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Editorial

Advances in Thermoelectric Materials—Bridging the Gap Between Discovery and Application

Marco Fronzi [1,*], Paolo Mele [2,*] and Giovanna Latronico [3]

[1] School of Physics, The University of Sydney, Sydney NSW 2050, Australia
[2] College of Engineering, Shibaura Institute of Technology, Saitama 337-8570, Japan
[3] National Research Council of Italy Institute of Condensed Matter Chemistry and Technologies for Energy (CNR-ICMATE), Via G. Previati 1/E, 23900 Lecco, Italy; giovannalatronico@cnr.it
* Correspondence: marco.fronzi@sydney.edu.au (M.F.); pmele@shibaura-it.ac.jp (P.M.)

Thermoelectric materials have gained considerable attention in recent years due to their ability to directly convert heat into electricity, making them a key focus in the development of sustainable energy technologies [1–3]. As global energy demands increase, and the need for alternative energy sources becomes more pressing, thermoelectric systems offer a viable opportunity to harvest energy from waste heat, which would otherwise be lost to the environment [4–6]. This capability positions them as potential contributors to energy efficiency in a wide range of industries, from automotive applications to power plants and consumer electronics [7–9]. The research progress in this field, however, is not only contributing to energy efficiency, but also addresses environmental sustainability by developing novel non-toxic materials and improving the lifespan and stability of technological devices [10].

This Special Issue of *Inorganics*, titled "Recent Advances in Thermoelectric Materials", brings together some pioneering papers that cover a broad spectrum of topics in the field, showcasing advancements in both theoretical frameworks and experimental techniques. The research featured in this issue not only focuses on enhancing the thermoelectric figure of merit (zT), but also emphasizes the scalability, environmental impact, and potential real-world applications of these materials.

One of the most significant contributions comes from the work of František Mihok et al., who explore the effects of multiple doping elements on the polarity switching of polycrystalline SnSe, a promising material for thermoelectric applications [11]. Their research shows that doping SnSe with elements such as Sb, Bi, Ag, Ni, In, and Mg can effectively alter its polarity. Of particular note is the impact of Bi doping, which induces polarity switching similar to that observed in monocrystalline Sb. Additionally, doping is shown to significantly boost the Seebeck coefficient, a key parameter for thermoelectric efficiency. The authors also developed an in-house apparatus for measuring the Seebeck coefficient, which not only offers practical value, but also enhances the understanding of how doping impacts thermoelectric performance, paving the way for further innovations in material design.

Building on the theme of advancing material properties, Sara Ghomi et al. introduce a novel method for the large-area growth of silver and gold telluride ultrathin films via chemical vapor tellurization [12]. This work is fundamental for nanotechnological applications, where the structural and electronic properties of these films are crucial. The study shows how these ultrathin telluride films hold the potential for thermoelectric and other technological uses due to their morphological characteristics, which were comprehensively analyzed using advanced characterization techniques. By establishing a scalable method for producing these materials, the authors contribute significantly to the broader goal of optimizing noble metal tellurides for future applications.

The integration of machine learning with traditional computational techniques is another exciting frontier in thermoelectric research, as suggested by the work of Kaja Bilińska and Maciej J. Winiarski [13]. Their study employs support vector regression models to predict critical thermoelectric properties of 18-electron half-Heusler phases, including lattice

Citation: Fronzi, M.; Mele, P.; Latronico, G. Advances in Thermoelectric Materials—Bridging the Gap Between Discovery and Application. *Inorganics* **2024**, *12*, 285. https://doi.org/10.3390/inorganics12110285

Received: 11 October 2024
Accepted: 23 October 2024
Published: 31 October 2024

parameters, bulk moduli, band gaps, and thermal conductivity. By combining machine learning with density functional theory (DFT), the authors are able to accelerate the discovery of new thermoelectric materials, providing a powerful tool for researchers seeking to optimize the performance of these materials. Their predictions offer promising insights that could streamline the process of identifying high-efficiency thermoelectric compounds.

Muhammad Isram et al. further contribute to this Special Issue by focusing on the thermoelectric performance of Fe-doped ZnSe nanoparticles, synthesized through the hydrothermal method [14]. Their study highlights how varying concentrations of Fe doping can significantly improve the thermoelectric properties of ZnSe, with power factors reaching as high as 9×10^{-3} W m^{-1} K^{-2} at 150 °C. The findings suggest that Fe-doped ZnSe nanoparticles are not only promising for thermoelectric applications, but also adaptable for performance optimization at elevated temperatures, expanding the potential uses of these materials in real-world applications.

The synthesis and crystal structures of Zintl phases are explored by Bayram Saparov and Svilen Bobev, who report on $Na_2CaCdSb_2$, $Na_2SrCdSb_2$, and $Na_2EuCdSb_2$. These materials exhibit layered structures with the potential for thermoelectric applications [15]. Through single-crystal X-ray diffraction, the study reveals the non-centrosymmetric structures of these compounds, characterized by $[CdSb_2]^{4-}$ layers. Additionally, the possibility of cation disorder in these structures is noted, contributing valuable structural insights that could inform future thermoelectric material design. Their work lays the groundwork for exploring the thermoelectric potential of these unique Zintl phases.

The exploration of cost-effective thermoelectric materials continues with the work of Ioanna Ioannou et al., who examine the effect of Hf/Zr substitution in mechanically alloyed (Hf,Ti)CoSb half-Heusler solid solutions [16]. Their research shows that reducing Hf content through Zr substitution lowers the material costs without significantly compromising the performance. Furthermore, the fine-tuning of the carrier concentration by substituting Sb with Sn leads to a high zT value of 0.77 at 960 K, demonstrating the potential of these materials for practical thermoelectric applications, especially in high-temperature environments.

Finally, Chengyu Zhao et al. provide a comprehensive review of the preparation methods for skutterudite-based thermoelectric materials [17]. Known for their excellent electrical transport properties at medium temperatures, skutterudites have garnered attention for applications in waste heat recovery and refrigeration. This review covers both the traditional and advanced preparation methods, offering insights into the rapid, low-cost, and large-scale production of high-performance thermoelectric materials, which is critical for their industrial scalability.

Together, these studies offer a broad and integrated view of the latest advances in thermoelectric materials, addressing both fundamental research challenges and practical applications. The contributions featured in this Special Issue push the field forward, offering new strategies for optimizing material properties, lowering costs, and scaling production, all of which are essential for realizing the full potential of thermoelectric technologies in addressing global energy challenges.

As the guest editors of this Special Issue, we are proud to present this collection of pioneering work. The diversity of approaches, from nanoscale engineering and machine learning to flexible devices and environmentally friendly materials, highlights the breadth of innovation in thermoelectric research today. We trust that these contributions will inspire continued advancements and serve as a valuable resource for scientists dedicated to solving the energy challenges of tomorrow.

Conflicts of Interest: The author declares no conflict of interest related to this publication.

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