Twisted layer structure: Electronic properties

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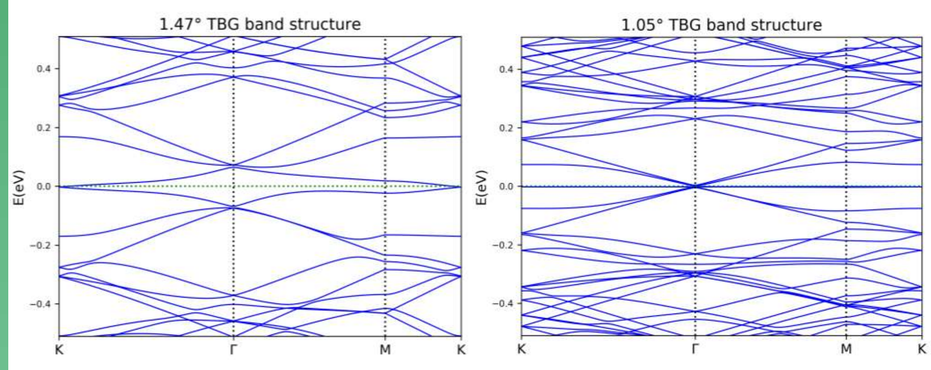
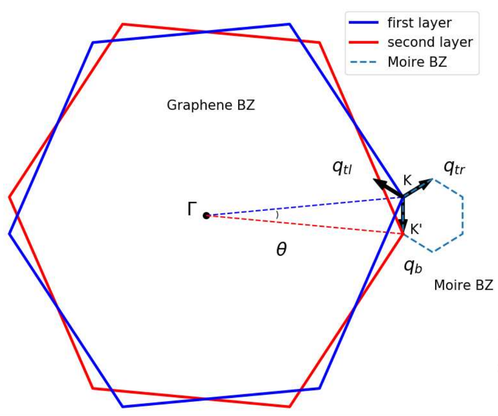
Abstract

Since 2011 the low energy continuum model of twisted bilayer graphene(TBG) has been solved [1], the researches about TBG has never decayed. In 2012, the tight binding model of TBG was proposed [2], short after, more and more van der Waals hetero-structure were gradually synthesized from experiments, and the theory also predicted many possible new materials and structures, including derivatives of graphene and popular two dimen-sional materials such as hexagonal boron nitride (hBN) and transition-metal dichalcogenide (TMD). However, for the twisted bilayer structure, there are relatively few examples of DFT calculations. The reason is that complex structures are not easy to build and too many atoms are difficult to DFT calculations. TBG is the most researched 2d material. In addition to TBG, we have also studied the electronic structure of other 2d materials after rotation. We hope that by exploring the energy bands, we can preliminarily judge whether they are magnetic or superconducting. Possibly, this will be a very important step for twistronics, because van der Waals forces will play an important role in this, and the effect on the electronic structure of superlattices with different sizes by changing the angle is very significant.

Low energy continuum model

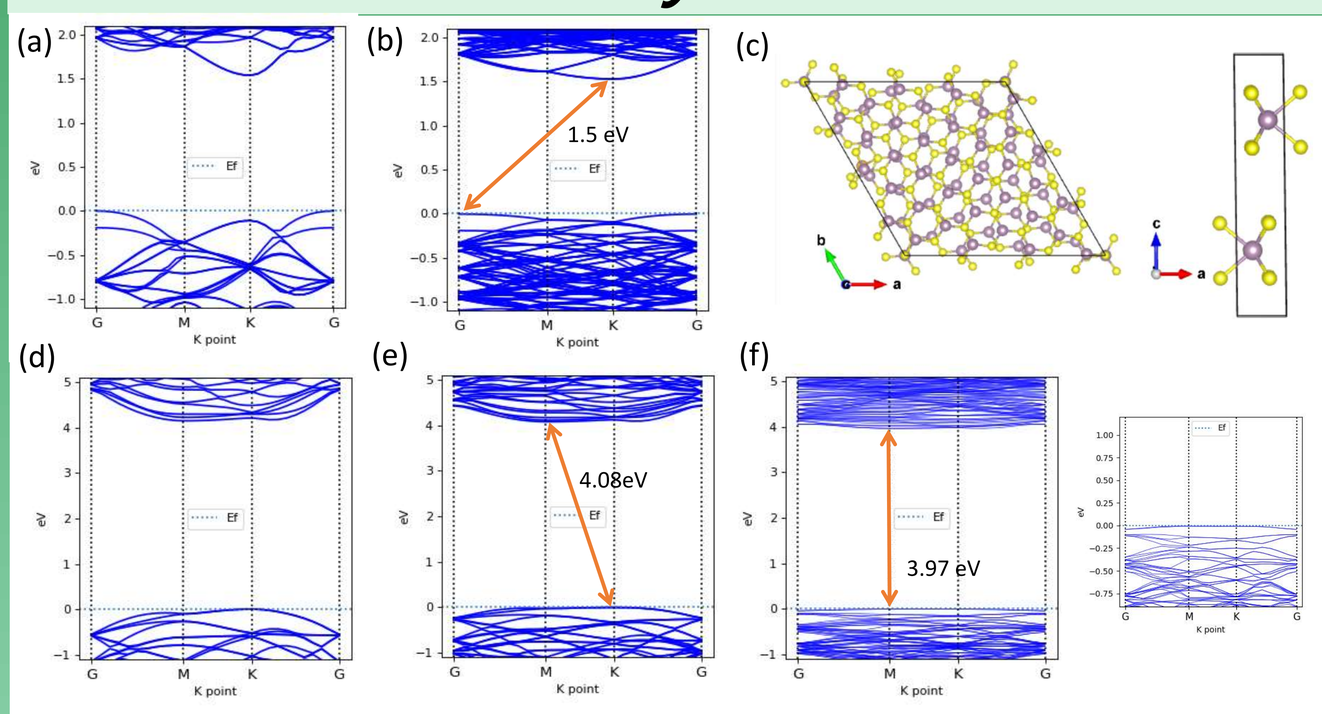


Based on Allan H. MacDonald's low energy continuum model, we calculated some twisted angle of twisted bilayer graphene (TBG). The low energy continuum model for gra-phene is just the k•p method, because we focus mainly on the behavior around the Fermi level, we can do Taylor exp-ansion around the K(K') point in Brillouin zone, thus we got the effective Hamiltonian of TBG. This model can produce band structure quickly, but the accuracy is lower than the density functional theory (DFT) and ab initio tight binding (TB), however, the arbitrariness choice of angle of this model is highest in these three methods.[3]



Brillouin zone of TBG, also called Moiré Brillouin zone

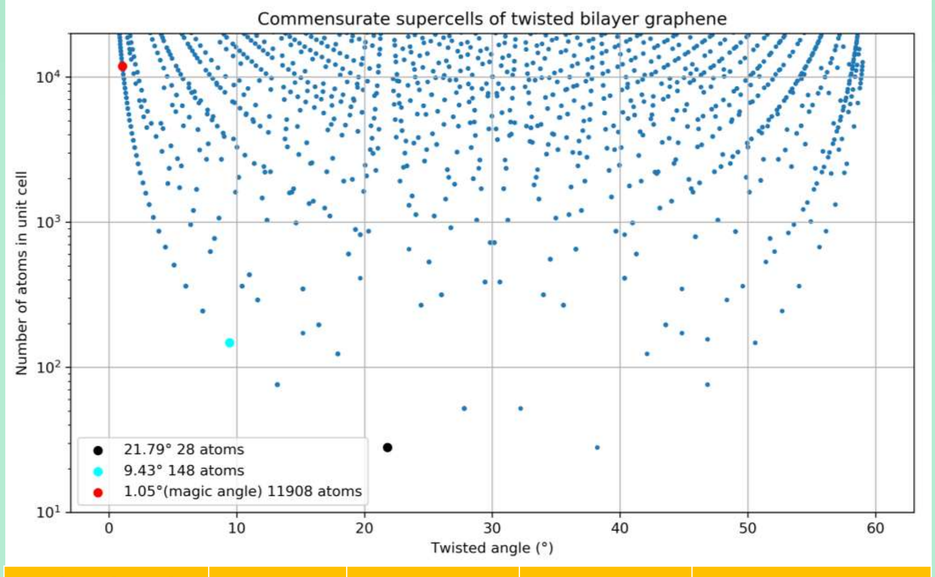
Twisted bilayer structure



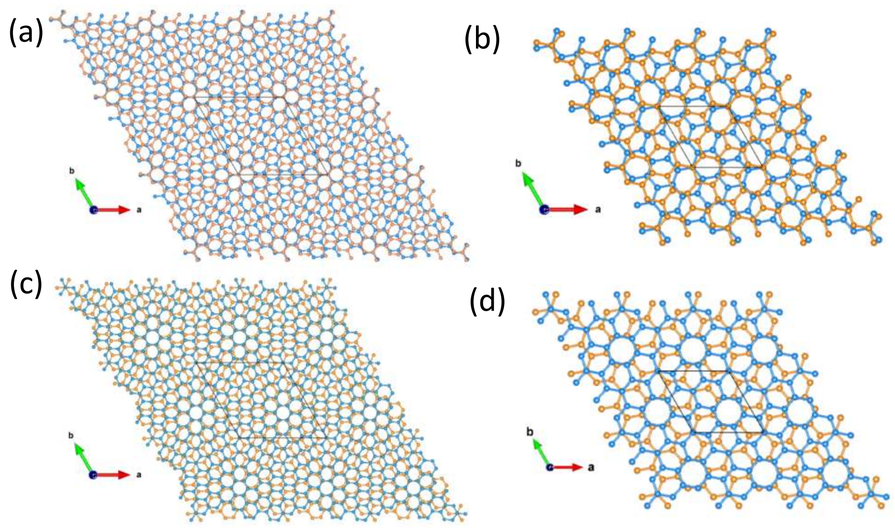
(a) 9.43° TB-MoS_2 (b) 5.09° TB-MoS_2 (c) 9.43° TB-MoS_2 supercell and the literal view of its untwisted unit cell (d) 13.17° TB-hBN (e) 9.43° TB-hBN (f) 5.09° TB-hBN

We try to stack and rotate two-dimensional materials other than bilayer graphene, because these two-dimensional materials are honeycomb lattice, so the commen-surate structure is the same as TBG. During the rotation process, as the angle bec-omes smaller and smaller, we found that the energy bands near the Fermi level of these semiconductors become flatter, and the magnitude of the band gap does not change significantly. However, the energy band of TB-hBN shows that it will switch between indirect-direct band gap semiconductor when twisted at different angles. In addition, because the energy band tends to be flat, we intercalate a gold atom at 5.09° TB-MoS2, which makes the material weakly ferromagnetic, with a magnitude of about 1.01. We also predict flat bands at smaller angles.

Structure of the system



Twisted angle	21.79	13.17	7.34	3.89
$\sqrt{\ } \times \sqrt{\ }$	$\sqrt{7} \times \sqrt{7}$	$\sqrt{19} \times \sqrt{19}$	$\sqrt{61} \times \sqrt{61}$	$\sqrt{217} \times \sqrt{217}$
Atoms[4]	28	76	244	868



(a) AA stacking 9.43° TBG (b) AA stacking 21.79° TBG
(c) AB stacking 9.43° TBG (d) AB stacking 21.79° TBG

Conclusion

In this study, we found that if the two-dimensional materials are rotated and stacked to each other, the electronic structure will be significantly affected. In addition to the discovery of superconductivity in graphene in 2018 [5], for semiconductor materials, this will make it indirect to direct band gap semiconductor transition, and we can control the energy band by adjusting its rotation angle and then design related optical devices. As the rotation angle becomes smaller and smaller, the energy band near the Fermi level becomes flatter. If some metal atoms are intercalated at this time, the material will become magnetic. In addition, for TB-TMD, consider spin orbital coupling (SOC) , its band gap will shrink, and the change of SOC to the energy band is relatively significant. We hope that more physics can be found in different twisted bilayer/few layer structures, especially superconducting phenomena, whic will greatly change our horizons, twistronics has not been fully explored.

Reference

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