Band Gap Engineering of Twisted Bilayer MoS2 Sheets

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Abstract—Density functional theory (DFT) calculations were performed to predict the modulation of band gap by twisting bilayer MoS2 sheets with different rotation angles. The electronic band structure results show that the rotations can make bilayer MoS2 sheets change from semiconducting to metallic. The band gap decreases from 1.24eV to 0.06eV. These results would open up possibilities for its applications in nanoelectronic devices simply by tuning band gaps of MoS2 with rotation angles.

1. INTRODUCTION

Graphene as a two-dimensional nanomaterial has attracted much attention due to its outstanding electronic, mechanical, optical and chemical properties [1-2]. However, the absence of a band gap in pristine graphene is a huge challenge for its application in semiconducting nanodevices, such as FET [3-4]. Therefore, more and more attention has been made to search for an alternative layered material to replace graphene. The promising candidate material is 2D molybdenum disulfide (MoS2) which is a semiconductor with an indirect band gap of about 1.2eV [5]. Unlike graphene, a monolayer MoS2 is a sandwich structure which is composed of three atomic layers: a Mo layer sandwiched between two S layers. Researches have shown that MoS2 has comparable or even better electronic properties than those of pristine graphene, such as high mobility, large on/off ratios (1 × 108) and tunable band gaps.

Several strategies have been developed by researchers to engineer band gaps of MoS2. Like graphene, some theoretical studies predicted that armchair MoS2 nanoribbons are semiconducting with an almost constant band gap, whereas zigzag MoS2 nanoribbons are metallic [6-7]. The band gap modulation in MoS2 sheets is investigated by applying external electric field using first-principles calculations [8-10]. Tensile strains and functionalization can also tune the electronic properties of monolayer and multilayer MoS2 sheets [11-14]. Nevertheless, the effect of rotation on the electronic properties of bilayer MoS2 sheets remains to be investigated.
In this paper, band gap engineering by twisting bilayer MoS$_2$ sheets is investigated through first-principles calculations. It’s shown that the electronic properties of bilayer MoS$_2$ sheets change from semiconducting to metallic with different rotation angles.

2. METHOD AND MODELS
The twisted bilayer MoS$_2$ sheets are constructed by fixing one layer and rotating another layer with an rotation angle $\theta$. In this case, Moiré patterns will be formed as depicted in Figure 1(a). The supercell model for all computations is shown in Figure 1(b).

All calculations were performed using the density functional based tight-binding (DFTB) method. The local Density Approximations (LDA) and a 150 Ry cutoff were used in all the computations. Periodic boundary conditions (PBC) along X and Y direction with a k-point sampling of 10*10*1 were applied. The structure optimization of twisted bilayer MoS$_2$ sheets is performed first.

3. RESULTS AND DISCUSSIONS
The band structures of bilayer MoS$_2$ sheets with different rotation angles are systematically studied. Figure 2 shows the band structures of the rotation angle $\theta$ changing from 0° to 10°. The results show that the band gaps are 1.24eV, 1.20eV, 1.10eV, 0.97eV, 0.85eV, 0.70eV, 0.46eV, 0.25eV, 0.11eV, 0.04eV and 0.06eV, respectively. The band gap of bilayer MoS$_2$ without rotation is agreement with the previous calculations [5]. Figure 3 shows the band gaps of bilayer MoS$_2$ with different rotation angles. When $0^\circ \leq \theta \leq 10^\circ$, the band gap decreases with the increasing of the rotation angles. The values decrease almost to 0.06eV. It indicates that the bilayer MoS$_2$ sheets change from semiconducting to metallic. When $10^\circ < \theta < 60^\circ$, the band gaps are basically around at 0.06eV.

Figure 1. The geometry structure of bilayer MoS$_2$ with different rotation angles. (a) Top view. (b) Side view.
Figure 2. The band structures of bilayer MoS2 sheets with different rotation angles.

To quantitatively characterize the interaction of the two layers, the binding energy per layer of the twisting bilayer MoS2 sheets is calculated as

$$E_{\text{binding}} = \frac{- (E_{\text{tot}} - E_{\text{fix}} - E_{\text{rot}})}{2}$$

where $E_{\text{tot}}$, $E_{\text{fix}}$, and $E_{\text{rot}}$ are the energies of the bilayer sheets, isolated fixed monolayer, and rotation monolayer, respectively. The binding energies of bilayer MoS2 sheets with different rotation angles are shown in Figure 4. The rotation can change the interaction of bilayer MoS2 sheets.
Figure 3. The band gap of bilayer MoS2 sheets with different rotation angles.

Figure 4. The binding energies of bilayer MoS2 sheets with different rotation angles.

4. CONCLUSIONS
2D materials have attracted much attentions in a lot of exhibited potential applications, such as sensors, transistors and solar cells. Although, graphene is first known 2D materials and has shown excellent performance in applications, the gapless nature is still a huge hurdle. Therefore, an increasing number of researchers have to searching other promising alternatives, such as transition metal dichalcogenides (TMDs). MoS2, a representative TMD, is a semiconductor with an indirect band gap. Therefore, it has many novel properties.
In this paper, we investigated the electrical properties of twisted bilayer MoS2 sheets with different rotation angles using first-principles calculations. The band structure results show that the rotations can make bilayer MoS2 sheets change from semiconducting to metallic. When the rotation angle $\theta$ changes from 0° to 10°, the band gaps decrease from 1.24eV to 0.06eV. These results would open up possibilities for its applications in nanoelectronic devices simply by tuning band gaps of MoS2 with rotation angles.

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