, benefiting from reduced lattice thermal conductivity and enhanced power factors due to quantum confinement and optimized carrier concentrations [44, 45]. Specifically, superlattices hold the record with  $zT$  values up to 2.4 at 300 K, while doped nanostructures (e.g., Pb-doped  $\text{Bi}_2\text{Te}_3$ ) [46] and alloyed systems (e.g., p-type  $\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_3$ ) [47] achieve  $zT \sim 1.6\text{--}1.9$  making them highly promising for thermoelectric applications. Overall, the advancements in nanostructuring and alloying have pushed  $zT$  values to new heights, highlighting their potential in high-performance thermoelectric devices [48].

Moving on to  $\text{CoSb}_3$ -based materials, binary skutterudites with a  $\text{CoAs}_3$ -type structure have been investigated [49], showing enhanced  $zT$  values as high as 1.1 at  $\sim 550^\circ\text{C}$  in n-type nanostructured  $\text{CoSb}_{3-x}\text{Te}_x$  skutterudite compounds. Additional substitution of IVB-group elements (Si, Ge, Sn, and Pb) for Sb, particularly Sn, was found to be the most effective in enhancing  $zT$  by extending the solubility limit of Te in  $\text{CoSb}_{3-x}\text{Te}_x$ , reducing thermal conductivity more significantly than electrical conductivity [50].

In another research study, a comprehensive exploration of the Mn doping effect on  $\text{CoSb}_3$ -skutterudite was reported, encompassing both theoretical and experimental investigations. An innovative approach was adopted, focusing initially on single Mn-doped  $\text{Mn}_x\text{Co}_{1-x}\text{Sb}_3$  samples before delving into co-doping with Te to prepare  $\text{Mn}_x\text{Co}_{1-x}\text{Sb}_{2.85}\text{Te}_{0.15}$  samples, evaluating their impact on both conduction types. Theoretical density functional theory (DFT) results unveiled the feasibility of single Mn doping, a finding successfully validated experimentally with the production of pure samples featuring a low solubility of Mn ( $x \leq 0.05$  in  $\text{Mn}_x\text{Co}_{1-x}\text{Sb}_3$ ) positioned at the Co site. Up to a certain level of Mn substitution, a minor amount of the binary MnSb phase was formed. In terms of transport properties, it was demonstrated for the first time that Mn stabilizes p-type conduction with a substantial Seebeck coefficient, resulting from a slight reduction of the valence electron concentration (VEC) per formula due to Co substitution. This led to an improvement in the power factor (PF) and the resulting figure of merit  $zT$  in the near-room temperature range ( $T < 450\text{ K}$ ). Co-doping with Te was subsequently undertaken, revealing an unexpectedly prevalent formation of the additional MnTe phase over Co substitution. Structural investigations highlighted that Te substitutes for Sb without filling the icosahedral voids present in the  $\text{CoSb}_3$  skutterudite. Moreover, a significant enhancement of the PF was achieved, reaching an ultrahigh value of  $4.7\text{ mW m}^{-1}\text{ K}^{-2}$  at 725 K,

rarely reported for rare-earth-free skutterudites. This was attributed to a remarkable increase in the Seebeck coefficient in the co-doped CoSb<sub>3</sub> skutterudite. The combined experimental and theoretical findings indicated that various factors contribute to the substantial enhancement of the Seebeck coefficient, allowing for a maximum  $zT$  value of 1 at 725 K. The controlled formation of the MnTe secondary phase was identified as a key factor, slightly reducing thermal conductivity and maximizing an unexpected PF to a level comparable to that reported for expensive rare-earth-filled skutterudites. This achievement contributes to the development of a new generation of sustainable thermoelectric (TE) materials by exploring the magnetic and composite effects, aiming to provide stable, cost-efficient, and high-performance materials for thermoelectricity based on unfilled skutterudites [51]. Ongoing research in CoSb<sub>3</sub>-based thermoelectric nanocomposites involves innovative cold sintering processes, such as CSP and post-annealing techniques. Aida Serrano et al. reported successful sintering of CoSb<sub>3</sub>-based thermoelectric nanocomposites by CSP with suitable mechanical integrity and similar morphological and structural properties as the starting powders. The thermoelectrical properties are shown to be dependent on the sintering process, with the highest power factor ( $1000(200) \mu\text{W m}^{-1} \text{K}^{-2}$ ) and  $zT$  (0.12(3) at RT) achieved for nanocomposites sintered by CSP followed by a subsequent post-annealing at 500°C, presenting the highest CoSb<sub>3</sub> phase content with adequate grain and crystallite size [52].

### *3.1.1 Recent advancements and improvements*

Recent years have shown renewed interest in the performance enhancement of traditional inorganic thermoelectric materials. Scientists have introduced a number of new synthesis methods and alloying and nanostructuring strategies to improve such material's figure of merit. The advances in material designs and fabrication have resulted in the optimization of thermoelectric properties, thus showing continuing efforts to improve the efficiency and applicability of inorganic thermoelectric materials.

This collection portrays a comprehensive view of diverse inorganic materials for thermoelectricity, from state-of-the-art thermoelectric materials to much less conventional ones but with huge potential for future applications. Although being concerned, like many authors, with the new figure of merit,  $zT$  max, we also emphasize the significance of the average  $zT$ , especially in the temperature region of interest, along with a few other significant thermoelectric parameters. Potential fulfillment of this important checklist has entered an era of exceptional materials advancement and discovery through a combination of data mining, machine learning, and high-throughput calculations, providing active research in modeling and experimental instrumenting. The pursuit of Earth-abundant, non-toxic starting materials remains a cardinal constraint for driving down cost and environmental impact. Coupling of atomistic and density of states calculations with band structure engineering will be instrumental in deciding upon effective additives to either enhance electrical conductivity or reduce thermal conductivity. In spite of these advances, the way is one of dealing with a vaster field: leading the material to the same level of performance as p-type, leading to good mechanical properties and stability, degrading mechanisms controlling, interfacing of thermoelectric modules, processing costs to levels where broad market competitiveness is attainable. A detailed assessment of the production costs, cost-effective material processing, and manufacturing routes has been considered long overdue for the purpose of wider adoption of thermoelectrics [53].



### 3.2 Organic and organic-inorganic hybrid materials

A paradigm change in the sector is shown by the introduction of organic and organic–inorganic hybrid thermoelectric materials. These materials provide new possibilities for thermoelectric applications because of their tunable electronic characteristics, cheap production cost, and flexibility.

Creating polymer–inorganic thermoelectric composites offers a viable strategy to address the poor electrical conductivity, low Seebeck coefficient, and inadequate power factor (PF) of polymers, as well as the expensive nature of inorganic materials. Multiple techniques have been utilized to produce these hybrid polymer–inorganic substances, including physical mixing, solution mixing, and in situ polymerization. It is important to note that the thermal conductivity of polymers is approximately an order of magnitude lower than that of conventional inorganic thermoelectric materials. This characteristic positions polymers like polyaniline (PANI), polythiophene (PTH), and poly(3,4-ethylenedioxythiophene) (PEDOT) as excellent candidates for the advancement of new thermoelectric materials [54]. One way to enhance the performance of this class of thermoelectric materials is through doping. This process, referred to as chemical or primary doping, can be accomplished via two methods: (1) A charge transfer (CT) mechanism that involves the incorporation of a redox-active molecule such as tetrakis (dimethylamino) ethylene (TDAE) into the conducting polymers, where the doping mechanism is founded on a CT interaction between the donor and the acceptor. 2) A comprehensive investigation was conducted to examine the complex effects of primary doping processes, which utilize acid-base ( $A^+ - B^-$ ) and charge transfer (CT) mechanisms via  $H_2SO_4$  and TDAE, respectively. Additionally, the study explored the secondary effects of ethylene glycol (EG) on the thermoelectric (TE) performance of both p-type Te/PEDOT:PSS and n-type  $Ag_xTe$ /PEDOT:PSS hybrids. In particular, the results have shown pronounced differences between EG post-treatment of pure PEDOT:PSS versus  $Ag_xTe$ /PEDOT:PSS hybrid systems. Unlike improved conformation exhibited in pure PEDOT:PSS systems, EG post-treatment mostly disturbs morphological conformations of PEDOT chains in hybrid systems. The upset negatively impacts on the lamellar domains, which raises the energy conversion layers (ECLs) full width at half maximum. This generally degrades the whole TE performance by increasing carrier mobility,  $\mu$ , and conductivity,  $\sigma$ . Besides, deep insight is given into how these numerous post-treatment processes create structural and electrical changes in hybrid organic–inorganic materials, underlining complex results realized in  $Ag_xTe$ /PEDOT:PSS hybrid systems in comparison with pure polymer systems. This work puts these strategies in the broader perspective of hybrid electronic material research and focuses on PEDOT-based hybrid materials for thin-film TEs [55].

### 3.3 Nanostructured organic-inorganic hybrid thermoelectric materials

Organic thermoelectric materials exploit the intrinsic features of carbon-based molecular structures and polymers. Tuning their electronic structure is a highly promising approach for designing materials with improved thermoelectric performance. Moreover, hybrid materials have been developed in which organic and inorganic components interact synergistically to provide flexibility without sacrificing stability, thereby expanding their potential for diverse applications.

### *3.3.1 Nanostructured materials*

Nanostructured materials represent a cutting-edge approach in the pursuit of high-performance thermoelectric materials. Gervino-Solona and colleagues claim a novel interconnected nanostructure of  $\text{Bi}_2\text{Te}_3$ , which achieves impressive thermoelectric performance despite using only 10% of the material typically required for thin films. The addition of sodium lignosulfonate during electrochemical deposition significantly improves the material's morphology and output performance. The fabrication method is scalable, offering the potential for flexible thermoelectric devices, particularly in energy-harvesting applications for wearable technologies [56]. Utilizing phonon scattering and quantum confinement processes, nanostructured thermoelectric materials such as nanowires and nanoparticles can dramatically change the thermal and electrical transport characteristics [57]. By overcoming the conventional trade-off between electrical and thermal conductivity [58], these materials seek to further the limits of thermoelectric efficiency [59]. Recent research shows that the addition of single-wall and multi-wall carbon nanotubes (SWCNTs and MWCNTs) to the conductive polymer base on PEDOT can significantly enhance its thermal conductivity. Researchers have demonstrated that these organic materials can increase the thermoelectric performance of flexible polymers. The authors claim that films with MWCNTs exhibit slightly higher electrical conductivity than those with SWCNTs. Using the LbL technique, the primary electrode made of MWCNTs achieved a conductivity of  $31.26 \text{ Scm}^{-1}$ , playing a critical role in subsequent polymerization. For SWCNTs, the conductivity was recorded at  $3.49 \text{ Scm}^{-1}$  under the same conditions [5].

For the development of thermoelectric generators that have nanometer thickness, increasing the electrical sheet resistance and thermal resistance is one of the challenges ahead. As a result, methods such as manufacturing thermoelectric micrometric strips with nanometer thickness and creating an interconnected network of these generators can be a way to overcome this problem. However, creating more costs for using the micrometric dimension manufacturing system and the need for more professional operators leads to an increase in the price of the final product. To find the optimal dimensions, theoretical methods and simulation software can help in finding the optimal dimensions quickly [59].

### **3.4 Advanced materials**

Advanced materials like topological insulators have a good talent for thermoelectric applications. Due to their special boundary states that are topologically shielded from backscattering at non-magnetic impurities and defects, topological insulators show enormous promise in the domains of electronics and magnetism. Interestingly, most topological insulators are also very good thermoelectric materials since they have comparable properties to thermoelectric compounds [60]. Quantized energy quanta linked to lattice vibrations, phonons are essential for a number of important physical processes, including heat capacity, electron-phonon/magnon-phonon interactions, thermal conduction, and lattice thermal expansion. Gaining better control over phonons, one of the main heat carriers in thermal transport, has important applications in a number of energy materials domains, such as waste heat recovery, phononic devices, and thermoelectric conversion. THz phonons in natural crystalline materials have gained interest recently because of the importance of atomic lattice vibrations in physics. Topological phonons in crystalline materials have been theoretically classified into a number of different forms, such as Dirac/Weyl point

phonons and [61] nodal-line phonons, using a framework akin to the topological classifications in electronic systems [62]. Wearable technology with maintenance-free batteries is necessary for the “Internet of Things” [63, 64] rapid development, and thermoelectric energy conversion based on large-area flexible materials has garnered a lot of interest. Recently, a fully printed origami thermoelectric generator (TEG) module has demonstrated significant advancements in power output, power density, and scalable manufacturing. By employing screen printing for the thermoelectric and contact materials, researchers developed a high-performance TEG module using synthesized n-type  $\text{Ag}_2\text{Se}$  and p-type Bi-Sb-Te materials. The design incorporates an origami-inspired folding process to enhance thermal impedance matching, with heat flow directed in-plane along the module’s height. The printed module achieves a low resistance of  $56\ \Omega$  and demonstrates substantial power output, indicating its potential for effectively powering IoT sensors [65]. Because of their superior transport characteristics and high-power factors, 2D materials—such as graphene and similar materials—are among the most promising large-area flexible materials for thermoelectric applications. The experimental reports on thermoelectric devices of graphene, black phosphorus, transition metal dichalcogenides, and other 2D materials are used in this review to survey both single-crystalline and polycrystalline 2D materials. Particular attention is paid to their carrier density-dependent thermoelectric characteristics and power factors that are optimized by Fermi level tuning methods. When the relevant performances of 2D materials and widely utilized thermoelectric materials are compared, it becomes clear that 2D materials have much higher power factors [66].

## 4. Methods for enhancing thermoelectric performance

In the pursuit of more efficient thermoelectric materials, various strategies have been employed to enhance the figure of merit ( $zT$ ), a critical parameter for assessing thermoelectric performance. This section explores key methodologies, including alloying, nanostructuring, doping, and the increasingly influential role of computational methods in material design.

### 4.1 Alloying

This is the classical strategy where alloying several different elements in a material can be deliberately combined to improve thermoelectric performance [67]. A proper choice of alloying elements could modify the electronic structure and phonon scattering mechanisms in a material [68]. That is to say, the optimization for increasing electrical conductivity and decreasing lattice thermal conductivity will contribute to elevating  $zT$ . Much success in alloying has already been achieved with traditional inorganic materials; for example, bismuth telluride alloys [69] have been prepared in tailored compositions and show considerable enhancement of thermoelectric efficiency. Bismuth telluride has long dominated TE technology, the scarcity of tellurium has shifted focus to abundant alternatives like  $\text{Mg}_3(\text{Sb,Bi})_2$ -based materials, which exhibit a high thermoelectric figure of merit ( $zT > 1$ ) over a broad temperature range (300–773 K) [70].

### 4.2 Nanostructuring

Manipulating materials at the nanoscale, or “nanostructuring,” has been proposed as a novel technique to improve thermoelectric qualities. Based on quantum

confinement, material design at the nanoscale modifies electrical and thermal transport properties through the use of nanowires, nanoparticles, and even hierarchical nanostructures. However, increased phonon scattering at the interfaces has been found to significantly inhibit thermal conductivity, and in some situations, quantum confinement effects in such nanostructured materials may even enhance electrical conductivity.  $zT$  values are enhanced when these two elements are combined. The inherent trade-offs between electrical and thermal conductivity have been particularly promisingly overcome by nanostructuring, which has led to unprecedented levels of thermoelectric efficiency.

Our group has achieved a significant advancement in the power factor augmentation of a conductive polymer by employing a sustainable technology aimed at improving the efficiency of a flexible thermoelectric module built on films based on carbon nanotubes infused with PEDOT. With an emphasis on conductivity and doping control through the incorporation of CNTs, a strategic combination of the Layer-by-Layer method for forming the layer of CNTs and electrochemical polymerization for the conducting polymer was utilized in the synthesis of effective thermoelectric nanocomposites. After measuring the Seebeck coefficient and assessing the samples' electrical conductivity, the samples were fully characterized. The power factor could be further estimated from these data. The synergistic combination of PEDOT and SWCNTs produced a competitive power factor of  $131.1 \mu\text{Wm}^{-1} \text{K}^{-2}$ , which is comparable to the performance of conventional inorganic thermoelectric materials. This method has the potential to be a very successful way to recycle heat waste because it is simple, affordable, and environmentally benign. Bright futures lie ahead for the advancement of flexible and effective thermoelectric module technology, thanks to green methods [5].

Antonios and coworkers have carefully investigated the effect of increasing the degree of modulation on the thermoelectric efficiency of width-modulated nanowires. More specifically, this work systemically elongates the modulation by adding modulation units and explains the effects of multiple modulation units on transport, keeping an eye on the optimization of the modulation profile toward maximum TE efficiency. The investigations took into consideration two-quantum dot and multiple-QD modulation scenarios, couplings between modulation units, and periodic and aperiodic sequences interacting with each other. Among the main observations made was that the electron transport property and thermoelectric power factor are augmented with an increase in modulation units and the maximum increase being for periodic modulation. The study went ahead to establish that phonon thermal conductance decreases with rising modulation, attaining the SL value for periodic modulation. Most importantly, the researchers uncovered the fact that a drastic increment in  $zT$  accompanies modulation, specifically for aperiodic modulation profiles where quasi-localized states for electrons are created. It will open new routes to optimize width modulation in order to achieve maximum TE efficiency, mostly in scenarios dominated by quantum effects in transport [71].

### 4.3 Doping

Doping is the deliberate introduction of foreign components into a material with the goal of altering its electrical structure. It is a very commonly used strategy. Researchers can manipulate the charge carrier concentration and mobility, which impacts the material's thermoelectric properties, by carefully selecting dopants [72]. Doping is a flexible approach that may be used with a wide range of thermoelectric

materials, both inorganic and organic. Optimizing electrical conductivity and the Seebeck coefficient by precise control of the doping process results in improved thermoelectric performance [73]. Zhibin and coworkers try to enhance the thermoelectric performance of BiCuSeO for its practical application in thermoelectric power generation and thermoelectric catalysis. According to the authors, the practical application of BiCuSeO is hindered by the fact that it shows lower thermoelectric efficiency. Bulk materials of BiCuSeO were prepared using the solid-phase reaction method combined with the ball milling method and spark plasma sintering. In this respect, the authors attempted to optimize thermoelectric performance through the synergistic enhancement of both carrier concentration and mobility. Enhancement was achieved by Al doping into a BiCuSeO matrix. Here, adjustments in carrier mobility were to be attained by an energy band adjustment. The results indicated that Al doping enlarged the bandgap and increased the carrier mobility of BiCuSeO; hence, it is a useful way to improve the thermoelectric properties at middle and high temperatures. Besides, Pb was used as a doping element to adjust the carrier concentration of BiCuSeO. Such Al and Pb dual-doping exhibited a great effect on improving carrier concentration without losing high carrier mobility. This method could improve electrical conductivity without sacrificing a large Seebeck coefficient. The power factor for the Al/Pb-doped BiCuSeO reached  $\sim 7.67 \mu\text{Wcm}^{-1} \text{K}^{-2}$  at 873 K. The thermal conductivity for all doped samples was found to be low in the measured temperature range. Finally, the  $zT$  of Al/Pb-doped BiCuSeO was  $\sim 1.14$  at 873 K, which is far greater compared to the pure phase. This successful dual-doping strategy eventually improved the thermoelectric properties of the BiCuSeO matrix [74].  $\text{Mg}_3\text{Bi}_2$ -based thermoelectric materials have also been recognized as highly promising materials for thermoelectric applications. The sample preparation of  $\text{Mg}_3\text{Bi}_2$  was carried out by a high-temperature synthesis. This study has focused on the influence of Mg/Sb content on the electrical transport properties and properties related to semiconductor-semimetal. The efficiency in terms of introducing electrons from excess Mg by high-temperature synthesis is relatively lower in comparison with that achieved by ball milling. This is mainly attributed to the high vapor pressure of Mg during synthesis. Herein, we present the substitution of Sb/Te at the Bi site, and its effect in bringing about a transition from p-type to n-type conduction. The increased content of the stronger Mg content weakens the material's behavior on the semiconducting side and strengthens the material's semi-metallic tendency with a corresponding enhancement of the material's conductivity. To this particular goal, the present results are of vital value regarding the optimization of the performance in the thermoelectric material series containing  $\text{Mg}_3\text{Bi}_2$  and help to shed light on factors like synthesis methods and elemental doping used for the tailoring of their electrical properties [75].

#### 4.4 Computational methods

Advances in computational methods have revolutionized the field of thermoelectric materials by enabling researchers to predict and design new materials with targeted properties. Quantum mechanical calculations, density functional theory (DFT), and high-throughput screening methodologies facilitate the exploration of vast material databases, accelerating the discovery of novel thermoelectric candidates. Computational tools It is now possible to predict and design new thermoelectric materials, thanks to advances in computational methods. Such efforts include quantum mechanical calculations, density functional theory, and high-throughput screening methodologies that allow for huge material databases to be mined quickly



and easily for a variety of thermoelectric candidates. The computationally determined electronic structure and bandgap engineering are helpful in developing phonon properties of materials that will turn out to be guiding experiments toward the synthesis of the best possible materials. What has happened, in view of this synergy of experimental and computational approaches, is a radical contraction of the cycle of development for materials and an expanded range of their application in the domain of thermoelectricity. Furthermore, these CFD tools prove exceedingly useful for researchers, designers, engineers, and analysts since they provide a view that assists in early decision-making, thereby saving much valuable engineering design process time [76]. On the other hand, Rodrigo et al.'s study explores the potential of novel silicide-tetrahedrite modules for energy generation. In the research, performance studies were carefully made on thermoelectric generators using computer simulations via the finite element method and the implicit finite difference method. For the verification of their computational models, the team uses validation against data measured on a specifically designed system working with commercial TE devices. It is found that high predictive capability is obtained with the developed models, with deviations of  $\leq 10\%$ . The implicit finite difference method (IFDM) analyzes the power performance developed by the silicide-tetrahedrite TEGs under different temperature differentials  $\Delta T$ , while the finite element method (FEM) [77] gives a detailed investigation of temperature distributions within the test system. This work thus shows the role computational modeling can play in understanding the behavior of new thermoelectric materials and proves the reliability of developed models in predicting the performance of TEGs [78]. Except for this, the search for identifying new high-performance TE materials that are economical and environmentally friendly remains a pressing task for the Thermoelectric society. However, the advancement in this task has been considerably exacerbated by the conventional trial-and-error approach being tedious and expensive. In fact, the field of TE materials research is now in the midst of a transformative change due to remarkable progress in the hardware of computers, efficient methods of computation, advanced artificial intelligence algorithms, and exponential growth in material data. Upon this paradigm shift, innovative strategies are built to transcend these limitations. A number of electrical and thermal performance descriptors for new materials have been advocated, accompanied by the creation of efficient high-throughput (HTP) calculation methods. The high-throughput methods, hence, allow the rapid screening of potential TE materials from large material databases. Moreover, a few HTP experiments using doped systems have been devised to gain a larger density of information in a single experiment, thus reducing the time and cost involved. In addition, the inclusion of machine learning (ML) methods in thermoelectrics has added to newer dimensions. The previous sections in this review present a description of the HTP strategies used in discovery processes in general, performance descriptors applications, HTP calculations, HTP experiments, and ML. Moreover, it highlights the challenges of using this area and explores the possible directions of future research [79].

On the other hand, Tiriyaki and coworkers have examined novel techniques for characterizing high-performance thermoelectric materials, specifically p-type  $\text{Sb}_x\text{Bi}_y\text{Ba}_z\text{B}_t\text{Yb}_w\text{Te}_3$  and n-type  $\text{Bi}_x\text{Ba}_y\text{B}_z\text{Yb}_t\text{Te}_3$ -based thermoelectric alloys. Two different cases of n-type  $\text{Bi}_{2-x}\text{Te}_3$  and p-type  $\text{Sb}_{1.5}\text{Bi}_{0.5-x}\text{Te}_3$  will be presented, where in all cases,  $x$  varies from 0 to 0.5 for Ba, B, and Yb, respectively, when tools for measuring electrical and thermal conductivity are not available. First, the experimental data at different temperatures for different compositions of these alloys were obtained. Then, training was performed using 26 machine-learning algorithms. More importantly,



some compounds' transport properties, like the p-type  $\text{Sb}_{1.5}\text{Bi}_{0.2}\text{B}_{0.3}\text{Te}_3$  and n-type  $\text{Bi}_{1.9}\text{Ba}_{0.1}\text{Te}_3$ , have been predicted only using the best ML algorithm. The predictive analysis is divided into two cases: case 1, in which only the Seebeck coefficient and electrical resistivity are forecasted, and case 2, for which heat capacity values  $C_p$  and thermal diffusivity were predicted. Both cases are under identical experimental conditions, classified just due to the availability of particular measuring equipment for thermoelectricity. Case 1 refers to situations in which the Seebeck coefficient and electrical resistivity-measuring device is not available and need an ML-driven prediction. Similarly, case 2 corresponds to the situation wherein the device measuring heat capacity and thermal diffusivity is not available and is in need of an ML-driven prediction. More importantly, as shown in this work, the challenge of the variation in the scales of the data during the training and test phases is addressed by normalization techniques [80].

Put another way, a rapidly expanding influence from computational approaches unites traditional methods of alloying and nanostructuring with doping, offering a potent toolkit for improving thermoelectric performance. When combined, these approaches are pushing thermoelectric materials toward increased efficiency and broader applications. Recently, researchers have demonstrated that integrating theoretical approaches with numerical computations for the Matrix Transfer Method can lead to the development of metamaterial structures. Ultimately, they successfully combined this structure with a thermoelectric conductive polymer to create a hybrid energy harvesting device [77].

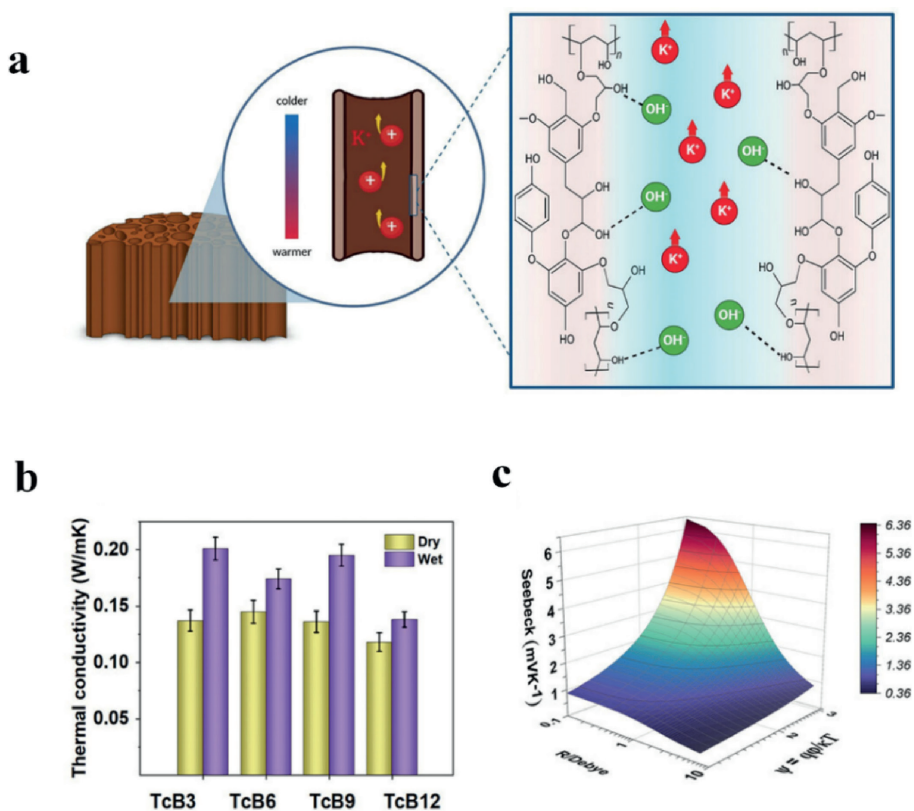
## 5. Applications

In this section, we try to show recent applications of thermoelectric materials. Here, we show in an ionic system, lignin-like sustainable material can be used to make a conductive membrane that can generate valuable Seebeck voltage. Also, it is interesting to discuss hybrid energy thermoelectric devices that combine metamaterial structure and organic conductive polymer. Furthermore, we demonstrate how thermoelectric technology can be scientifically combined with electrical generator technology in space to mitigate global warming. Finally, we explore the applications of thermoelectric materials in the automotive and sensor industries.

### 5.1 Lignin-derived ionic conducting membranes

In recent research, the ionic thermoelectric properties of lignin-derived membranes were investigated in the low-temperature heating zone. Membranes infused with aqueous KOH electrolyte were evaluated for ionic conductivity and Seebeck coefficients. The selective ion transport mechanism, thermal ion diffusion, and intermolecular bonding were illustrated, with phenolic groups on lignin surfaces converting into anionic alkoxides upon KOH immersion. This transformation induced negatively charged channels that attracted  $\text{K}^+$ , forming an electric double layer (EDL) and facilitating selective ion diffusion. The membranes demonstrated an ionic Seebeck coefficient of up to  $5.7 \pm 0.4 \text{ mV K}^{-1}$ , attributed to increased lignin content enhancing nanochannel dominance and thermoelectric diffusion efficiency [8].

According to **Figure 2**, thermal conductivity was measured in both dry and wet membranes. Dry membranes exhibited low thermal conductivity ( $0.10\text{--}0.14 \text{ W m}^{-1}\cdot\text{K}^{-1}$ ), while KOH infiltration increased conductivity to



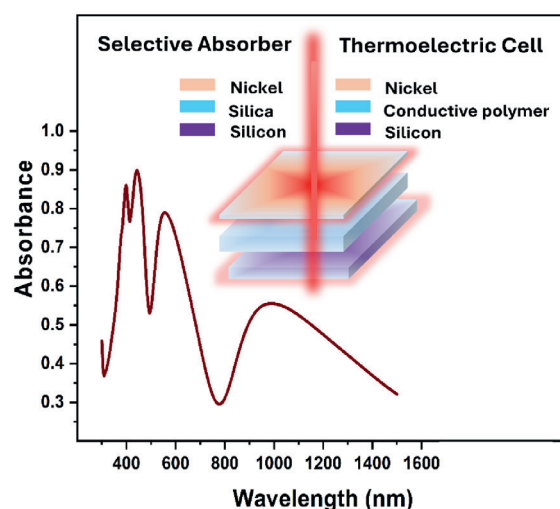
**Figure 2.**

(a) Schematic representation of selective ion diffusion within the channels of lignin-derived ionic conducting membranes, and ionic thermoelectric performance of synthesized membranes in terms of (b) thermal conductivity, and (c) estimated ionic Seebeck value in lignin-derived membranes (parallel) at channel radii and EDL potential. Reproduced with permission [8] (Copyright 2023, Wiley-VCH).

0.17–0.20  $W m^{-1} K^{-1}$  due to water uptake. Numerical modeling further confirmed that narrower channel radii and higher EDL potentials optimized the ionic Seebeck effect. Enhanced lignin content increased functional group ionization, leading to higher EDL potentials and thermopower. However, the experimental thermopower (5.71  $mV K^{-1}$ ) fell slightly below the modeled maximum (6.36  $mV K^{-1}$ ) due to channel size variation and tortuosity in real samples. These findings validate the potential of lignin membranes for efficient thermoelectric applications [8].

## 5.2 Integration of organic thermoelectric materials with metamaterial structures

**Figure 3** shows that enhancing light absorption is crucial for advancing solar thermoelectric generators. Conventional light absorbers often rely on a back mirror, typically a thick metal film, to minimize reflectivity by facilitating interference between incident and reflected light. However, such continuous metal films pose a challenge for thermoelectric applications as they can short-circuit the Seebeck voltage. Recently, researchers introduced a back mirror-free selective light absorber tailored for thermoelectric devices. The design optimizes the combination of materials with high and low refractive indices coated with a semi-transparent electrode. Unlike a back mirror, the semi-transparent electrode can be patterned to preserve

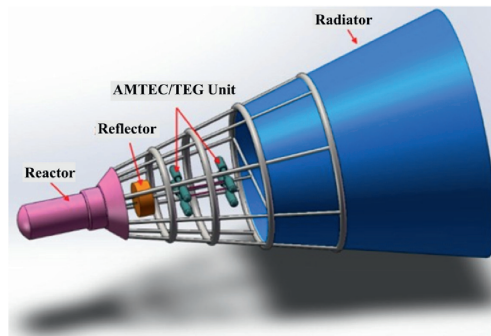


**Figure 3.**  
 An illustration of the integration of thermoelectric materials with metamaterial structures [77]. (Copyright 2024, Advanced Optical Materials).

the Seebeck voltage. This approach also allows the low-refractive-index material to be substituted with a transparent thermoelectric material, enabling efficient heat-to-energy conversion without compromising absorption performance [77]. The researchers show a back mirror-free selective absorber for thermoelectric applications has been numerically simulated and experimentally realized. Designed with layers of nickel, silica, and silicon on a transparent substrate, the structure has demonstrated scalable fabrication potential. By eliminating the back mirror, improved thermoelectric performance has been achieved, along with greater tolerance to fabrication parameter variations, such as layer thickness or refractive index. The silica layer has been replaced in some cases with a transparent thermoelectric polymer (conductive PEDOT: PSS) for light-to-electricity applications. Devices fabricated in this way have shown over 60% absorption and a Seebeck coefficient exceeding  $22 \mu\text{VK}^{-2}$ , paving the way for innovative combined thermoelectric-photovoltaic.

### 5.3 Space exploration

For decades, thermoelectric materials have played an important role in space exploration. Inherent in these materials is the ability to power long-duration missions and deep-space probes with radioisotope thermoelectric generators at the core of space exploration. RTGs convert heat emanating from radioactive isotopes into electric power. The technology has been used since the Voyager, Cassini, and Mars rovers [82]. Xinyu Miao et al. present a coupling system integrating alkali metal thermoelectric converter (AMTEC), TEG, and microwave power transmission (MPT) subsystems to enhance thermoelectric efficiency in rovers and lunar bases by recycling AMTEC's waste heat (**Figure 4**). Thermodynamic analyses reveal that AMTEC primarily determines system performance, with output power and efficiency varying by key parameters ( $J$ ,  $i$ , and heat exchange area). The combined system achieves maximum efficiency at 37% under optimal conditions, suggesting potential for efficient, low-cost, high-power spacecraft applications in space exploration [81].



**Figure 4.** Nuclear space power stations (NSPS) with unit alkali metal thermoelectric converter (AMTEC) with TEG combined unit. Reproduced with permission [81] (Copyright 2024, Journal of Annals of Nuclear Energy).

## 5.4 Automotive and sensor industry

In the automotive sector, high-efficiency thermoelectric materials apply to more than just waste heat recovery. First, they can be used in advanced cooling systems to improve the efficiency of temperature control in e-vehicles and traditional combustion engine vehicles. Second, the thermoelectric modules in hybrid vehicles capture and turn into electricity part of the energy wasted as heat through the exhaust system, thereby contributing to total energy efficiency. Kim et al. developed a fiber-shaped thermoelectric temperature sensor tailored for advanced wearable applications. This sensor utilizes a continuous graphene fiber with two halves in distinct reduction states, achieved by treating each half with hydroiodic acid (HI) at different concentrations. The differing reduction levels create a seamless junction with varied Seebeck coefficients, enabling thermoelectric functionality. This flexible graphene thermocouple demonstrates high sensitivity ( $12.5 \mu\text{V/K}$ ), linearity, and fast response time (0.24 s), making it suitable for integration into wearable textiles, like gloves, without needing external power [83].

## 6. Challenges and future directions

Several challenges still remain, and future directions beckon toward more efficient, cost-effective, and far-reaching applications as high-performance thermoelectric materials continue in the process of evolution. Addressing these challenges is very critical to unlocking the full potential of thermoelectric technology.

### 6.1 Challenges and future

#### 6.1.1 Challenges

In this section, it was highlighted the challenging points for researchers that need to be addressed to advance the development of thermoelectric materials and their applications. In order to advance the thermoelectric industry, factors such as cost and scalability, efficiency, operating temperature range, and environmental protection are crucial to address.

#### *6.1.1.1 Cost and scalability*

One of the primary challenges lies in the cost of manufacturing and scalability of high-performance thermoelectric materials [73]. Many of the materials with superior thermoelectric properties, such as certain rare or toxic elements, can be expensive and hinder large-scale deployment. Finding cost-effective alternatives without compromising performance is a critical challenge.

#### *6.1.1.2 Efficiency trade-offs*

Traditional thermoelectric materials often face a trade-off between electrical conductivity and thermal conductivity. Enhancing one property tends to negatively impact the other, limiting the overall efficiency of the material. Striking the right balance and overcoming this trade-off is an ongoing challenge in material design [84].

#### *6.1.1.3 Temperature range*

Many thermoelectric materials exhibit optimal performance only within specific temperature ranges. This limitation hinders their applicability in environments with fluctuating or extreme temperatures. Developing materials that maintain high performance across a broader temperature spectrum is a challenge for achieving versatility in applications [85].

#### *6.1.1.4 Environmental impact*

A few high-efficiency thermoelectric materials may include elements that are environmentally sensitive or might have a possible negative impact on the environment during mining and manufacturing. The sustainability of thermoelectric materials to the environment remains the latest concern [86].

### *6.1.2 Future*

#### *6.1.2.1 Future directions*

**Materials Discovery and Design:** Improvements in the area of computational methods, using machine learning and artificial intelligence, open up exciting avenues for the accelerated discovery and design of new thermoelectric materials. High-throughput simulations and predictive modeling guide researchers toward the identification of materials with optimal properties and reduce the time and resources required for experimental exploration [87].

#### *6.1.2.2 Multidisciplinary approaches*

In this respect, if the challenges that now exist are to be surmounted, it will be incumbent upon at least some diversified fields of disciplines, such as materials science, physics, chemistry, and engineering. It is expected that multidisciplinary study may awaken creativity and facilitate an understanding of the complex interactions among multiple factors that influence thermoelectric performance [77].

#### *6.1.2.3 Flexible and stretchable thermoelectric materials*

With the rising demand for wearable devices and flexible electronics, the development of thermoelectric materials that are not only efficient but also flexible and stretchable is a promising avenue. Such materials could open up new possibilities for energy harvesting in unconventional settings [88].

#### *6.1.2.4 Nanostructured and 2D materials*

By adjusting electrical and thermal transport characteristics at the nanoscale, more studies in nanostructured materials such as nanowires and 2D materials such as graphene, could help overcome efficiency trade-offs. These materials present special chances to customize thermoelectric performance [89].

#### *6.1.2.5 Hybrid and composite materials*

Investigating hybrid and composite materials, which combine the best features of several material classes, may have a positive feedback loop and enhance overall performance. This strategy might lessen the difficulties brought on by personal material constraints [90].

#### *6.1.2.6 Real-world integration*

One of the most important future directions is to close the gap between laboratory-scale demonstrations and real-world implementations. Incorporating thermoelectric materials into useful devices, systems, and infrastructure necessitates taking technical and financial concerns into account in addition to material obstacles [91].

In conclusion, although the creation and use of high-performance thermoelectric materials have not yet been successful and are really difficult to execute, continuous efforts have opened up new ways for research and development. Potential applications of thermoelectric technology can create tremendous changes in energy harvesting, waste heat recovery, and the use of widely available, environmentally friendly materials. Thermoelectric materials present an exciting pathway for sustainable energy solutions, offering opportunities for energy harvesting and waste heat recovery. However, challenges such as cost, efficiency trade-offs, environmental impact, and scalability remain significant barriers. Addressing these hurdles requires advancements in computational design, multidisciplinary collaborations, and the exploration of nanostructured, hybrid, and flexible materials. Looking ahead, the integration of thermoelectric technology into real-world applications holds transformative potential, driving innovations in energy systems and contributing to a greener, more sustainable future.

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## Conflict of interest

The authors declare no conflict of interest.

## Nomenclature

$\alpha_n$	Seebeck coefficient for electrons	$VK^{-1}$
$E$	electric field	$Vm^{-1}$
$\nabla T$	temperature gradient	$Km^{-1}$
$S$	Seebeck coefficient	$VK^{-1}$
$k_B$	Boltzmann constant	$1.38 \times 10^{-23} JK^{-1}$
$e$	elementary charge	$1.602 \times 10^{-19} C$
$\sigma(E)$	energy-dependent electrical conductivity	$Sm^{-1}$
$\sigma$	total electrical conductivity	$Sm^{-1}$
$T$	absolute temperature	$K$
$E_F$	fermi level energy	$eV$
$E_v$	valence band edge energy	$eV$
$zT$	thermoelectric figure of merit	Dimensionless
$\kappa$	thermal conductivity	$Wm^{-1}.K^{-1}$
$\kappa_L$	lattice thermal conductivity	$Wm^{-1}.K^{-1}$
$K_e$	electronic thermal conductivity	$Wm^{-1}.K^{-1}$
$PF$	power factor	$Wm^{-1}.K^{-2}$
$L$	Lorenz factor	$2.44 \times 10^{-8} W\Omega K^{-2}$
$n$	charge carrier density	$m^{-3}$
$\mu_c$	charge carrier mobility	$m^2V^{-1}.s^{-1}$
$q_h$	rate of heat flow from hot to cold section	$W$
$P_0$	electrical power output	$W$
$\eta$	thermoelectric conversion efficiency	Dimensionless
$\eta_C$	Carnot efficiency	Dimensionless
$T_H$	hot-side temperature	$K$
$T_C$	cold side temperature	$K$

Nomenclature: Key terms and symbols in advanced thermoelectric materials.

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