

Twisted layer structure: Electronic properties

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Since 2011 the low energy continuum model of twisted bilayer graphene(TBG) has been solved, the researches about TBG has never decayed.

In 2012, the tight binding model of TBG was proposed, 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 dimensional 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.

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