Two-dimensional layered architecture constructing energy and phonon blocks for enhancing thermoelectric performance of InSb

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ABSTRACT InSb is a narrow-bandgap semiconductor with a zinc blende structure and has been widely applied in photo-detectors, infrared thermal imaging, and Hall devices. The facts of decent band structure, ultrahigh electron mobility, and nontoxic nature indicate that InSb may be a potential mid-temperature thermoelectric material. The critical challenges of InSb, such as high thermal conductivity and small Seebeck coefficient, have induced its ultrahigh lattice thermal conductivity, and thus low ZT values. In view of this, we have developed a competitive strategy typified by the cost-efficient nanocompositing of z wt% QSe_2 ($Q = Sn, W$). Specifically, the Q_{In}^{+} and Se_{Sb}^{+} point defects were introduced in the InSb system by nanocompositing the vested two-dimensional layered QSe_2 . In addition, the enlarged valence band maximum of intrinsic WSe_2 acted as ladders can scatter a fair number of hole carriers, resulting in the relatively enhanced Seebeck coefficient of high temperature. Moreover, the disorderly distributed nanosheets/particles, and dislocations acting as obstacles can effectively delay the heat flow diffusion, inducing the strong scattering of thermal phonons. Consequently, an enhanced power factor of $\sim 33.3 \mu W cm^{-1} K^{-2}$ and ZT value of ~ 0.82 at 733 K have been achieved in the 3% WSe_2 sample, accompanied with the engineering output power density $\omega_{max} \sim 233 \mu W cm^{-2}$ and thermoelectric conversion efficiency $\eta \sim 5.2\%$. This artificially designed approach indicated by suited nanocompositing can integrate several engineering strategies such as point defects, nanoengineering, and energy filtering into one, providing a reference to optimize the thermoelectric performance of other thermoelectric systems.

Keywords: thermoelectric, InSb, energy barrier, WSe_2 nanosheets, output power density

INTRODUCTION

Thermoelectric generators (TEGs) can convert the industrial waste heat into electricity, which is of great significance to alleviate the energy crisis and the greenhouse effect [1–4]. For generating electricity through the thermoelectric effect, a thermoelectric module and a temperature difference between its hot and cold side are necessary. The most commonly used commercial thermoelectric materials are SiGe [5], Bi_2Te_3 [6] and PbTe [7], and recently, some new materials such as half-Heusler

[8] and SnSe [9] have been demonstrated to have a better efficiency but require higher temperature difference. The conversion efficiency of thermoelectric devices is closely related with the $ZT = S^2\sigma T/k$ of TE materials, where S , σ , k , T are the Seebeck coefficient, electrical conductivity, thermal conductivity, and absolute temperature, respectively. Among them, $k = k_e + k_l$ is derived from the carrier thermal conductivity (k_e) and lattice thermal conductivity (k_l) [10–12]. The classic theory of phonon glass electron crystal (PGEC) provides a route to design a high- ZT thermoelectric material with higher electrical performance and low thermal conductivity. Therefore, numerous separate approaches have been devoted to optimizing the electrical and thermal properties, thus increasing the ZT value, and the electrical performance can be optimized via point defects (PDs) [13,14], band engineering [15,16], and high-entropy engineering [17,18]. In contrast, the microstructure engineering induced by nanocompositing [19,20], dislocations [21,22], and hierarchical architecture [23,24], has been employed and proven to be effective in reducing the thermal conductivity.

InSb is a narrow-bandgap (~ 0.18 eV) semiconductor with a zinc blende structure, and its characteristics of high electron mobility ($\sim 78,000 cm^2 V^{-1} s^{-1}$) [25,26] and Pb-free composition indicate that it may be a promising mid-temperature thermoelectric material. Numerous effects have been employed to improve the thermoelectric properties of InSb in recent years. For instance, Su *et al.* [27] obtained a ZT value of ~ 0.49 at 700 K for polycrystalline InSb by a Melt-MS-SPS (MS: melt spinning; SPS: spark plasma sintering) process. Zhang *et al.* [28] reported an improved ZT value of ~ 0.73 at 650 K in a Ga-doped InSb compound. Jiang *et al.* [29] got a decreased lattice thermal conductivity of $\sim 10 W m^{-1} K^{-1}$ in InSb via *in situ* introducing NiSb precipitates and more recently, Yang and co-workers [30,31] achieved a large reduction of lattice thermal conductivity in a narrow temperature range with the help of InSb-Sb eutectic structure. However, the thermoelectric performance of InSb is far inferior to the currently mid-temperature thermoelectric materials such as PbTe [32] and $CoSb_3$ [33], which is mainly due to its high thermal conductivity and small Seebeck coefficient. As is known, the thermal conductivity of TE materials can be largely reduced through introducing multi-scale second phases, and the electrical transport properties such as carrier mobility may also get deteriorated. Meanwhile, inducing PDs via single- or co-doping is an effective approach to increase the carrier

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concentration, except for the decreased Seebeck coefficient due to the Mott relationship [34].

As is known, WSe_2 and SnSe_2 are emerging two-dimensional layered compounds with ultra-low thermal conductivities, and their partial elements of anion and cation sites may be dissolved into the InSb crystal lattice during hot pressing. In this scenario, we develop a merged strategy for regulating the electrical and thermal properties *via* subtly building thermal and energy barriers, which can be detailed by the nanocompositing of z wt% QSe_2 ($Q = \text{Sn}, \text{W}$) with the InSb system. Benefiting from it, the enhanced electrical conductivity originated from the generated Q_{In}^+ and Se_{Sb}^+ PDs. Meanwhile, the suitable energy ladder constructed by the valence band maximum between the InSb and WSe_2 can effectively scatter low energy carriers, thus leading to an enhanced Seebeck coefficient compared with SnSe_2 -composited sample. As a result, a 43.2% increased power factor of $33.3 \mu\text{W cm}^{-1} \text{K}^{-2}$ has been achieved in the 3% WSe_2 sample. Moreover, the hierarchical microstructure such as nanosheets/particles, abundant dislocations, and strain fields can effectively scatter multi-scale phonons, leading to a decreased lattice thermal conductivity of 1.1 and $1.02 \text{ W m}^{-1} \text{K}^{-2}$ with the additives of 9% SnSe_2 and 3% WSe_2 , respectively. Ultimately, an enlarged thermoelectric performance of ZT value ~ 0.82 at 733 K has been achieved in the 3% WSe_2 -composited sample, which results in 30% and 134% improvement compared with the SnSe_2 composites ($ZT \sim 0.63$) and pristine InSb ($ZT \sim 0.35$). This work realizes multiple functions of PDs, energy filtering, and microstructure engineering *via* cost-efficient QSe_2 nanocompositing, synchronously optimizing the electrical and thermal properties of InSb, which could be taken as an example for other high thermal conductivity thermoelectric systems.

EXPERIMENTAL SECTION

Fabrication of thermoelectric materials

Indium powder (99.99%, Changsha Asian Light Co., Ltd.) and antimony powder (99.99%, Changsha Asian Light Co., Ltd.) were mixed in an exact metage according to nominal composition $\text{In}_{1.0}\text{Sb}$, slowly heated to 973 K at a rate of 117 K h^{-1} and held at this temperature for 6 h. Then the InSb ingots were ground into fine powders in an agate mortar. As for the preparation of QSe_2 ($Q = \text{Sn}, \text{W}$), the acquisition of SnSe_2 was referred to the previous work [35], and the WSe_2 was obtained through the melting-quenching method [36]. The QSe_2 ingot was ground into uniform powder and performed in an ultrasonic vibrator for 6 h to obtain QSe_2 nanopowders. Subsequently, the prepared QSe_2 was mixed with the sieved pristine InSb well and then moved to a graphite mold for SPS sintering, consolidated at 733 K for 10 min in a graphite mold (20 mm in diameter) with a compressive stress of 60 MPa. All the cylinders were obtained and characterized with relative densities at least 95%.

DFT calculated details

The density functional theory (DFT) was implemented in the Vienna *ab initio* simulation package (VASP) [37]. The geometry of system is fully relaxed until the magnitude of the force acting on all atoms is less than $10^{-5} \text{ eV \AA}^{-1}$ with a kinetic energy cutoff of 520 eV. The $2 \times 2 \times 2$ supercells with the Gamma centered k-point grid of $6 \times 6 \times 6$ (InSb) and $9 \times 9 \times 2$ (WSe_2) were adopted for the Brillouin zone to calculate the total energy and density of

states (DOS), respectively.

Characterizations of phases and microstructures

The powder X-ray diffraction (PXRD) was characterized on a PANalytical Empyrean diffractometer. The *in situ* PXRD was performed on Rigaku Smartlab equipped with $\text{Cu K}\alpha$ ($\lambda = 1.5418 \text{ \AA}$). The electron probe micro-analysis (EPMA) measurements were carried out on the EPMA-8050G instruments, in which the analysis accuracy of the element content is less than 5%. The high-resolution transmission electron microscopy (HRTEM), energy-dispersive X-ray spectroscopy (EDS), and high-angle annular dark-field (HAADF) analysis of sheared InSb specimen were completed by the TEM observation performed on a Talos F200X microscope equipped with corresponding advanced accessories.

Measurements of thermoelectric properties

The temperature-dependent Hall coefficient (R_H) was obtained by using the van der Pauw technique under a reversible magnetic field ($\sim 1.5 \text{ T}$) [38]; the Hall carrier concentration (p_H) and Hall mobility (μ_H) were then calculated by the equation of $n_H = 1/(eR_H)$ and $\mu_H = R_H/\rho$, respectively. The Seebeck coefficient and electrical resistivity were measured by a commercial thermoelectric measurement system (ZEM-3, ULVAC). The longitudinal (v_L) and transverse (v_T) velocities were obtained from the measurement based on the OLYMPUS model 5072PR. The relative densities (d , refer to Table S1) and thermal diffusivity (D) of bulk samples were measured by the Archimedes method and laser flash method (LFA 427, NETZSCH); heat capacity (C_p) was derived from the Debye model (Supplementary information Note), and thus the thermal conductivity (κ) was derived from $\kappa = dDC_p$. The deviation of ZT values was considered as 20% [39], which can be detailed explicitly by the uncertainty of 10%, 5%, and 3% of thermal conductivity, Seebeck coefficient, and electrical resistivity, respectively.

RESULTS AND DISCUSSION

Phase characterizations and microstructure observations

Fig. 1 depicts the XRD patterns of InSb + z wt% QSe_2 -composited samples detailed by the z wt% SnSe_2 ($z = 0, 3, 6, 9$) and z wt% WSe_2 ($z = 0, 3, 6, 9$). Except for the well-matched main diffraction peaks of zinc-blende InSb, traces of second phases such as Se (PDF#54-0500), and SnSb (PDF#33-0118) were observed in the SnSe_2 composites as shown in Fig. 1a. The intensity of WSe_2 phase (PDF#71-0600) was increased with increasing concentration of z wt% (Fig. 1b). Especially, the PXRD analysis displayed in Fig. S1 confirms that the pure SnSe_2 and WSe_2 powders had been obtained, which clearly reveals that the WSe_2 is compatible with the InSb matrix while the SnSe_2 is not. According to the principle of lowest energy, the formation energy/atom of SnSe_2 and WSe_2 is -0.345 and -0.558 eV , respectively [40], which means that the SnSe_2 is more unstable than the WSe_2 at the same condition. Moreover, these nanocomposited samples were prepared at 733 K under 60 MPa; this high temperature and pressure may provide a suitable environment for SnSe_2 to react with InSb. Ulteriorly, EPMA was applied on the SnSe_2 - and WSe_2 -composited samples, as shown in Fig. 2a and Fig. S2. The back-scattered electron (BSE) image and corresponding EDS characterizations indicate that the elements of In and Sb are spread evenly in the matrix except for

Figure 1 The room-temperature XRD patterns of (a) InSb + z wt% SnSe₂ ($z = 0, 3, 6, 9$) and (b) InSb + z wt% WSe₂ ($z = 0, 3, 6, 9$) SPS-sintered samples.

Figure 2 (a) The BSE electron pattern of 3% WSe₂ sample, (b–e) the corresponding EDS element mapping accompanied by the EPMA measurement.

Table 1 The EDS analysis of the spots marked in Fig. 2a

Spots	Se	In	Sb	W	Se:W
1#	–	49.75	50.25	–	–
2#	58.50	0.68	0.98	39.84	1.47
3#	57.47	1.52	1.44	39.58	1.45

some fibrous W- and Se-rich regions. Moreover, the element analysis of area (Fig. 2b–e) and spots (Table 1) for the 3% WSe₂ sample manifests that these long W- and Se-rich inclusions are WSe₂ phases. The ratio of Se:W is slightly lower than the intrinsic nominal (~2), indicating that part of Se and W may be dissolved into the InSb crystal.

To further explore the microstructure of QSe₂-composited samples, we also adopted an advanced TEM technique to observe the 3% WSe₂ and SnSe₂ samples in an HAADF mode, as shown in Fig. 3 and Fig. S3a, respectively. It can be seen that the WSe₂ second phases were detected inside the composites (Fig. 3a). Moreover, a part of elongated fibrous WSe₂ inclusions (~300 nm) were embedded in the InSb matrix (Fig. 3b), a small amount of W and Se are uniformly dissolved in the matrix, and this can be formed as the W_{In}⁺, Se_{Sb}⁺ PDs suchlike. Similarly, several inhomogeneous phases with different Z-contrasts can be clearly observed in the SnSe₂ sample (Fig. S3a), and the corre-

sponding EDS results reveal that these impurities are indeed SnSb and Se, which is also consistent with the previous XRD measurement. The low-resolution TEM images in Fig. 4a, b and Fig. S3b, c affirm the ample hierarchical microstructures, and the inset of Fig. 4a is the corresponding selected area electron diffraction (SAED) pattern well indexed by the cubic InSb structure. A large amount of WSe₂ nanofibers (Fig. 4a, b), abundant dislocation clusters (Fig. 4c) and SnSb/Se nanoinclusions (Fig. S3b–d) germinated well in the InSb grains. Thereinto, the WSe₂ generated a good heterogeneous interface with the matrix due to the stable nature of WSe₂ and its congenial crystal formation energy with InSb. Strain simulation detailed by the geometric phase analysis (GPA) [41] was performed on the HRTEM image of Fig. 4d, which shows some drastically distorted regions between Grain A and Grain B. This can be directly revealed in the elastic strain map (inset of Fig. 4d) with aligned strain centers, facilitating an extensive phonon scattering

Figure 3 (a, b) The HAADF images of 3% WSe₂ sample and the corresponding EDS characterizations of surface scanning.

Figure 4 (a–c) The low-resolution TEM images of 3% WSe₂ sample with an inset of the SAED pattern in (a), displaying some embedded WSe₂ nanofibers and abundant dislocation clusters. The HRTEM images of (d) heterogeneous interface. Inset is the corresponding GPA. (e) WSe₂ nanostructure and (f) highly crystalline InSb matrix with the lattice spacing of ~0.33 nm.

induced by a heterogeneous interface. Overall, these hierarchical structures, as well as the dispersed clusters of dislocations and dense stacking faults (SFs, Fig. S3e, f) combined with a number of distorted centers (marked in the inverse fast Fourier transform image), play an important role in multi-scale phonon propagation barriers in the electrical and thermal transport properties for the InSb system, and this will be discussed in the following sections.

Electrical transport properties

The electrical properties of QSe₂-composited samples were displayed in Fig. 5, and the detailed properties of *z* wt% SnSe₂ and WSe₂ (*z* = 0, 3, 6, 9) samples are shown in Figs S4–S6. The electrical resistivity ρ of QSe₂ shows an obvious decrement with

elevating temperature compared with the pristine InSb (Fig. 5a), which are both far lower than the ultra-high electrical resistivity of WSe₂. Moreover, we conducted the Hall measurements as shown in Fig. 5b. It can be easily seen that the carrier concentrations of QSe₂ are increased, even though the mobilities are lower than that of the InSb matrix. The significant enhancement of carrier concentration can be ascribed to the implants of Sn, W and Se observed in the microstructure characterizations for QSe₂ samples. It should be noted that the concentration of nano WSe₂ is very low, and thus the p-type carriers of intrinsic WSe₂ cannot compensate the largely enhanced carrier concentration induced by PDs. The Seebeck coefficient $|S|$ of WSe₂-composited samples is larger than that of SnSe₂ (Fig. 5c), and the calculated conduction and valence band [42–44] aligned at Fermi level

Figure 5 The temperature dependence of (a) electrical resistivity, (b) Hall measurement, (c) Seebeck coefficient for InSb and QSe₂ (Q = Sn, W) composites with the cited experimental results of WSe₂ [36]. (d) The calculated energy structure of InSb matrix and WSe₂. (e) The evaluated energy gap obtained by the equation $E_g = K_B \ln(|n|/T^{1.5})/(T^{-1})$, where K_B , n is the Boltzmann constant and carrier concentration. (f) The deformation coefficient E_{def} calculated from the two-band model compared to the experimental results.

between InSb and WSe₂ indicate that the valence band maximum (VBM) of WSe₂ (~ -1.40 eV) is lower than that of the matrix (~ -0.62 eV) (Fig. 5d), which can effectively filter partial hole carriers, thus enhancing the whole Seebeck coefficient. With the measured Hall coefficient, the evaluated energy gap E_g values of InSb and QSe₂ samples are displayed in Fig. 5e. The reduced energy gap (~ 0.06 eV) of composited samples is consistent with the increased carrier concentration induced by the Q and Se co-doping. Furthermore, based on the Kane energy model (Supplementary information Note 1), the deformation coefficient (E_{def}) accompanied with the measured data for InSb and QSe₂-composited samples are displayed in Fig. 5f. The E_{def} differences between 323 and 673 K such as $E_{\text{def}}@_{\text{InSb}}$ from 31 to 44 eV, $E_{\text{def}}@_{\text{SnSe}_2}$ from 32.5 to 79 eV and $E_{\text{def}}@_{\text{WSe}_2}$ from 24 to 63 eV, suggest that the scattering effect between electrons and phonons increases significantly with increasing temperature, which is beneficial for decreasing the lattice thermal conductivity.

Thermal transport properties

The total thermal conductivities k_{tot} of InSb + z wt% QSe₂ (Q = Sn, W) samples as a function of temperature are depicted in

Fig. 6a. The k_{tot} of 9% SnSe₂ and 3% WSe₂ samples reduce significantly than the pristine InSb matrix; one of the reasons is the low intrinsic thermal conductivity of WSe₂ (~ 2.1 W m⁻¹ K⁻¹ at 300 K) as shown in Fig. 6a, and on the other hand it is mainly because of the reductions in lattice thermal conductivity k_{lat} thus leading to the decreased k_{tot} . More specifically, the k_{lat} of InSb decreases from ~ 14.1 to ~ 7.65 W m⁻¹ K⁻¹ in 3% WSe₂ and ~ 7.65 W m⁻¹ K⁻¹ in 9% SnSe₂ at room temperature, ~ 4.92 to ~ 2.73 and ~ 2.43 W m⁻¹ K⁻¹ at 673 K, respectively. For better analyzing the possibilities of k_{lat} -reduction, the calculated k_{lat} based on the well-known Callaway and two Kane band model (Supplementary information Note 2) with the consideration of various phonon scattering centers such as EP (electrons-phonons), GB (grain boundaries), PD, NP (nanoparticles) and SF are shown in Fig. 6b. The confirmed W_{In}⁺/Se_{Sb}⁺ PDs and observed WSe₂ nanosheets contribute most of the phonon scattering, thus significantly decreasing the k_{lat} . As presented in Fig. 6c, d, we further simulated the thermal transport and strain distribution (details refer to Supplementary information Note 3) with the comparison between nanofiber-based WSe₂ and pristine InSb. Assuming that the ambient heat flow (673 K) is transferred from the hot-side to the cold-side of composites (Fig. 6c), the

Figure 6 (a) The temperature-dependent total thermal conductivity k_{tot} of InSb and QSe₂ (Q = Sn, W) composites. (b) The lattice thermal conductivity k_{lat} vs. temperature with the comparison of theoretical k_{lat} obtained from the Callaway model. (c, d) The simulated thermal transport analysis of WSe₂-composited samples based on the heat transfer and structural mechanics module in COMSOL Multiphysics software.

Figure 7 (a) The ZT values vs. temperature for QSe_2 -composited InSb compared with the reported WSe_2 [36] and $SnSe_2$ [35] systems. (b) The engineering output power density ω_{max} and thermoelectric conversion efficiency η dependent on hot-side temperature T_h assumed by the single thermoelectric leg length $L = 5$ mm. The available mid-temperature SnTe thermoelectrics are included.

disorderly distributed WSe_2 nanosheets acting as obstacles can effectively delay the heat flow diffusion due to the mismatch of thermal conductivity, which is advantageous for building the internal temperature difference in composites or thermoelectric devices. Moreover, the localized thermal stress and temperature (Fig. 6d) indicate that the nanosheet-based WSe_2 disrupts the homogeneous thermal stress especially localized at the interface between WSe_2 and InSb matrix, enhancing the effect on suppressing the propagation of phonons and reducing the lattice thermal conductivity. The corresponding heat transfer model of InSb (Fig. S7) shows anhyseretic heat conduction and uniform thermal stress distribution. Thus the heat flow can be quickly transferred from hot- to cold-side, which is also consistent with the experimental thermal transport properties with a high thermal conductivity.

Thermoelectric performance of QSe_2 ($Q = Sn, W$) composites

In view of the anionic-cationic PDs (Q_{In}^+ , Se_{Sb}^+) and the favorable energy barrier between WSe_2 composites and InSb matrix, the power factor of 6% WSe_2 sample (Fig. S6c) was significantly improved to $33.3 \mu W cm^{-1} K^{-2}$ at 733 K, with a 60.1% and 43% increment compared with z wt% $SnSe_2$ composites (Fig. S5c) and pristine InSb, respectively. In addition, the abundant hierarchical microstructures such as heterogeneous interface and dislocations steadily reduce the total thermal conductivity and lattice thermal conductivity, thus enhancing the ZT values for z wt% QSe_2 composites as illustrated in Fig. 7a. The ZT increases significantly from ~ 0.35 for InSb to ~ 0.63 for 9% $SnSe_2$ and ~ 0.82 for 3% WSe_2 at 733 K, suggesting that the low-cost technology detailed by QSe_2 nanocompositing can synergistically regulate the electrical and thermal properties and effectively enhance the thermoelectric performance. Besides, the evaluation of potential power generation based on the Thomson and Joule heat [45,46] (Supplementary information Note 4) for optimized sample (3% WSe_2) was displayed in Fig. 7b, including a comparison to mid-temperature SnTe system [13] from 300 to 733 K. The engineering output power density ω_{max} of WSe_2 nanocomposites increases to $\sim 235 \mu W cm^{-2}$ at 733 K, superior

to pristine InSb as well as referred $Sn_{0.98}V_{0.02}Te$, enabling a thermoelectric conversion efficiency $\eta \sim 5.1\%$ assumed by the single thermoelectric leg length $L \sim 5$ mm. These encouraging results reveal that the mid-temperature InSb-based thermoelectrics may possess a promising prospect in practical power generation with further reduction in thermal conductivity.

CONCLUSIONS

In this work, we have simultaneously regulated the electrical and thermal properties of InSb-based thermoelectrics in virtue of a low-cost and efficient nanocompositing of QSe_2 ($Q = Sn, W$). More precisely, the improved electrical conductivity originated from the Q_{In}^+ and Se_{Sb}^+ PDs, since the deeper valence band of WSe_2 is conducive to hindering these appreciate hole carriers, thus leading to a relatively increment of Seebeck coefficient when exceeding the intrinsic excitation temperature. Compared with $SnSe_2$ composites and InSb, the enhanced power factor of $\sim 33.3 \mu W cm^{-1} K^{-2}$ at 733 K was achieved in the 3% WSe_2 sample. As for thermal transports, the thermal conductivity and lattice thermal conductivity were thus significantly reduced due to the hierarchical microstructures such as PDs, nanosheets/particles, and dislocations that constructed strong barriers to scatter multi-scale thermal phonons. Consequently, an enhanced ZT value of ~ 0.82 at 733 K with a 135% improvement was obtained in 3% WSe_2 sample, in combination with the engineering output power density ω_{max} of $\sim 233 \mu W cm^{-2}$ and thermoelectric conversion efficiency η of $\sim 5.2\%$ in the single InSb-based thermoelectric leg. To sum up, motivated by selecting suitable compounds, nanocompositing can artificially merge effective strategies such as PDs, nanoengineering, and energy filtering into one, which may provide an ingenious way to optimize the thermoelectric properties of other thermoelectric systems.

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Conflict of interest The authors declare that they have no conflict of interest.

Supplementary information Experimental details and supporting data are available in the online version of the paper.

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通过二维层状结构搭建能量和声子势垒提高InSb热电性能

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摘要 InSb是一种具有闪锌矿结构的窄带隙半导体, 在光电探测器、红外热成像、霍尔器件等领域有着广泛的应用。良好的能带结构、超高的电子迁移率和无毒性表明InSb可能是一种潜在的中温热电材料。InSb当前面临着一些关键挑战, 如高导热系数和小Seebeck系数, 导致其超高的晶格导热系数, 进而低的ZT值。鉴于此, 我们发展了一种z wt% QSe₂ (Q = Sn, W)纳米复合的高效策略, 即通过对二维层状QSe₂的纳米复合, 在InSb体系中引入Q_{In}⁺和Se_{Sb}⁺点缺陷。此外, 本征WSe₂的价带作为势垒可以散射相当数量的空穴载流子, 导致本征激发阶段的Seebeck系数升高。此外, 无序分布的纳米片/粒子和位错可以有效地阻碍热流扩散, 形成热声子的强散射。结果表明, 3% WSe₂样品的功率因子提高到~33.3 μW cm⁻¹ K⁻², 733 K时ZT值提高到~0.82, 工程输出功率密度 $\omega_{\max}$ ~233 μW cm⁻², 工程热电转换效率 η ~5.2%。