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Special Topic: Thermoelectric Materials and Devices

Advancing thermoelectrics: From microstructures to applications

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Mitigating the forthcoming energy crisis necessitates extensive research and investment in sustainable, low-carbon energy alternatives. As a key sustainable energy solution, thermoelectric materials enable direct heat-to-electricity conversion, enhancing waste heat recovery and solid-state refrigeration efficiency. These semiconductor-based systems offer a promising path to alleviate energy challenges while simultaneously mitigating CO_2 emissions through cleaner energy utilization.

The merits of thermoelectric conversion lie in the solid-state operation, gas-free emissions, without any moving parts and chemical reactions, environmental friendliness, long-term durability with minimal maintenance, and wide applicability. The widespread application of thermoelectric technologies is fundamentally determined by the development of advanced materials with superior energy conversion efficiency and cooling performance, which is governed by the dimensionless figure of merit zT, defined as $zT=S^2\sigma T/\kappa_{\mathrm{tot}}$, where S, σ, and T are the Seebeck coefficient, the electrical conductivity, and the absolute temperature, respectively, κ_{tot} is the total thermal conductivity that is composed of electronic (κ_e) and lattice (κ_L) contributions.

To show recent advancement in thermoelectric materials and devices from microstructures to applications, we have organized a Special Topic on Thermoelectric Materials and Devices in *National Science Open* (NSO). This special topic includes eight representative reviews and articles, showcasing cutting-edge research in characterization techniques, novel materials for both power generation and cooling, with top-up mechanical flexibility.

A fundamental challenge in thermoelectrics lies in deciphering the nanoscale mechanisms governing defect behavior and carrier transport, as well as mechanical properties. Nan *et al*. [1] demonstrated the pivotal role of transmission electron microscopy (TEM), leveraging high-energy resolution electron energy loss spectroscopy (EELS) to analyze defect phonon dispersion relations, low dose or low temperature techniques to characterize beam-sensitive materials such as Ag_2S and Ag_2Se, and *in situ* TEM measurements integrated with micro-electrochemical systems to enable atomic-scale correlation of microstructure and performance. Building upon these experimental advances, Zeng *et al*. [2] summarized the theoretical frameworks of

Wigner transport equation (WTE) and quasi-harmonic Green-Kubo (QHGK) theory to model phonon behavior in both crystalline and amorphous systems. Their work elucidates how atomic disorder and crystal symmetry govern lattice thermal conductivity, providing a theoretical foundation for designing materials with intentionally suppressed heat transport via controlled defect scattering.

Material innovation emerges as a cornerstone of progress, with studies showcasing breakthroughs in both inorganic and organic systems. Chen *et al*. [3] reported a landmark achievement in diamondoid Cu_2SnSe_3, where Cd doping triggers a monoclinic-to-cubic structural transition, enhancing carrier mobility by 85%, and Ag off-centering effect reduces lattice thermal conductivity to an extremely low value of 0.3 W m^{-1} K^{-1}. This synergy yields a high zT of 1.3 at 800 K, showcasing how crystal symmetry and atomic off-centering behavior can decouple electrical and thermal transport.

For lower temperature applications, Zhu's group [4] summarized advanced strategies to enhance thermoelectric cooling performance, addressing the limitation of conventional Peltier-effect materials whose zT decreases with temperature. It highlights two key approaches: magneto-enhanced Peltier effects in Bi-Sb alloys and topological semimetals, Ettingshausen effect in semimetals for transverse heat transport, enabling theoretical cooling to 60 K. This is critical for enabling efficient cooling in infrared detectors and cryogenic electronics. Meanwhile, Ma *et al*. [5] demonstrated unipolar performance in bipolar polymers ($FeCl_3$-doped PDPP4T films) by separating electron and hole contributions via the transverse thermoelectric effects, revealing ultrahigh thermopower at low temperatures and expanding the application potential of organic materials in cold environments.

Flexibility and mechanical robustness are paramount for deploying thermoelectrics in wearable and miniaturized devices. Chen *et al*. [6] reported $Ag_2Se_{1-x}Te_x$ alloys exhibiting robust mechanical properties combined with competitive thermoelectric performance (zT=1.1 at 380 K). They revealed that the remarkable mechanical properties originate from the dense dislocations and possible sub-grain rotations. Furthermore, Shen *et al*. [7] comprehensively dissected elastic thermoelectric generators based on hot-rolled Ag_2Se and $Ag_2Se_{1-x}S_x$, achieving recoverable bendability (withstanding 10^6 bending cycles) and high strength via dislocation engineering and grain refinement. These materials maintain high power factors, effectively overcoming the intrinsic brittleness of traditional inorganics and paving the way for wearable electronics. In $Bi_{0.5}Sb_{1.5}Te_3$ thin films, Qu *et al*. [8] demonstrated that optimized magnetron sputtering parameters and annealing process induce strong (00l) preferential orientation. This crystallographic control significantly enhances in-plane carrier transport, enabling a record-high zT of 1.49 at room temperature. Their work underscores the critical role of texture engineering and defect configuration optimization in thin-film thermoelectrics.

Collectively, these studies illustrate the interdisciplinary nature of thermoelectric research, where progress in microscopy characterization, theoretical modeling, material synthesis/optimization, device fabrication with mechanical strengthening, and working mode involving transverse thermoelectric effects have addressed long-standing challenges. We believe that this special topic will provide valuable perspectives and meaningful insights into waste heat recovery and cooling applications.

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