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Introduction to advances in emerging thermoelectric materials and devices

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Due to the growing global energy demand and the increasing adoption of sustainable and clean energy solutions, research in thermoelectric generators (TEGs) has intensified, leading to the development of novel materials that are earth-abundant, non-toxic, and produced at low cost. The direct conversion of heat into electricity is enabled by thermoelectric materials, which have gained significant attention because of their potential for clean energy harvesting. TEGs have recently gained popularity mainly due to their simple device structure and operation, being lightweight, noise-free and solid-state (there is no ongoing maintenance as there are no moving parts), and the possibility to integrate them with various devices that produce heat as a by-product. The performance of TEGs is determined by the dimensionless thermoelectric figure of merit (*ZT*). Organic and hybrid thermoelectric materials are becoming increasingly popular because of their flexibility and low cost of production in the near future. These materials are being explored due to the huge demand for sustainability using self-powered devices for applications in wearable electronics and IOT devices.[1] Currently, ample research activities are ongoing to improve the properties of

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TEGs. Some of the strategies used to achieve high-performance TEGs include the use of quantum-confinement effects, point-defect engineering, exploration of nanocomposite materials, synthesis of 2D composite materials, controlling carrier effective mass, and doping. It is important to mention that the commercially and most widely used TEG material is Bi_2Te_3 due to its excellent thermoelectric properties at room temperature. Other emerging and experimentally studied materials include lead telluride (PbTe) (ZT = 1.0–2.0), silicon–germanium (Si–Ge) (ZT = 0.5 to 1.5), skutterudites (*e.g.*, $CoSb_3$) (ZT = 1.5 to 2), half–Heusler compounds (ZT 0.5 to 1.5), and tin selenide (SnSe) (ZT = 2.0 to 2.6).[2,3] In the power generation mode, these materials are used in automotive waste-heat recovery, industrial power generation, deep-space probes, high-temperature power generation, and space power generation (*e.g.*, NASA radioisotope thermoelectric generators (RTGs)). TEGs are also proposed for thermal management (refrigeration, cooling, and thermal switching) in batteries, high-power electronics, and medical devices. Although there have been many advancements, challenges remain in enhancing the ZT of non-conventional and non-toxic materials to levels suitable for widespread commercial applications that need to be implemented at room temperature. Ongoing research focuses on strategies such as nano-structuring, band engineering, alternative novel compound materials, 2D layered materials, and the development of hybrid materials to overcome current challenges posed by commonly used bulk thermoelectric materials. In contrast, recently, silicon and silicon-based compounds have gained huge interest in the thermoelectric community. For example, SiGe Thermagy modules are already available for commercial use.[3] Nanostructured silicon has shown ZT = 0.3.[4] In comparison, silicon nanowires have shown a 100-fold decrease in thermal conductivity as compared to the bulk silicon, with ZT = 0.6 at room temperature.[5] A newly synthesized silicon allotrope, Si_{24}, features an intrinsic nanoscale porous structure that effectively hinders heat conduction while maintaining electrical conductivity.[6] In addition, authors have proposed a practical solution to further reduce the thermal conductivity of Si_{24} without hindering the electric conductivity (this is the most important criterion for obtaining high ZT) by adding guest atoms of specific size exactly within the pores. Silicon nanocomposites with hierarchical structures, including nanograins, nanopores, and metal nanoprecipitates, have shown $ZT > 0.3$ at room temperature.[7] 2D materials are also contenders for thermoelectric materials due to their unique properties that are best suited for thermoelectricity. Some of their advances will be mentioned later in this editorial. This themed collection has covered the most recent progress in the

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synthesis, preparation, characterisation, simulations, and properties of emerging thermoelectric materials to reflect the need for these materials to be further explored and used in TEGs for clean energy applications, especially in converting waste heat to electricity at higher efficiency.

With the emerging exploration of 2D materials, borophene has gained huge interest due to its higher strength-to-weight ratio. Bilayer β_{12}-phase borophene has demonstrated superior thermoelectric properties that have been theoretically studied for borophene on a Cu(111) substrate, thus demonstrating its application as an efficient heat-energy converter. In this study, authors have concluded that the Cu(111) substrate is more suitable compared to Ag(111) for wide range and high temperatures (https://doi.org/10.1039/D3MA01121F). Another dominant and widely explored 2D material is graphene, which is a suitable material for various applications including thermoelectric devices. A recent article has adapted the well-established Su–Schrieffer–Heeger (SSH) model Hamiltonian to study the thermal effects on graphene nanoribbons (GNRs). Simulations carried out at 0 K indicate that the bipolarons are stable, and interestingly 50% (approximately) of the ensemble states contain stable polarons at higher temperatures. This study indicates that the next generation of thermoelectric devices should be able to manage and control the number and movement of charge carriers to obtain more efficient TEGs (https://doi.org/10.1039/D3MA01181J).

Simulations based on density functional theory (DFT) have shown a *ZT* value of approximately 1.01 for $K_2GeMnCl_6$, 1.00 for $K_2GeMnBr_6$, and 0.99 for K_2GeMnI_6 at room temperature. The *ZT* values determined using these materials are due to their ultra-low thermal conductivity. Thus, halide double perovskites K_2GeMnX_6 (X = Cl, Br, I) exhibit promising ferromagnetic and thermoelectric properties, making them suitable candidates for semiconductor spintronics and thermoelectric applications (https://doi.org/10.1039/D3MA01160G). Although double-perovskite halides have shown good power conversion efficiency in solar cells, recently they have been studied to find their suitability in thermoelectric applications. Density functional theory (DFT) simulations of these halides (A_2YAuI_6 (A = Rb, Cs)) have demonstrated potential use in thermoelectric applications with *ZT* values being very close to "1". These compounds thus provide some insights to the experimental community to unfurl the research with these ionic compounds for applications in thermoelectricity (https://doi.org/10.1039/D4MA00090K). First-principles DFT calculations and Boltzmann transport theory were applied to study the effect of iodine monochloride (ICI) doping in single-wall carbon nanotube (SWCNT) networks. Doping has significantly enhanced the thermoelectric power factor of SWCNT networks, with an increase from 0.28 to 2.4 mW m^{-1} K^{-2}. This study clearly indicated that the ICI intercalation and filling in SWCNTs effectively improve the thermoelectric properties (https://doi.org/10.1039/D4MA00319E). An experimental study on a 60-nm-thick crystalline silicon fabricated using a silicon-on-insulator substrate showed a significant reduction in thermal conductivity (up to 88% compared to bulk Si and 42% compared to plain Si membranes) at room temperature. Importantly, a *ZT* of 0.04 is shown on the Si membrane, which is considerably higher than that of bulk Si (*ZT* = 0.001) (https://doi.org/10.1039/D4MA00095A). The growth of a p-type $CuSbSe_2$ single crystal with the vertical Bridgman technique resulted in excellent thermoelectric and optoelectronic properties, making it a promising material for renewable energy applications. This material showed a *ZT* value of ≈ 0.976 and a power factor of 0.00672 μW cm^{-1} K^{-2} at 543 K. Hence, it is worth mentioning that $CuSbSe_2$ single crystals will be a promising contender amongst the new generation of thermoelectric materials (https://doi.org/10.1039/D4MA00298A). Another study has interestingly shown that dual substitutions could hinder the thermoelectric properties as compared to single substitution of atoms in Yb_4Sb_3. A La and Bi co-substituted Yb_4Sb_3 compound was synthesised and a detailed investigation of the transport properties concluded that the substituted compounds exhibited similar Seebeck coefficients to the pristine material, but their resistivity significantly increased. This further prevented improvement in the *ZT* and a maximum value of 0.5 was measured at 1273 K for the parent and co-substituted Yb_4Sb_3 compounds. Thus, it is clear that more work is required to further understand and optimise this material before adapting it for TEG devices (https://doi.org/10.1039/D3MA00903C). Recent exploration of thermoelectric materials based on relatively earth-abundant and nontoxic raw materials has emerged with a new compound, argyrodite (Ag_8SiSe_6). This material was studied in more detail for the first time and has exhibited n-type thermoelectric performance at room temperature. Currently, this material is highly sensitive to its cooling history, hence precise control over synthesis conditions is important to achieve good thermoelectric properties. Quenching conditions were optimised, and a notable enhancement in *ZT* value was observed and exceeded 0.7. This material further promises a better alternative to conventionally used Bi_2Te_3-based compounds that are used for room-temperature TEG applications (https://doi.org/10.1039/D3MA01190A).

In summary, it is very clear that researchers are exploring various nanostructuring materials and moving away from commonly used bulk materials for thermoelectric applications. All the efforts are focused towards improving the Seebeck coefficient and reducing the thermal conductivity, thus leading to higher *ZT* values for making highly efficient TEGs. At the nanoscale, these materials exhibit reduced thermal conductivity, hindered heat conduction, increased phonon boundary scattering, and reduced phonon mean free paths. Considering sustainability, toxicity, and earth abundance, nanostructured silicon and germanium are the next promising materials for high-efficiency thermoelectric materials. This themed collection features the latest research on new and novel thermoelectric materials and their uses in thermoelectric generators (TEGs) for energy harvesting applications. It

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covers novel thermoelectric materials for TEGs, advanced synthesis, processing, and characterisation techniques for thermoelectric materials, as outlined above.

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