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Tunable Electronic Structure in Twisted Bilayer WTe$_2$

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The moiré pattern restricts the electronic states of transition metal bilayers, thus extending the concept of the magic angle found in twisted bilayer graphene to semiconductors. Here, we have studied the electronic structure of the twisted bilayer WTe$_2$ using first-principle calculations. Our result shows that a twist significantly changes the band structure, resulting in the bandgap engineering when the twisted bilayer of WTe$_2$ is turning to a specific angle. The electronic structure is changed by the change of the twist angle. Interestingly, a semiconductor-to-metal phase transition is found at a twist angle of 15°. Our results provide a reference for the regulation of two-dimensional band structures. These results are important for understanding the electronic structure of twisted systems and for future applications in electronic devices.

Keywords: twisted angle, WTe$_2$, electronic structure, first-principle calculations, twisted bilayer

INTRODUCTION

Twisted bilayer graphene (TBG) has been investigated in recent years to find the existence of strongly correlated [1–5] insulating insulators [6] and superconducting states [4] in magic angle [7]. The combination of theory and experiment has facilitated the development of research in this area. The emergence of insulator behavior and unconventional superconductivity in magic-angle twisted bilayer graphene (TBG) has attracted great interest in this field of research [8–10].

In recent years, the extended family of transition metal dichalcogenide (TMDC) [10–17] has provided a wide range of possible rotational stacked bilayer systems. TMDC has prompted a large number of experimental [18, 19] and theoretical [20, 21] studies to understand such limited moiré states in semiconductor materials, especially in WTe$_2$. Recently, it has been reported that the bandgaps of both monolayer and bilayer twisted 2H-MoTe$_2$ from indirect bandgap to direct bandgap transitions, and also, semiconductor-to-metal phase transitions occur [22]. Lately, the effect of the stacking mode on the electronic structure of the multilayer MoSe$_2$ has been emphasized. Then, it has been reported that the photoluminescence intensity ratio of ions and excitons reaches a maximum at a twist angle of 0 or 60° for twisted bilayer MoSe$_2$/WSe$_2$ [21]. Twisted bilayer MoS$_2$ was found to show flat bands at the twist angles of 5 and 6°, and the average velocity disappears at a twist angle of 2° [18, 23]. The presence of flat bands has also been found in twisted bilayer WSe$_2$. For example, it has been recently reported that the electronic structure of twisted bilayer WSe$_2$ samples was found to have flat bands at the twist angles of 3 and 57.5° by scanning tunneling spectroscopy [24]. The optical detection of strongly correlated phases in the WS$_2$/WSe$_2$ superlattice reveals Mott insulator states at one cavity at each superlattice position and surprising insulating phases of 1/3 and 2/3 filling of the superlattice. It is found that the transport of WSe$_2$/WS$_2$ is also dependent with distortion [25]. For example, by transient absorption microscopy combined with first-principle calculations to study the

WS$_2$/WSe$_2$ heterogeneous bilayer interlayer exciton dynamics and transport in the time, space and momentum domains of the molecular layers are studied. It was found that exciton motion around 100 meV is modulated by a moiré potential dependent on the twist [26].

WTe$_2$ is a type-II Weyl semi-metal (WSM). The topologically protected valence bands and conduction bands lead to contacting points between electrons and holes near the Fermi level. WTe$_2$ has promising applications in the fields of low dissipation electrons, semiconductors, spintronics, optoelectronics, thermodynamics, and catalysis [27, 28]. However, WTe$_2$ has been less studied so far and has not been fully investigated. Theoretical guidance is also needed for conductivity, unlike some 2D materials such as graphene [29]. A recent theoretical work [30–33] predicts that WTe$_2$ is a new type of Weyl half-metal with a strongly tilted Weyl cone. This Weyl cone arises from the crossover with excellent properties such as chiral anomaly, non-saturable large magnetoresistance (MR), pressure-induced superconductivity, and ultra-low thermal experiments.

Previous studies have not made a systematic pattern of bandgap evolution with a twist angle. Here, our studies have made a systematic pattern of bandgap evolution with a twist angle. The study of twisted bilayer WTe$_2$ confirms that it is possible to modulate the electronic structure by twisting to make the electrons correlate stronger. These findings serve as a sufficient theoretical basis for guiding experiments and provide a highly tunable experimental platform for strong correlation physics.

METHOD AND MODELS

The density functional theory (DFT)-based Vienna *ab initio* simulation package (VASP) [34] is used for the theoretical calculations with the projector augmented wave (PAW) method [35]. The generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) function [36, 37] is used for the exchange and correlation potential. The experimental crystal constants for non-twisted bilayer WTe$_2$ are $a = b = 3.550$ Å, $c = 15$ Å, $\alpha = \beta = 90°$, and $\gamma = 120°$ [38]. To study the electronic structure of the twisted bilayer WTe$_2$ system, we constructed a supercell containing two 3×3 WTe$_2$ monolayers with 54 atoms, where the first layer is stationary and the other layer is rotated by an angle, and a vacuum region of 15 Å, which is added in the vertical direction of the WTe$_2$ layer. We sampled a range of interlayer orientation angles from 0 to 15°. The space group of all twisted systems was P6$_3$/mmc. In the relaxation of non-twisted and twisted bilayer WTe$_2$ structures, all atoms are relaxed until the force on each atom is 0.02 eV Å^{-1} and the energy convergence criteria of 1×10^{-6} eV is met. A plane wave cutoff energy of 500 eV was used. The Brillouin zone (BZ) was sampled by using $12 \times 12 \times 1$ Monkhorst–Pack grids for non-twisted and twisted bilayer WTe$_2$ structures. Because van der Waals correction is important for the bilayer WTe$_2$ system, the DFT-D3 van der Waals correction was taken into account. Spin-orbit coupling (SOC) is considered in the calculation of electronic properties [39].

RESULTS AND DISCUSSION

AB stacking is the most stable form of stacking [38]. We used the AB stacking form when calculating the twisted bilayer WTe$_2$ structure, as shown in **Figure 1A**. With the increase of the twist angle, the symmetry and periodicity of the system inevitably break. The inevitable breaking of symmetry and periodicity of systems lead to a change in the twisted bilayer WTe$_2$ band structure and the van der Waals (vdW) coupling between the layers changes at the same time. Depending on previous studies, the vdW interlayer interaction plays a decisive role in MX$_2$ [25]. So the effect of DFT-D3 on the twist angle between the layers was considered in the calculation. **Figures 2A,D** show the band structure of the twisted bilayer WTe$_2$ along with the high symmetry point, and the bandgap of the electronic structure shows a very interesting pattern with the variation of the twist angle. For instance, the structure with a twist angle of 0° has a direct bandgap, with the valence-band maximum (VBM) and the conduction-band minimum (CBM) are all located at the G point. For the structure with a twist angle of 0°, the maximum bandgap is about 0.74 eV, which is the largest bandgap from 0 to 15°. However, the structure with a twist angle of 15° has a direct bandgap, with VBM and CBM all locating at the G point, as shown in **Figure 2D**. When the twist angle goes to 15°, VBM increases and CBM decreases with the increase in the twist angle and finally becomes zero. The maximum bandgap is zero, which is the smallest bandgap from 0 to 15°, indicating that the bandgap is very sensitive to the change in the twist angle. When the twist angle is 14°, the bandgap is a direct bandgap. For the structure with a twist angle of 14°, the bandgap is about 0.06 eV. Direct bandgap semiconductors facilitate better utilization of light, as shown in **Figures 2A,D**.

The valence-band maximum and conduction-band minimum for the systems of 0, 10, 14, and 15° are located at the G point. The bandgaps for non-twisted and twisted systems of 0, 10, 14 and 15° are different. The results show that the bandgap changes very significantly for larger twist angles from 0 to 15°. For example, for structures with a twist angle of 15°, the bandgap is zero. The change of the bandgap with the twist angle may be a common feature of the twisted structure WTe$_2$, and significant changes in its luminescence properties are expected. Twists along the superposition direction change the interlayer distance and thus significantly alter the interlayer vdW interaction [22]. Previous studies have also found that twists can sensitively change the electronic properties of the edges of molybdenum disulfide [16–19, 22, 40].

From the aforementioned band structure diagram, we observe that the bandgap and ΔE vary with the twist angle. We present this regularity in the following, as shown in **Figures 3A,B**. The bandgap of WTe$_2$ is very sensitive to the change of the twist angle. The bandgap changes accordingly as the twist angle changes continuously. The bandgap decreases trends from 0 to 15°. The bandgap determines the energy required for the valence-band electrons to leap to the conduction band. The larger the bandgap, the higher the leap energy, the less likely the electrons will be excited. Therefore, when the twist angle is from 0 to 15°, the bandgap shows an overall decrease tendency, which is favorable

FIGURE 1 | Top view of the twisted bilayer WTe₂ crystal structure with twist angles of **(A)** 0˚, **(B)** 10˚, and **(C)** 15˚. Side view of the twisted bilayer WTe₂ corresponds to the twist angles of 0˚. Blue and purple represent W and Te atoms, respectively.

FIGURE 2 | Band structures of bilayer WTe₂ with twist angles **(A)** 0˚, **(B)** 10˚, **(C)** 14˚, and **(D)** 15˚. Specific torsional values are indicated accordingly in the plots. Light black dashed dots represent Fermi energy.

for the valence-band electrons to jump to the conduction band. When the twist angle is from 0 to 15˚, the bandgap shows an overall decrease tendency, and the binding effect on the valence-band

electrons is weaker, which is favorable for the valence-band electrons to get rid of the valence bonds and also favorable for conductivity. When the angle is turned to a particular angle, the appearance of the reduced bandgap may reduce the carrier, when the kinetic energy of the carrier is quenched, the enhanced electron–electron interaction may lead to the appearance of a strongly correlated phase [6, 41–44].

The ΔE varies with the twist angle trend of fluctuation and is very large. The ΔE of the twisted bilayer WTe₂ is obtained by subtracting the energy without the twist angle from the energy after the twist angle. As the twist angle increases, the energy change of the twist angle also shows the result of certain changes. When the twist angle is from 0 to 15˚, the energy tends to decrease overall. It can be seen from the relationship between ΔE and the twist angle as described before, as shown in **Figure 3B**. When the twist angle is 1˚, the corresponding energy is the largest, which means that the system is the most unstable compared to twisted systems with other twisted angles. But when the twist angle is 15˚, the corresponding energy is the smallest, which means that the system is the most stable compared to other twisted systems with other twisted angles.

We explain it in terms of the projected density of states (PDOS), as shown in **Figures 4A,D**. The PDOS of twisted bilayer WTe₂ mainly has the d-orbitals of W and the p-orbitals of Te atoms as the contributions near the Fermi level. As the twist angle increases, the density of states moves toward

FIGURE 3 | (A) Bandgap of bilayer WTe₂ as a function of the twist angles. **(B)** ΔE (the total energy difference that is relative to the untwisted WTe₂) as a function of the twist angles.

FIGURE 4 | Projected density of states (PDOS) of WTe₂ with and without twist angles. PDOS of twisted bilayer WTe₂ with twist angles **(A)** 0°, **(B)** 10°, **(C)** 14°, and **(D)** 15°.

FIGURE 5 | (A) Distance between Te and Te atoms as a function of twist angles. **(B)** Side view of WTe₂, where d [d represents the Te–Te distance in Figure **(B)**] is the distance between Te and Te atoms.

FIGURE 6 | (A,B) Charge density difference with the charge density at 10° and 15° subtracting the charge density at 0°. The isosurface value is 7×10^{-2} e per bohr^3. The yellow isosurface indicates gained electrons, while the blue isosurface indicates lost electrons.

the Fermi level and the bandgap of the system substantially decreases for 10, 14, and 15°. At 14°, the system shows an approximate zero bandgap state with a bandgap of only 0.07 eV, while at 15°, the bandgap of the system is completely closed and the system appears metallic.

Interestingly, the PDOS are shown in **Figures 4A,D**. When the twist angle is turned from 0 to 15°, we derive that the PDOS is localized in peaks. This new localization significantly changes the transport properties [19–21, 45, 46]. Because of the localization of PDOS, there are sharp peaks at the Fermi level of the PDOS. The peaks of PDOS lead to a strong change in the density of states. As the twist angle increases, the sharp peaks move toward near the Fermi level, with the sharp peaks of 1.4 eV for a twist angle of 0°, 1.3 eV for a twist angle of 10°, 1.0 eV for a twist angle of 14°, and
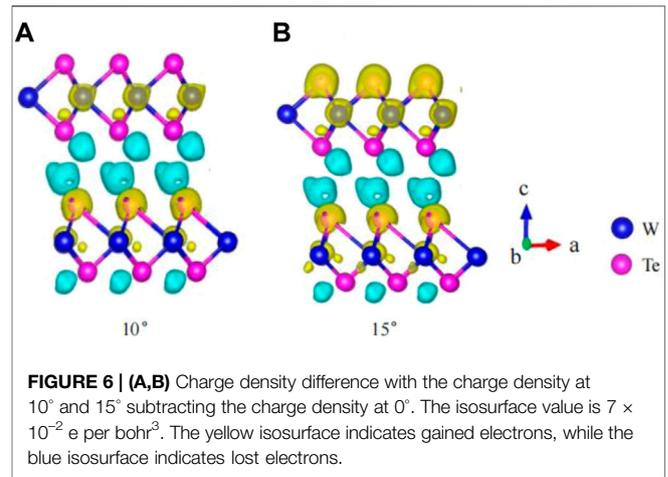
0.9 eV for a twist angle of 15°. These peaks are due to the relatively localized electrons in the d-orbital of the W atom. We conjecture that the change of the bandgap is influenced by the changes of these peaks.

When the twist angle reaches 15°, the PDOS is localized compared to 0° twisted systems. When the twist angle reaches 15°, the appearance of sharp peaks near the Fermi level and the movement of electrons in the p-orbitals of the Te and d-orbitals of W atoms move toward near the Fermi level resulting in a bandgap of 0 eV. Therefore, the bandgap changes due to the electrons of the p-orbitals of Te and d-orbitals of W atoms move toward near the Fermi level, and there are sharp peaks near the Fermi level.

Next, we explain it in terms of the distance between Te and Te atoms, as shown in **Figures 5A,B**. As the twist angle increases, there is an overall tendency for the distance between Te and Te atoms to decrease when the twist angle is from 0 to 15°. The bandgap shows an overall decrease tendency when the twist angle is from 0 to 15°. Therefore, as the twist angle increases, the bandgap decreases as the distance between Te and Te atoms decreases when the twist angle is from 0 to 15°. The bandgap is affected as the overall distance between Te and Te atoms tends to decrease.

Figure 6 depicts the charge density difference at the twisted bilayer WTe₂ interlayer, which is defined by subtracting the charge density at the twist angle from the charge density without the twist angle. Finally, it is explained by the charge density difference, as shown in **Figures 6A,B**. With the increase of the twist angle, the electron gaining the ability of W atoms is enhanced, and the number of electrons gained is increased, which affects the change of bandgap due to the transfer of electrons. When the twist angle is 10°, the W atoms gain electrons. In the case of equal planes, it is advantageous for the W atoms, and the covalent bond is enhanced. When the twist angle is 15°, it is favorable for W atoms to gain electrons more easily.

From **Figure 6**, we know that W atoms with 15° get more electrons than those of 10°. The charge density overlapping at a twist angle of 15° is more than that with the twist angle of 10°. So the bandgap of 15° is smaller than that of 10°. The bandgap at 10° is 0.45 eV, while the bandgap at 15° is zero. It means that the transfer of charge affects the bandgap.

CONCLUSION

In summary, we have performed first-principle calculations of the electronic structure of twisted bilayer WTe₂. The bandgap is very sensitive to the variation of the twist angle. When the twist angle is 0°, the bandgap is the largest compared to other twisted systems, and the bandgap is a direct bandgap. However, when the twist angle is 15°, the bandgap is the smallest compared to other twisted systems, and the bandgap is a direct bandgap. Twist significantly changes the band structure resulting in bandgap engineering when the twisted bilayer WTe₂ is turning to a specific angle. The calculations demonstrated that the twist significantly changes the band structure of the bandgap. A semiconductor-to-metal phase transition is found at 15°. The same VBM/CBM and the components of the orbitals near the Fermi level exhibit drastic change under twist. These significant changes near the Fermi level for a twisted system will result in a significant change in optical and electronic transport properties. Twisted layered materials have potential applications in future electronic devices. The realization of twisted layered materials provided a platform in the future to study strongly correlated superconducting behavior and the unconventional superconductivity of insulator states.

DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article/Supplementary Material, further inquiries can be directed to the corresponding authors.

AUTHOR CONTRIBUTIONS

KZ and J-MZ: conceived and supervised this work. Z-SC: performed the calculations. Z-SC and KZ: wrote the manuscript. LH, W-TG, and ZH: analyzed the data and provided valuable and constructive suggestions.

ACKNOWLEDGMENTS

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