

Research Advances of Typical Two Dimensional Layered Thermoelectric Materials

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Abstract:

Thermoelectric technologies have caught our intense attention due to their ability of heat conversion into electricity. The considerable efforts have been taken to develop and enhance thermoelectric properties of materials over the past several decades. Recently, two-dimensional layered materials are making the promise for potential applications of thermoelectric devices because of the excellent physical and structural properties. Here, a comprehensive coverage about recent progresses in thermoelectric properties of typical two dimensional (2D) layered materials, including the theoretical and experimental results, is provided. Moreover, the potential applications of 2D thermoelectric materials are also involved. These results indicate that the development of 2D thermoelectric materials take a key role in the flexible electronic devices with thermoelectric technologies.

Keywords: thermoelectric properties; transport properties; 2D layered materials; figure of merit, first-principle calculations

1 Introduction

Thermoelectric (TE) conversion technology, which is a kind of green energy technology and can convert waste heat into electricity, has been considered to be an alternative for relieving energy shortage. TE devices have been used in different directions, including solid state cooling and deep space exploration^[1-2], and also shown the high potential in other areas, such as sensors and power generators^[3-5]. These make TE materials a kind of important compounds which support the development of sustainable energies and technologies with high efficiency. The performance of TE materials usually is characterized by the figure of merit ZT which is a dimensionless parameter and expressed as^[6], $ZT=S^2\sigma T/\kappa$, where S is the Seebeck coefficient and σ is the electrical conductivity. κ presents the thermal conductivity and T is the abbreviation of absolute temperature. There are two parts for the thermal conductivity κ which are including the electronic (κ_e) and lattice contributions (κ_l). These parameters are coupled to each other and strongly depend on the electronic structure and carrier concentration of the materials. There are usually two approaches to improve the TE performance. One way is to decrease the thermal conductivities κ_e and κ_l , and the other is to increase the power factor $S^2\sigma$. In the past few decades, the TE field has made great progress, including various strategies to increase

the power factor and reduce the thermal conductivity. In the TE materials family there are a lot of candidates which have been reported to achieve an obvious enhancement for the value of ZT ^[7-12]. Among these kinds of strategies, low-dimensional material system has become a focus with the development of the nanotechnologies and has been applied to the thermoelectrics. Moreover, TE devices on the basis of flexible materials with large size have shown the great potential with the rapid emergence of the concept of the "Internet of Things (IoT)"^[13], especially in flexible wearable devices. It has many advantages, such as long lifetime and maintenance-free. In addition, the devices of TE energy conversion don't give rise to the vibrations or noises, while they are suitable at moderate temperatures^[14]. Thus, TE properties of low-dimensional materials have attracted much attention^[15-16].

To date, the research of TE materials has shown the prominent progress with the enhancement of ZT value, due to the inspirations by the design of low-dimensional structures, mainly two-dimensional (2D) structures for TE proposed in 1990s^[17]. The core idea behind with low-dimensional structures to enhance the TE performance is to introduce the dramatic differences in the electronic density of states (DOS) near the Fermi level. In this way, the electrical conductivity, thermal conductivity and Seebeck coefficient can be modulated quasi-independently by

quantum-confinement effects from three-dimensional to two-dimensional^[18]. With the development of preparation technologies, A series of 2D materials have been fabricated successfully^[19-28]. It is possible to develop new low-dimensional TE materials from the perspective of two-dimensional materials.

Initially, the research on 2D TE materials was mainly focused on quantum well and super-lattice thin film materials^[29-31], such as GaAs/AlAs, Bi₂Te₃/Sb₂Te₃ and SrTiO₃/SrTi_{0.8}Nb_{0.3}O₃. To date, although there have been some summaries on the related researches about 2D TE materials and the progress of the TE devices based on 2D materials^[14-15, 32], an interesting review about new layered 2D materials with different structure types for the potential applications in TE field is still missing. In this short review, we are focused on the progress in the new 2D thermoelectric materials theoretically and experimentally, such as group IV-VI layered materials, III-VI layered materials, group IV-V compounds and transition metal dichalcogenides (TMDs). We review the new TE properties in these types of 2D structures and also provide some insight for designing the new layered TE materials in the future.

2 TE Properties of typical 2D TE Materials

2.1 Group IV-VI two-dimensional layered materials

As a typical one of layered group IV-VI materials, SnSe with the special atomic structure has the excellent electronic transport and thus has attracted wide attention. It possesses a orthorhombic structure with layered atomic arrangement under space group of *Pnma*^[21]. In figure 1a, its structure is along the *b*-axis in the perspective view. Due

to this special layered structure, the carriers' mobilities are highly anisotropic along different transport directions. As depicted in figure 1b, the carrier's mobility at room temperature is 250 cm² V⁻¹s⁻¹ along the *b*-axis. This value is 10 times as high as that of *a*-axis which is outside the plane. Due to the folded plane, the mobility of carrier along *c*-axis is also obvious different, compared with that along the *a*-axis. On account of the lone electron pairs of the Sn²⁺ atoms, SnSe also exhibits ultralow thermal conductivity of 0.34 W m⁻¹ K⁻¹ at 773 K along the *b*-axis. Combined superior mobility and ultralow thermal conductivity, the SnSe shows a high *ZT* value along *b*-axis at 773K for *p*-type which is 2.3, as shown in figure 1c. This value is a higher value among the recent experimental reports in the published literatures. Moreover, because of the layers' weak van der Waals interaction, the single-layer with in-layer strong covalent bonds can be fabricated from the bulk SnSe. The cleavage energy for splitting layers is about 200 meV/atom theoretically^[33]. The calculation results show that the single-layer SnSe is with an energy gap of 1.28 eV and possesses the thermodynamic stability^[34-35]. It has been reported that the *ZT* value of single-layer SnSe at 773 K could reach to 3.27. Furthermore, it has been demonstrated that SnSe with orthorhombic *Pnma* symmetry (denoted as α -SnSe) has a phase transition at 796 K and becomes to be the β -SnSe with orthorhombic structure under space group *Cmcm*^[36]. These suggested that the new phases may be realized by changing growth temperature. Since then, the electronic and TE properties of many potential new phases (the polymorph structures of SnSe are shown in figure 1d) have been researched^[37]. The theoretical results show that the β -SnSe phase has a *ZT* value of 2.06 at room temperature^[37].

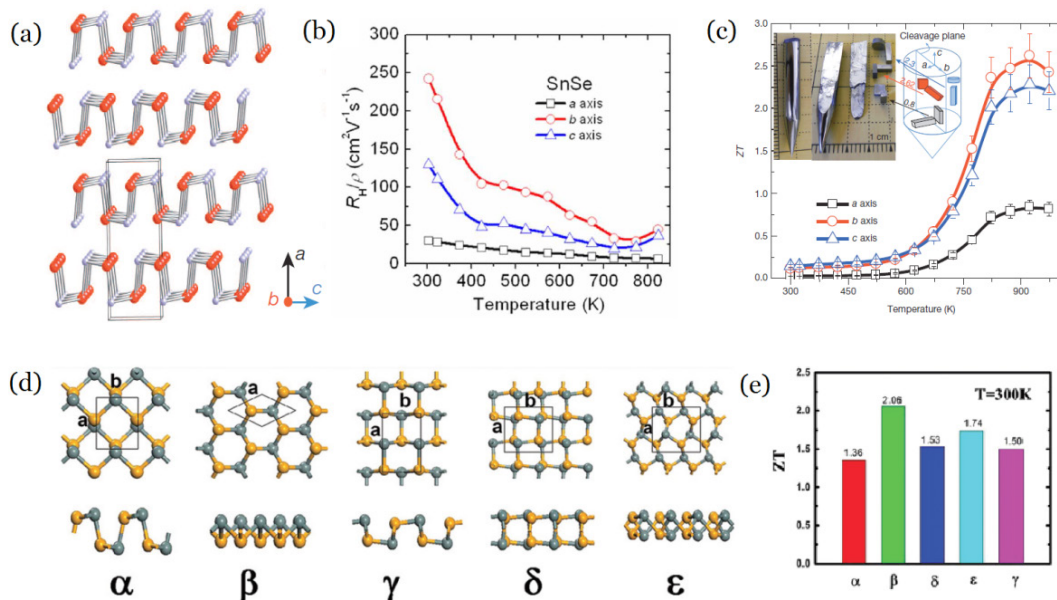


Figure 1 (a) Crystal structure of SnSe. (b) R_H/ρ (ρ , electrical resistivity) of SnSe along different axial directions. (c) *ZT* values of SnSe along different directions. Reproduced with permission from ref. 21. Copyright 2014, NPG. (d) Geometric structures of α -, β -, γ -, δ - and ϵ -SnSe monolayers. Gray atoms denote Sn atoms and yellow atoms denote Se atoms. (e) *ZT* values of different monolayer SnSe phases at 300 K. Reproduced with permission from ref.37. Copyright 2017, RSC.

These results above have sparked interest in exploring other group IV-VI two-dimensional materials^[38-42], such as GeSe, SnS, GeS, SnS₂, SnSe₂, SiS and SiSe. Theoretical calculations have revealed that group IV-VI compounds with folded structure could exhibit high Seebeck coefficient, relative low thermal conductivity and had the potential toward TE applications^[43]. The thermal transport property of group IV-VI single-layer materials (GeS, GeSe, SnS and SnSe) has been investigated by first-principles calculations^[42]. The average thermal conductivity calculated is 6.38 Wm⁻¹K⁻¹, 5.23 Wm⁻¹K⁻¹, 3.08 Wm⁻¹K⁻¹ and 2.77 Wm⁻¹K⁻¹, respectively. Among these IV-VI materials studied, GeS has the largest Seebeck coefficient (2810 VK⁻¹) at room temperature^[41]. Compared with their bulk materials, the optimal *ZT* values of single-layer GeSe, GeS and SnS are high and 1.99, 1.85 and 1.88, respectively. Therefore, these materials are expected to have the potential applications in TE devices. In addition, as typical group IV-VI materials, SiSe and SiS possess high Seebeck coefficient arising from the sharp DOS near Fermi level^[44]. The calculation results about the power factor indicate that the peak values of the *p*-type and *n*-type are 16 mWm⁻²K⁻² and 11 mWm⁻²K⁻², respectively. these values are similar to the experimental report on the state-of-the-art material SnSe with the layered structure^[35].

2.2 Group III-VI two-dimensional layered materials

As the potential TE materials, the compounds which belong to III-VI group have aroused much attention during the past few years. These materials, including InSe, GaSe, GaS and Tl₂O, have been extensively studied in the TE field^[45-47]. Taking InSe as an example, with the stoichiometric ratio of 1:1, it has the typical structure of group III-VI layered materials shown in figure 2a. It has been also noticed that In-Se system is complex and there are other different stoichiometric ratios^[48], such as In₄Se₃^[49], In₂Se₃^[50], InSe^[51], In₆Se₇^[52] and In₃Se₄^[53]. In addition, with the same stoichiometric ratio, different phases and crystal structures may coexist. Geim *et al.*^[54] reported that the carrier's mobility of the thin InSe was very high. It exceeds 10³ cm²V⁻¹s⁻¹ at RT and is about 10⁴ cm²V⁻¹s⁻¹ at liquid-helium temperature. Moreover, experimental studies show that the thermal conductivity of bulk In₄Se_{2.35} is very low along the *b-c* plane (1.2 Wm⁻¹K⁻¹ at 300 K), and it decreases with increasing temperature (0.74 Wm⁻¹K⁻¹ at 705 K)^[55].

Based on the analysis of the electronic structure of III-VI compounds with single-layer and multi-layer, it is found that the valence band of these materials have a “Mexican hat” dispersion^[56-59], which can increase the density of states near the band edge (as seen in figure 2b), and further increases the Seebeck coefficient. Single- and multi-layer materials of InSe, GaSe and GaS have been successfully fabricated experimentally^[60-63]. Subsequently, the electronic and TE properties of these materials from single-layer to multi-layer have been researched extensively. The results show that the power factor increases, following the material's thickness decreases^[64-65]. As an example, the maximum power factor of single-layer InSe reaches to

16 mWm⁻²K⁻². The TE performance of single-layer InSe has been also investigated theoretically through using mechanical strain. Under the strain, the energy bands will converge and thus lead to an increase of power factor, while the thermal conductivity is also found to decrease^[66].

Some works have revealed that the sharp conduction band edge with high DOS due to the quantum confinement could lead to the enhancement of the Seebeck coefficient^[67]. The DOS and the information of electronic wave functions at conduction band maximum CBM for 9-layers and 36-layers InSe films are shown in figure 2c. With the combination of theoretical simulations and experimental tests, it is found that the power factor is increased obviously, by following the thickness of InSe sample decreases, especially less than the thermal wavelength (seen in figure 2d). This may provide a guideline for further optimizing the TE properties of 2D layered structures.

2.3 Group IV-V two-dimensional layered materials

With the emergence of group IV and group V 2D layered materials, including graphene, silicene, germanene, phosphorene and antimonene, group IV-V 2D compound materials have been also explored^[68-70]. Group IV-V compounds are known to form the layered structures. A few structures have been synthesized at high pressure^[71], such as SiP, SiAs, GeAs and GeP. The layered crystal structure with space group *C2/m* is shown in figure 3a.

As a typical one, GeAs with anisotropic atomic structure has demonstrated highly anisotropic properties of transport^[72]. As shown in figure 3b, the resistivity perpendicular to the layers is very high due to large distance of layers with weak coupling. It is 2 orders of magnitude higher than that along the layers at 300 K. The TE properties of Sn-doped GeAs have been studied. The results revealed that at high temperature, Sn-doped GeAs exhibited superior transport properties, compared to the pristine GeAs. It has shown that Sn-doped GeAs possesses a remarkable *ZT* with a maximum of 0.35 at 660 K (as shown in figure 3c)^[72]. On the Ge-As phase diagram, there are another compound GeAs₂ with an orthorhombic crystal structure (in figure 3d)^[73]. It exhibits the strong interlayer coupling due to its special stacking of layers with small layers' spacing along vertical direction (about 1 Å). The power factor of the *n*-type GeAs₂ along the *b*-axis can reach to 4.2 mW/mK². This are comparable to the value (4 mW/mK²) of SnSe^[74]. Monolayer GeAs₂ has complex bonding characteristic, and this is similar to the structural characteristic of SnSe. The calculated in-plane lattice thermal conductivities is 0.68 Wm⁻¹K⁻¹ along the *a*-axis and 6.03 Wm⁻¹K⁻¹ along *c*-axis at RT, respectively^[75]. These research achievements suggest that the group IV-V compound materials are the promising candidates for environmentally friendly TE applications.

2.4 TMD materials

It has been well known, TMDs are with typical layered stacking and the coupling of layers is by van der Waals interaction. For the singer layer, there are usually two different structural types. One is the hexagonal structure (H-phase). The typical materials include Mo and W based

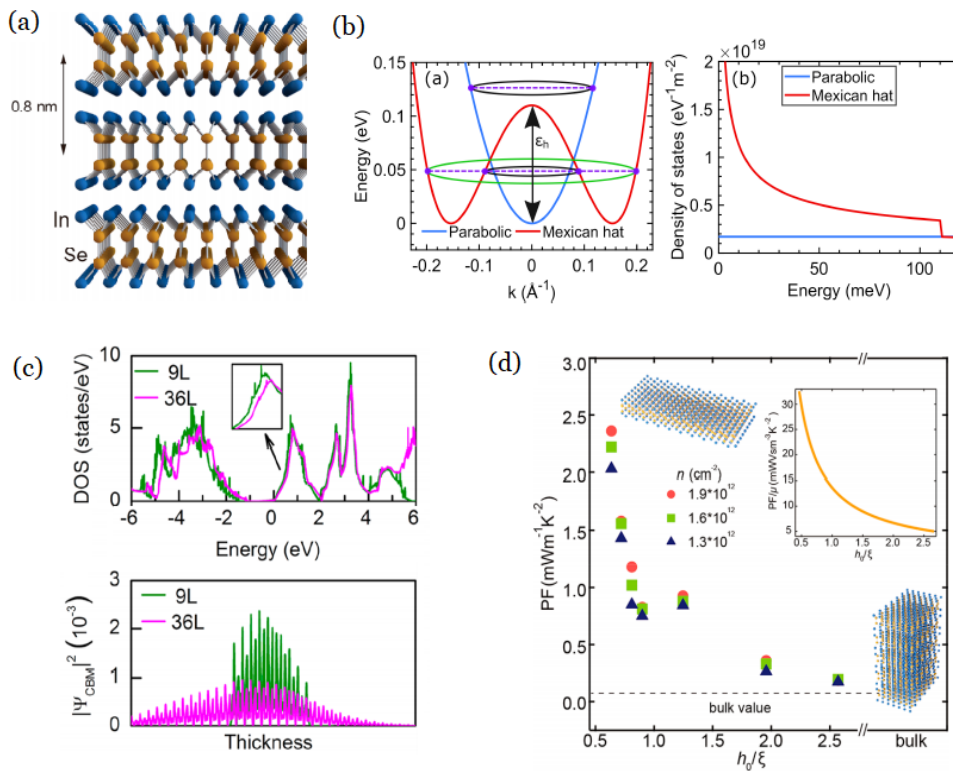


Figure 2 (a) Crystal structure of InSe. Reproduced with permission from ref. 67. Copyright 2018, ACS. (b) Comparison of a parabolic and Mexican hat dispersion and density of states of both. Reproduced with permission from ref. 59. Copyright 2019, APS. (c) Total density of states and planar-averaged squared magnitude of wave functions (which are from the states of conduction band maximum and plotted along the direction perpendicular to layers) of 9-layers and 36-layers InSe films (upper panel), (lower panel). (d) Power factor as functions of films' thickness with quantum confinement effect (h_0/ξ) for the different carrier concentrations. (h_0 is for quantum confinement of length, and ξ is for heat wavelength). Reproduced with permission from ref. 67. Copyright 2018, ACS.

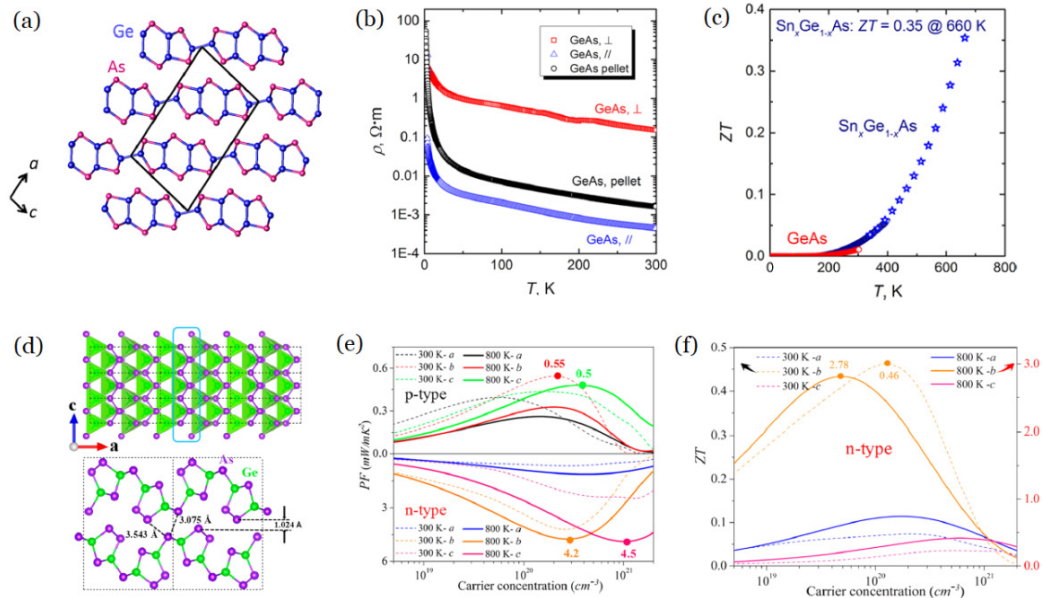


Figure 3 (a) Crystal structure of GeAs. (b) Resistivity of GeAs pellet and the GeAs crystal as functions of temperature. (c) ZT value as functions of temperature for $\text{Sn}_x\text{Ge}_{1-x}\text{As}$ pellet and GeAs. Reproduced with permission from ref. 72. Copyright 2016, ACS. (d) Top view and side view of GeAs_2 atomic structure. (e) Power factors as functions of carrier concentration with different temperature for the *p*-type and *n*-type along different axes. (f) Calculated ZT value for the *n*-type GeAs_2 . Reproduced with permission from ref. 73. Copyright 2017, ACS.

dichalcogenides, such as MX_2 ($\text{M}=\text{Mo}, \text{W}$, and $\text{X}=\text{S}, \text{Se}, \text{Te}$). The other one is the 1T- CdI_2 type with trigonal structure^[76]. In both structures, single layer of metal atoms is sandwiched between two chalcogen layers. Hexagonal structure is shown in figure 4a. They have been widely explored in various fields, such as electronics and optoelectronics, due to their diverse physical and chemical properties^[77]. TMDs have been also researched as candidate materials for TE devices because of their high Seebeck coefficients and low thermal conductivities^[78-82].

The TE properties of 2D TMDs, such as MoS_2 , have been studied by both theoretical calculations and experimental works. The electronic structure has a significant layered effect for TMDs. For an example, their indirect band gap in multi-layers and bulk changes into direct band gap in their monolayer limit^[83]. The band structure exhibits obvious changes by following the increase of atomic layer's number from monolayer to multilayer^[84-86]. The TE transport properties of few-layer MoS_2 have been reported^[87]. As shown in figure 4b and 4c, the electrical conductivities, Seebeck coefficient and power factor have been measured^[87]. The power factor increases correspondingly, by following the increase of applied gate voltage V_g on account of increasing electrical conductivity. Apparently, the device with double layer MoS_2 has a large effective mobility of $64 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ with a maximum power factor of $8.5 \text{ mWm}^{-1}\text{K}^{-2}$ at RT. The value of power factor is the highest one among that measured in semiconducting TMDs as the TE materials. The enhancement of transport performance is not only due to the quantum-confinement effect but also due to their valley degeneracies and large effective masses. Similar behavior was also found in other TMDs, such as MoSe_2 , WS_2 , and WSe_2 ^[88-89].

The 2D materials, such as TiX_2 , Zr X_2 , and HfX_2 , are typically with CdI_2 type. They have attracted much attention because of their lower lattice thermal conductivity than those of W and Mo based TMDs. The lower thermal conductivity is originated mainly from the strong hybridization between low lying optical phonon modes and acoustic phonon modes^[90-91]. For instance, the theoretical calculation results indicate that the lattice thermal conductivity at RT are $1.2 \text{ Wm}^{-1}\text{K}^{-1}$ for ZrSe_2 and $1.8 \text{ Wm}^{-1}\text{K}^{-1}$ for HfSe_2 , which is lower than those values of MoS_2 -type monolayers^[79, 92-93] and comparable to those of some popular bulk TE materials, such as Bi_2Te_3 ^[94] and PbTe ^[95].

Recently, another class highly desirable 2D material has been theoretically predicated and explored experimentally^[96-100]. They are formed by the combination of chalcogens and noble metals, such as Pt and Pd. They have usually bulked or puckered pentagonal structure with low symmetry. Oyedele *et al.* has been exfoliated monolayer PdSe_2 from its bulk crystals^[98]. This typical 2D noble transition metal dichalcogenide monolayer with a puckered morphology is air-stable. The theoretical results demonstrate that the mobility of holes can reach $1929 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ for monolayer PdSe_2 . It possesses the lower lattice thermal conductivity of $3.7 \text{ Wm}^{-1}\text{K}^{-1}$ ^[100], which is much

lower than that of MoS_2 . It indicates that PdSe_2 monolayer could have a quite potential for TE applications. Recently, a novel Pd_2Se_3 monolayer phase, which is reconstructed from a few layers of PdSe_2 by the interlayer fusion, has been reported experimentally^[101]. Figure 4d shows the experimental TEM image with atomic resolution (grey) of the monolayer and correspondingly theoretical TEM image by the simulation. The ultralow lattice thermal conductivity has been found in Pd_2Se_3 monolayer. Theoretical analysis reveals that in the region of low frequency a strong hybridization is between $[\text{Se}_2]^{2-}$ ion and Pd^{2+} , as verified by the phonon DOS in figure 4e^[102]. Thus, it is proposed that the low thermal conductivity is due to the softening of phonon modes and the anharmonicity between covalently bonded $[\text{Se}_2]^{2-}$. The lattice thermal conductivity of Pd_2Se_3 is calculated and is about $2 \text{ Wm}^{-1}\text{K}^{-1}$. This small value is 90, 27, and 6 times lower than that of MoS_2 ^[103], WSe_2 ^[79], and TiS_3 ^[104], respectively.

3 Potential applications of two-dimensional thermoelectric materials

Traditionally, TE materials are mainly used as TE power generation and TE refrigeration. The TE generator can be applied in the TE power station with the long distance and unmanned maintenance, such as in man-made satellite. They can be applied in the low-grade TE generation, such as industrial waste heat, waste heat in our daily life and heats from vehicle exhaust. TE materials with the characteristics of both cooling and heating can control easily the temperature timing and are used to provide the constant temperature environment for different systems, such as electronic computers, cameras with CCD and communication devices. They are also used as the sensors and temperature controllers with extensive applications in microelectronic systems and devices. Here, we won't discuss these traditional applications in details. Following the device miniaturization, TE materials will expand their applications in other potential areas further. Especially, two-dimensional TE materials have wide application prospect in wearable/flexible systems.

With the recent appearing of the IoT era, and the wide range use of microelectronic devices by that people can communicate with each other at anytime and anywhere, the research of wearable electronic systems is growing. However, it still remains a problem for the power supplies of wearables. At present, batteries can power these wearable devices. But the frequent recharging and replacement are unavoidable problems. To solve this issue, one of most effective strategy is to integrate self-powered system with wearable electronic devices. Here, the energy conversion by TE effect on basis of large-area flexible materials is expected to serve as the energy harvester with self-powered way. This has received large attention because of its advantages^[105-109]. For examples, the heat energy from body may be enough and the long lifetime prevents them from frequent replacement. In addition, the TE conversion process don't create any noise¹⁴.

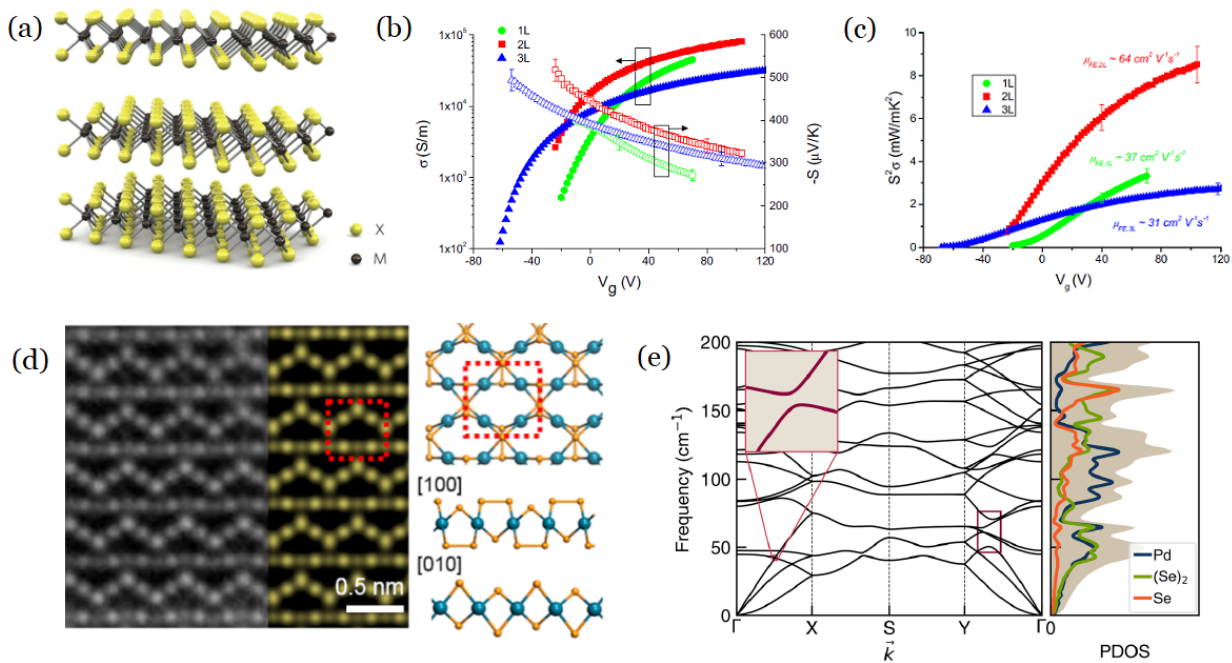


Figure 4 (a) Three-dimensional schematic representation of typical hexagonal MX₂ structure. Reproduced with permission from ref. 77. Copyright 2012, NPG. (b) Electrical conductivities σ and Seebeck coefficients S at RT as functions of V_g for single layer MoS₂. (c) Power factor $S^2\sigma$ as a function of V_g . Reproduced with permission from ref. 87. Copyright 2017, APS. (d) High resolution TEM (grey) and simulated (yellow) image for monolayer Pd₂Se₃. Reproduced with permission from ref. 101. Copyright 2017, APS. (e) Phonon band structure and density of states of monolayer Pd₂Se₃. Reproduced with permission from ref. 102. Copyright 2018, ACS.

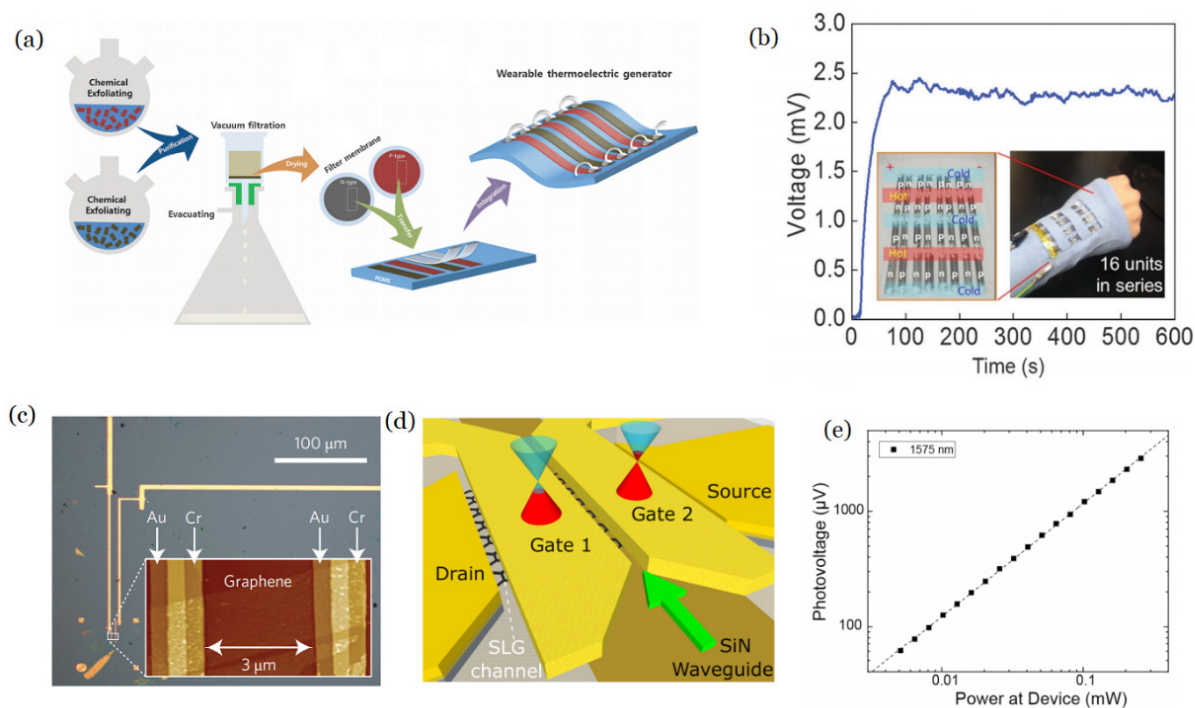


Figure 5 (a) Fabrication processes of wearable thermoelectric devices using TMDs nanosheets. (b) Output voltage from the human wrist's heat by thermoelectric generator. Reproduced with permission from Ref. 111. Copyright 2016, RSC. (c) Optical micrograph and atomic force microscopy of graphene photo detector. Reproduced with permission from Ref. 112. Copyright 2014, NPG. (d) Schematic illustration of the graphene photo detector with SiN waveguide. (e) The relation between photo voltage and optical power. Reproduced with permission from ref. 113. Copyright 2019, ACS.

Originally, the TE generator consisting of bulk Bi_2Te_3 and Sb_2Te_3 printed on a flexible glass fabric has been reported^[107]. A bend ability radius of up to 20 mm is shown in this kind of devices. This basically meets the demand of flexible wearables. Kim *et al.*^[110] have fabricated a novel wearable TE generator, which could attach to human skin and use the heat energy from body. Thus, it is expected to be with various potential applications. Because of unique electrical and mechanical properties, TMDs have given risen to great attention due to their potential in next-generation microelectronics and wearables. Oh *et al.*^[111] developed a method by combining chemical exfoliation and vacuum filtration to construct the TE generators directly which are parallel-connected on flexible substrates (seen in figure 5a). As shown in figure 5b, NbSe_2 and WS_2 nanosheets were used as the *p*-type and *n*-type materials, respectively. In this way, the TE generators were fabricated. This kind of devices has very high flexibility and durability. They can be used as the glove-type wrist-band thermal sensor.

Moreover, based on the Seebeck effect, the photo TE device can generate a photocurrent. With the adsorbed light, the temperature gradient between lighting region and dark region is built and thus the electric voltage is formed. This phenomenon has several advantages in designing the optoelectronics devices with high performance. The graphene TE terahertz photo detector has been investigated^[112] (figure 5c). This kind of device demonstrates an outstanding sensitivity more than 10 VW^{-1} at RT with noise-equivalent power less than $1100 \text{ pW Hz}^{-1/2}$, referenced to the incident power. If based on absorbed power, the sensitivity exceeds 700 VW^{-1} at RT with noise-equivalent power less than $20 \text{ pW Hz}^{-1/2}$. A photo-thermoelectric-based graphene photo detector has been designed to generate a photovoltage directly (seen in figure 5d)^[113]. It exhibits an external responsivity of about 12.2 V/W with a roll-off frequency up to 42 GHz and 3dB bandwidth. Figure 5e shows the relation between photovoltage and optical power. With TE effect, the voltage generated by temperature gradient due to the lighting has a linear response to optical power^[113].

4 Conclusion and Outlook

Over the last few decades, TE materials have made a great progress. In this review, we are focused on the TE properties of new two-dimensional materials and the possible applications. In particular, the relevant theoretical and experimental results for group IV-VI, group IV-V, group III-VI and layered transition metal dichalcogenides have been highlighted. We also compared the TE properties between new two-dimensional materials we considered and state-of-the-art layered structure materials. In these new two-dimensional materials, both low thermal conductivity and high power factor have been revealed. Finally, the current potential applications in TE device, including flexible generator and optoelectronics devices using two-dimensional film materials have also been presented.

Although the tremendous advances have been

achieved during the past decades, there are still problems and challenges for the practical applications. The phonon and electrical transport mechanism are still obscure. The mechanism of increasing the power factor has been proposed in two-dimension materials, but it still remains challenge to decouple the different transport coefficients. We also need a deeper understanding of transport mechanisms to help enhance TE properties and design new TE materials in the future.

Conflicts of interest: The authors declare no competing financial interest.

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