Spin–orbital coupling effect on the power factor in semiconducting transition-metal dichalcogenide monolayers

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Abstract

The electronic structures and thermoelectric properties of semiconducting transition-metal dichalcogenide monolayers MX$_2$ (M = Zr, Hf, Mo, W and Pt; X = S, Se and Te) are investigated by combining first-principles and Boltzmann transport theory, including spin–orbital coupling (SOC). It is found that the gap decrease increases from S to Te in each cation group when the SOC is opened. The spin–orbital splitting has the same trend with the gap reducing. The calculated results show that SOC has a noteworthy detrimental effect on the p-type power factor, while it has a negligible influence in n-type doping except for the W cation group, which can be understood by considering the effects of SOC on the valence and conduction bands. For WX$_2$ (X = S, Se and Te), SOC leads to an observable enhanced power factor in n-type doping, which can be explained by SOC-induced band degeneracy, namely the bands converge. Among all of the cation groups, the Pt cation group shows the highest Seebeck coefficient, which leads to the best power factor, if we assume that the scattering time is fixed. The calculated results show that MS$_2$ (M = Zr, Hf, Mo, W and Pt) have the best p-type power factor of all the cation groups, and that MSE$_2$ (M = Zr and Hf), WS$_2$ and MTe$_2$ (M = Mo and Pt) have a more excellent n-type power factor in their respective cation group. Therefore, these results may be useful for further theoretical prediction or experimental research of excellent thermoelectric materials from semiconducting transition-metal dichalcogenide monolayers.

Keywords: transition-metal dichalcogenide monolayers, spin–orbit coupling, power factor

(Some figures may appear in colour only in the online journal)

Introduction

Due to the Seebeck effect and Peltier effect, hot-electricity conversion can be achieved in thermoelectric materials to solve energy issues, and the dimensionless figure of merit [1, 2], $ZT = S^2\sigma T/(\kappa_e + \kappa_L)$, can characterize the efficiency of thermoelectric conversion, where $S$, $\sigma$, $T$, $\kappa_e$ and $\kappa_L$ are the Seebeck coefficient, electrical conductivity, absolute temperature, and the electronic and lattice thermal conductivities, respectively. It is interesting and challenging to search for high $ZT$ materials, and one of the key parameters is the power factor ($S^2\sigma$), which depends on the electronic structures of materials. As is well known, SOC has an important effect on the electronic structures of materials containing heavy elements like famous topological insulators [3, 4]. Recently, spin–orbital coupling (SOC) has proved to be very important for power factor calculations [5–12]. For thermoelectric material Mg$_3$Sn, when the SOC is included, the best n-type power factor is higher than the best in p type doping, which agrees with the experimental results [13]. Therefore, it is very important to consider SOC for theoretical analysis of the power factor.

The discovery of graphene has led to much attention being focused on two-dimensional (2D) nanostructures due to their unusual physical, mechanical and chemical properties. 2D transition-metal dichalcogenides (TMDs) have potential
applications in nanoelectronics and nanophotonics [14–22]. The physical and chemical properties of 2D-TMDs can be tuned by strain and applied electric field, controlling the composition and functionalizing [23–29]. Thermoelectric properties of low-dimensional materials have been a hotspot for their applications into high-performance thermoelectric devices, such as Bi₂Te₃ nanowire, 2D-phosphorene and silicene [30–34]. Compared with conventional bulk thermoelectric materials, the density of states (DOS) of 2D materials shows sharp changes near the Fermi level, which is a benefit for the Seebeck coefficient [35]. Low-dimensional materials have lower phonon thermal conductance, which benefits from higher phonon scattering [35]. These advantages of 2D materials may produce higher ZT values. The thermoelectric properties related to low-dimensional TMDs, including few layers, monolayers and nanotubes, have been widely investigated [36–40]. However, the SOC is neglected in these theoretical calculations of thermoelectric properties related to low-dimensional TMDs. Recently, we prove that SOC has a very obvious effect on the p-type power factor for MoS₂ [41].

Here, we systematically investigate the electronic structures and thermoelectric properties of semiconducting TMD monolayers MX₂ (M = Zr, Hf, Mo, W and Pt; X = S, Se and Te) by first-principles calculations and semiclassical Boltzmann transport theory within the generalized gradient approximation (GGA) plus SOC. It is found that both SOC-induced gap reducing and spin–orbital splitting increase from S to Te in each cation group. Calculated results show that SOC can not only reduce the power factor in p-type doping, but also can enhance the n-type doping, especially for the W cation group. These can be understood by considering their energy band structures. It is found that PtX₂ (X = S, Se and Te) may have more excellent thermoelectric properties due to the very high Seebeck coefficients.

The rest of the paper is organized as follows. In the next section, we briefly describe the computational details. In the third section we present the electronic structures and thermoelectric properties of semiconducting TMD monolayers. Finally, we give our discussions and conclusion in the fourth section.

**Computational detail**

First-principles calculations of semiconducting TMD monolayers are performed using density functional theory [42] within the full-potential linearized augmented-plane-waves method, as implemented in the package WIEN2k [43]. The GGA of Perdew, Burke and Ernzerhof (PBE) [44] is used for the exchange-correlation potential. The full relativistic effects are calculated with the Dirac equations for core states, and the scalar relativistic approximation is used for the valence states [45–47]. The SOC was included self-consistently by solving the radial Dirac equation for the core electrons and evaluated by the second-variation method [48]. We use 6000 k-points in the first Brillouin zone for the self-consistent calculation. We make harmonic expansion up to ℓₘₐₓ = 10 in each of the atomic spheres, and the plane-wave cutoff is determined by $R_{\text{mt}} * k_{\text{max}} = 8$. The self-consistent calculations are considered to be converged when the integration of the absolute charge-density difference between the input and output electron density is less than 0.0001|e| per formula unit, where e is the electron charge. Transport calculations are performed using the semiclassical Boltzmann transport theory within the constant scattering time approximation (CSTA) and rigid band approach as implemented in BoltzTrap [49] (note: the parameter LPFAC cannot choose the default value 5, and should choose a larger value; here, we choose a LPFAC value of 20), which has been applied successfully to several materials [50–52]. To enable accurate Fourier interpolation of the Kohn–Sham eigenvalues, we use 90000 k-points in the first Brillouin zone for the energy band calculation.

**Main calculated results and analysis**

The single-layer MX₂ contains three atomic sublayers with the metal atom M in the center sublayer, while X atoms locate in the top and bottom sublayers. The different stacking of top and bottom X sublayers leads to two crystal structures, namely a 1T structure (M = Ti, V, Zr, Hf and Pt) and 2H structure (M = Nb, Mo, Ta and W), which are shown in figure 1. The ionicity of MX₂ leads to two distinctive structures, and the 1T structure supports higher ionicity, which is due to a longer distance between the X atoms of the top and bottom sublayers. In [53], Zhuang et al predict that 27 single-layer MX₂ can be fabricated from bulk crystals due to small formation energies (some of them have been achieved experimentally, such as MoS₂, MoSe₂ and WS₂). 13 MX₂ of which are semiconductors. Because good thermoelectric materials are usually narrow-gap semiconductors, we focus on semiconducting TMD monolayers MX₂ (M = Zr, Hf, Mo, W and Pt; X = S, Se and Te). The crystal structure of single-layer MX₂ is built with the vacuum region of 18 Å to avoid spurious interaction. The optimized lattice constants $a$ [53] are used to do our DFT calculations, which are listed in table 1.

We investigate their electronic structures by using GGA and GGA+SOC, and plot their energy band structures in figures 2 and 3 (note: the high-symmetry path K-Γ-M-K is chosen for the 1T structure, and Γ-K-M-Γ for the 2H structure).
constant or a lattice constant obtained using the HSE functional is used. The minimum energy of the valley between the \( \Gamma \) and \( K \) points in the conduction band depends quite sensitively on the lattice constant.) The \( \text{ZrX}_2 \) and \( \text{HfX}_2 \) are indirect band gap semiconductors with the VBM at the \( \Gamma \) point and CBM at the \( M \) point. The VBM appears at the \( \Gamma \) point, while the CBM is between the \( \Gamma \) and \( K \) points for \( \text{PtS}_2 \) and \( \text{PtTe}_2 \). The VBM of \( \text{PtS}_2 \) is between the \( \Gamma \) and \( K \) points, while the CBM appears between the \( \Gamma \) and \( M \) points. The GGA gaps, GGA+SOC gaps and the differences between them are listed in table 1. The calculated GGA gaps are consistent with other theoretical values [36, 53]. To clearly see the gap trend, the related gap values also are plotted in figure 4. It is found that the gap of \( \text{MX}_2 \) decreases from \( \text{S} \) to \( \text{Te} \) with the same \( M \), while the difference between the GGA and GGA+SOC gaps gradually increases. The larger gap decrease means the larger movement of conduction bands toward low energy, which reflects the SOC effects on the conduction bands. The SOC effects on the valence bands near the Fermi level can be described by spin–orbit splitting at the \( \Gamma \) point with 1T structure or the \( K \) point with 2H structure near the Fermi level in the valence bands, which are listed in table 1 and plotted in figure 4. Our GGA spin–orbit splitting values agree with other calculated ones [55, 56]. From \( \text{S} \) to \( \text{Te} \), the spin–orbital splitting value increases in each cation group. These data show that SOC produces more obvious effects on the valence bands than the conduction bands.

The semi-classic transport coefficients are calculated within the CSTA Boltzmann theory. Calculating scattering time from first-principles calculations is challenging due to the complexity of various carrier scattering mechanisms. To mimic the doping effects on the transport coefficients, the rigid band approach is used, and only the Fermi level is shifted to change the doping level. If the doping level is low, the rigid band approximation is reasonable, which has been widely used for theoretical study of thermoelectric materials [49, 57–59], and the calculated transport coefficients agree well with the experimental results. The Seebeck coefficient \( \mathcal{S} \), electrical conductivity with respect to scattering time \( \sigma/\tau \) and power factor, with respect to scattering time \( S\sigma/\tau^2 \) as a function of doping level at the temperature of 300 K by using GGA and GGA+SOC, are shown in figure 5. The n-type doping (negative doping levels) with the negative Seebeck coefficient is related to the conduction bands, while p-type doping (positive doping levels) with the positive Seebeck coefficient is connected to the valence bands. When the Fermi level is located in the middle of the band gap, the Seebeck coefficient has a very large value, but low electrical conductivity due to low carrier concentration leading to a very small power factor. As the Fermi level moves into the conduction bands or valence bands (change the doping level), the electrical conductivity increases and the Seebeck coefficient decreases, and the power factor reaches its maximum at a certain doping level.

Firstly, we consider SOC effects on transport coefficients \( S \), which is independent of scattering time \( \tau \), and can be directly compared with experimental results. It is found that SOC has a detrimental influence on \( S \) (absolute value) in

![Figure 2. The energy band structures of monolayer MX2 (M = Zr, Hf, X = S, Se) by using GGA (black solid lines) and GGA+SOC (red short dash-dot lines).](image)

**Table 1.** The optimized lattice constant \( a (\text{Å}) \); the calculated gap values with GGA \( E_1 \) (eV) and GGA+SOC \( E_2 \) (eV); \( E_1 - E_2 \) (eV); spin–orbit splitting \( \Delta \) (eV) at the \( \Gamma \) point with 1T structure or the \( K \) point with 2H structure near the Fermi level in the valence bands. These values in the parentheses are else theoretical values in [53, 55].

| Name   | \( a \)    | \( E_1 \) | \( E_2 \) | \( E_1 - E_2 \) | \( \Delta \) |
|--------|------------|-----------|-----------|----------------|-------------|
| \( \text{ZrS}_2 \) | 3.68       | 1.16 (1.19)| 1.12      | 0.04           | 0.09        |
| \( \text{ZrSe}_2 \) | 3.80       | 0.50 (0.50)| 0.35      | 0.15           | 0.28        |
| \( \text{HfS}_2 \)  | 3.64       | 1.22 (1.27)| 1.16      | 0.06           | 0.13        |
| \( \text{HfSe}_2 \) | 3.76       | 0.59 (0.61)| 0.42      | 0.17           | 0.32        |
| \( \text{MoS}_2 \)  | 3.18       | 1.70 (1.68)| 1.63      | 0.07           | 0.15 (0.148)|
| \( \text{MoSe}_2 \) | 3.32       | 1.44 (1.45)| 1.34      | 0.10           | 0.18 (0.184)|
| \( \text{MoTe}_2 \) | 3.55       | 1.09 (1.08)| 0.96      | 0.13           | 0.21        |
| \( \text{WS}_2 \)   | 3.18       | 1.86 (1.82)| 1.60      | 0.26           | 0.42 (0.430)|
| \( \text{WSe}_2 \)  | 3.32       | 1.56 (1.55)| 1.28      | 0.28           | 0.46 (0.466)|
| \( \text{WTe}_2 \)  | 3.55       | 1.09 (1.07)| 0.78      | 0.31           | 0.48        |
| \( \text{PtS}_2 \)  | 3.57       | 1.76 (1.81)| 1.73      | 0.03           | 0.21        |
| \( \text{PtSe}_2 \) | 3.75       | 1.37 (1.41)| 1.20      | 0.17           | 0.34        |
| \( \text{PtTe}_2 \) | 4.02       | 0.77 (0.79)| 0.38      | 0.39           | 0.49        |
Figure 3. The energy band structures of monolayer MX\textsubscript{2} (M = Mo, W, Pt; X = S, Se, Te) by using GGA (black solid lines) and GGA+SOC (red short dash-dot lines).
pressure or doping [10, 63]. Figure 6 shows that SOC can lead to 2D-like DOS of conduction bands near the Fermi level for WS$_2$. Secondly, the SOC has little effect on $\sigma/\tau$ for MX$_2$ ($M = $ Zr, Hf and Mo) in n-type doping, but has observable effects for MX$_2$ ($M = $ W and Pt). In [54], the work shows that the SOC can lead to spin polarization of the bands, and therefore certain scattering processes will be prohibited in the presence of SOC. Here, we only consider that the SOC leads to changes in the effective masses and degeneracy between different minima in the band structure, which gives rise to the changes of $\sigma/\tau$, and ignores the fact that the SOC leads to spin-polarization of the bands and hence certain selection rules in the scattering processes. For p-type doping, the SOC influences on $\sigma/\tau$ are more obvious with respect to the ones in n-type doping. These can be understood by SOC-induced band localization or delocalization.

Finally, the SOC effects on the power factor are considered, which is a comprehensive physical quantity for the electrical performance of thermoelectric materials. Due to the power factor being proportional to $S$ and $\sigma$, the SOC has a remarkable detrimental influence on the power factor in p-type doping, while it has a weak influence in n-type doping except for WX$_2$. The power factors of WX$_2$ can be significantly improved in the presence of SOC. To clearly see the SOC effects on the power factor, the power factors with the doping level 0.01 electrons or holes per unit cell by using GGA and GGA+SOC at $T = 300$ K are plotted in figure 7. Although the scattering time $\tau$ is unknown, comparison of the relative power factor values among these TMD monolayers MX$_2$ may be useful for experimental guidance on searching for excellent thermoelectric materials. For Zr, Hf, W and Pt series, the n-type doping has better power factors than p-type doping. For MoX$_2$, the p-type power factor of MoS$_2$ is larger than the one in n-type doping, while it is opposite for MoSe$_2$ and MoTe$_2$. These can be easily observed from figure 7. If we assume the scattering time $\tau$ is constant for MX$_2$, the Pt series have a larger power factor due to the larger Seebeck coefficient $S$. It is worth noting that the local Rashba spin polarization and spin-layer locking have been observed in monolayer PtSe$_2$, which can realize electrically tunable spintronics [64]. For each cation group, we summarize the best power factors for both n-type and p-type, as shown in figure 8. It is found that MS$_2$ has the best power factor in p-type doping for all the cation groups. For n-type, MS$_2$ ($M = $ Zr and Hf), WS$_2$ and MTe$_2$ ($M = $ Mo and Pt) have a more excellent power factor in their respective cation groups.

**Discussions and conclusion**

As is well known, the SOC removes the band degeneracy by spin–orbit splitting, which can modify the outlines of energy bands. These SOC effects can lead to a remarkable influence on the Seebeck coefficient, and further affect the power factor. The SOC-induced detrimental influence on the power factor in Mg$_2$Sn [5, 10] and half-Heusler ANiB ($A = $ Ti, Hf, Sc, Y; $B = $ Sn, Sb, Bi) [6], especially for p-type doping, has been
observed. For monolayer MX$_2$, SOC can reduce the power factor for p-type in the considered doping range, but can also improve the one in n-type doping for some of them, especially for WX$_2$. The SOC can also lead to the conversion of the best power factor between n- and p-type doping. For example, in the absence of SOC, the p-type has a better power factor for PtS$_2$. However, including SOC, the n-type doping shows a more excellent power factor. So, it is very important for power factor calculations to include SOC for semiconducting TMD monolayers MX$_2$. 

Figure 5. At $T = 300$ K, transport coefficients, including Seebeck coefficient $S$ (left), electrical conductivity with respect to scattering time $\sigma/\tau$ (middle) and power factor with respect to scattering time $S^2\sigma/\tau$ (right), as a function of doping level calculated with GGA (solid lines) and GGA+SOC (short dash-dot lines). The doping level is defined as electrons (minus value) or holes (positive value) per unit cell.
Symmetry-driven degeneracy, low-dimensional electronic structures and accidental degeneracies can lead to an enhanced power factor. Here, SOC-induced degeneracy of the conduction band extremum produces a significantly improved power factor for WX₂ (W = S and Se). In fact, strain is a very effective way to tune the electronic structures of materials, which can achieve an improved power factor. The electronic structures of the monolayer MX₂ have a sensitive strain dependence, which provides a platform to realize a higher power factor. In [41], the first-principle calculations predict that both compressive and tensile strain at the critical strain of the direct-indirect gap transition can induce the accidental degeneracies for MoS₂, which can produce a more excellent power factor in a certain doping range. For Pt cation group, the outlines of valence bands near the Fermi level are very distinct. However, the valence bands’ outlines of PtS₂ near the Fermi level can be attained from recently-synthesized PtSe₂ [66] by tensile strain, and the ones of PtTe₂ can also be achieved by compressive strain. (These results have been tested by the first-principle calculations.) Therefore, it is possible to realize a higher power factor for semiconducting monolayer MX₂ by strain tuning.

In summary, we investigate electronic structures and thermoelectric properties of semiconducting TMD monolayers using GGA+SOC, based mainly on the reliable first-principle calculations and Boltzmann transport theory. It is found that the inclusion of SOC is crucial for power factor calculations, due to the remarkable SOC influences on the energy band structures of TMD monolayers. The calculated results show that the Pt series may be potential thermoelectric materials due to the large Seebeck coefficient S. The present work is useful for further theoretical calculations and experimental guidance on searching for excellent thermoelectric materials from TMD monolayers.

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