

Electronic properties of low-angle twisted bilayer graphene

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Abstract

Twisted bilayer graphene (tBG) at and around specific magic angles [1] exhibiting correlated insulating phases and superconductivity has boosted the new field of “twistronics” [2] where strong electron-electron interactions play a dominant role in the electronic properties of the system. Below a threshold twist angle $\theta_c \sim 1^\circ$, this superlattice undergoes self-organized lattice reconstruction [3], forming a periodic domain and thus modifying strongly its electronic structure, compared to those observed above such threshold angle. Although low-angle tBG has been intensively investigated using effective electronic approaches (see an example in [4]), an in-depth investigation using more accurate calculations is still highly desirable. In this work, we developed and performed atomistic calculations using the Green’s function techniques to solve tight-binding models, where the lattice reconstruction obtained by simulations as in [5] is taken into account. Indeed, it was shown that the lattice reconstruction presents very significant effects on the electronic structure of low-angle (around and below θ_c) tBG systems. Especially, the second magic angle around $\theta \approx 0.5^\circ$ predicted in [1] is no longer observed (see Fig.1), which is a direct consequence of the mentioned lattice reconstruction. In addition, the local electronic properties and the helical network in these tBG systems were systematically investigated. Our work thus presents valuable contributions, that could be helpful for further development of the field “twistronics”, e.g., as it helped to interpret the experimental data [6].

REFERENCES

- [1] Rafi Bistritzer and Allan H. MacDonald, PNAS **108** (2011) 12233-12237.
- [2] Allan H. MacDonald, Physics **12** (2019) 12.
- [3] H. Yoo *et al.*, Nature Materials **18** (2019) 448-453.
- [4] S. Carr, S. Fang, Z. Zhu, and E. Kaxiras, Phys. Rev. Research **1** (2019), 013001.
- [5] Michael Lamparski, Benoit Van Troeye and Vincent Meunier, 2D Materials **7** (2020) 025050.
- [6] Andreij C. Gadelha *et al.*, [arXiv:2006.09482](https://arxiv.org/abs/2006.09482)

FIGURES

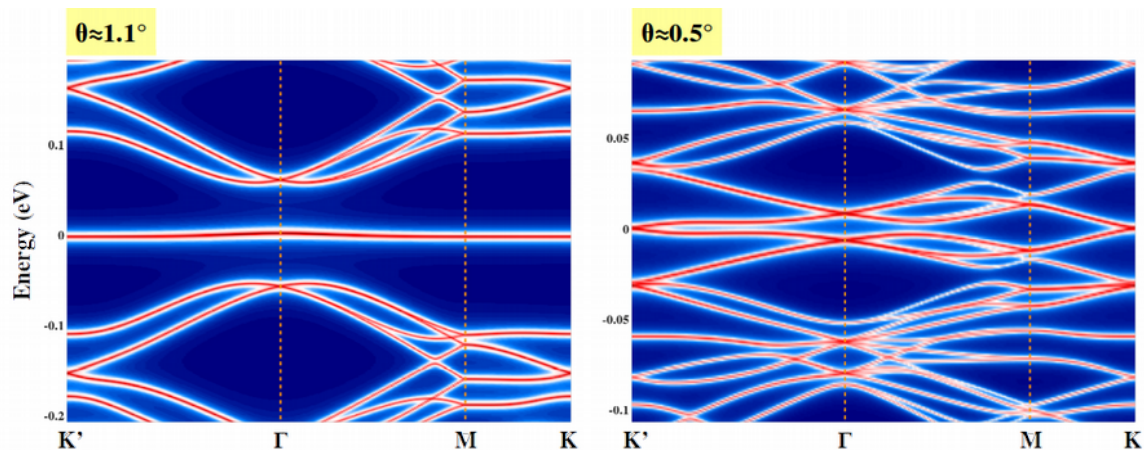


Fig.1: Electronic bandstructure of twisted bilayer graphene around the expected first (left) and second (right) magic angles reported in [1]. The lattice reconstruction obtained as in [5] was taken into account.