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Editorial: A Brief Perspective to the Development of Emerging Thermoelectric Materials

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Editorial on the Research Topic

A Brief Perspective to the Development of Emerging Thermoelectric Materials

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The ever-growing energy issue brings forth a strong impetus for efficient harvesting and conversion of heat into electrical energy, where thermoelectric (TE) materials play a pivotal role. Such materials provide a simple and environmentally friendly solution for the thermoelectric conversion, applicable for automobiles and high-power electrical appliances which produce lots of waste heat.

The development of high-performance TE materials and their optimization have attracted intensive attention in the materials science and energy communities, with one of the main goals to boost the TE figure of merit $ZT = \frac{S^2\sigma}{\kappa}T = \frac{S^2\sigma}{\kappa_e+\kappa_l}T$, where S is the Seebeck coefficient, σ is the electrical conductivity, κ_e is the electronic thermal conductivity, κ_l is the lattice thermal conductivity, and T is the absolute temperature. In this regard, ZT can be efficiently enhanced by lowering the thermal conductivity, which can be achieved by lots of possible manners, such as designing the geometry structures at the micro/nanoscales. For instance, the strain-modulated phonon transport behavior of the monolayer H-decorated pentagonal silicene (penta-SiH) and bilayer pentagonal silicene (penta-Si), and one hexagonal H-decorated silicene structures (H-silicene) are comparably studied from first-principles (Liu et al.). For both pentagonal silicene structures, the thermal conductivity first shows a large improvement (90% for monolayer penta-SiH and 400% for bilayer penta-Si) as tensile strain increases from 0 to 10% and then stabilizes with a strain larger than 10%. A detailed analysis shows that the phonon group velocity and phonon lifetime of both structures increase with applied strain, and the phonon lifetime plays the major role in the improvement of thermal conductivity. Furthermore, based on the detailed analysis between the pentagonal (penta-SiH) and hexagonal silicene structures (H-silicene), the difference in out-of-plane phonon scattering cannot be ignored. Furthermore, the thermal conductivities of Mg- and Si-doped GaN are studied based on the first-principles method combined with the solvent of phonon Boltzmann transport equation (BTE) (Li et al.). Li et al. found that both the thermal conductivities of Mg- and Si-doped GaN reach the ultra-low values, and the thermal conductivity of Si-doped GaN is even an order of magnitude lower than that of Mg-doped GaN.

In recent years, two-dimensional (2D) materials have been extensively investigated for fabricating miniaturized electronic devices, where the thermal management and thermoelectric conversion become essential. Interestingly, an increasing number of 2D materials have been predicted to have the potential applications in TE via high-throughput calculations

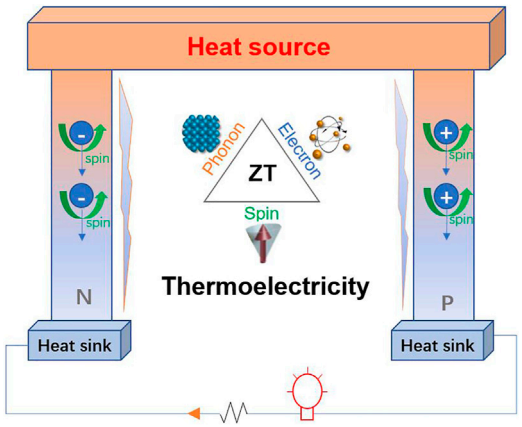

FIGURE 1 | Schematic diagram of thermoelectricity.

(Jia et al., 2020; Sarikurt et al., 2020). Electronic fitness function as a new descriptor to estimate TE performance of semiconductors is usually used for screening novel TE materials. Among them, the monolayer GeS_2 has been recently confirmed as a good candidate for 2D materials with weak interlayer coupling from theory and experiment study (Yan et al., 2022). In this topic, Wang et al. systematically investigated the TE performance of monolayer GeS_2, including both the electronic and the thermal transport properties (Wang et al.). As compared with other typical TE monolayer materials, the monolayer GeS_2 exhibits excellent electronic transport properties but a relatively high lattice thermal conductivity of 5.71 $W\,m^{-1}\,K^{-1}$ at 500 K. Thus, an unsatisfactory ZT value of 0.23 is reached. Such a low ZT value indicates that beyond the electronic transport properties, it is necessary to also consider the thermal transport properties through high-throughput calculations to screen the thermoelectric materials with excellent performance.

This collection on the investigation of TE materials or the closely related thermal conductivity provides a comprehensive perspective, which is expected to stimulate research inspiration in the TE field and advance the fundamental understanding of TE performance. Due to the role of electrons, spins, and the lattice vibrations (phonon) and their couplings have a significant effect on the thermal transport and thermoelectric performance (**Figure 1**), more novel strategies are expected to boost TE performance in future, such as spin modulation, etc. Notably, the Rashba effect modulation is expected to optimize the electronic and the thermal transport properties simultaneously. In addition, for searching high performance TE materials through high-throughput calculations and machine learning techniques, new descriptors are also deserved to be explored, such as by constructing from existing descriptors of bandgap, effective mass, etc.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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