

Electron localization in small-angle twisted bilayer graphene

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Owing to the outstanding and nicely tunable properties, twisted bilayer graphene (TBLG) systems display many fascinating features, especially, those related to the electronic flat bands and the corresponding strong electronic localization observed when the twist angle is close to magic ones. Indeed, superconductivity, correlated insulating states, magnetism, and quantized anomalous Hall states have been explored in magic-angle TBLGs [1], thus giving rise to the nascent research field of “twistronics”. A comprehensive and accurate understanding of the intrinsic electronic properties of TBLG is therefore very mandatory. However, while its electronic properties at large twist angles down to $\sim 1.1^\circ$ have been well clarified, there are still discrepancies between theoretical explorations and experimental observations for small-angle TBLGs. In particular, theoretical studies [2] have predicted a recurrent series of magic angles $\leq 1.1^\circ$. However, only the first magic angle at $\sim 1.1^\circ$ has been experimentally demonstrated [3,4] but there is no evidence pointing to the existence of smaller ones. In this work [5], using a tight-binding framework performed on fully relaxed TBLG lattices, the twist angle $\sim 1.1^\circ$ is found to be a unique magic angle and concurrently is the critical case where the electron localization is maximum, thus separating TBLGs into two classes with clearly distinct electronic properties. For large twist angles $> 1.1^\circ$, low-energy Dirac fermions are preserved. For small-angles ($\leq 1.1^\circ$), TBLG systems present common features such as large spatial variation and strong electron localization stably observed in the AA stacking regions. However, the global electronic localization (maximum at $\sim 1.1^\circ$) is shown to progressively reduce when the twist angle decreases, confirming that isolated electronic flat bands (as observed at 1.1°) can no longer be observed for smaller angles. In very good agreement with recent nano-Raman/STM/STS spectroscopies [4,6], our study clarifies essentially the reasons of the absence of magic angles below 1.1° previously reported [2], and on the other hand, provide a more comprehensive and accurate understanding of the electronic properties of small-angle ($\leq 1.1^\circ$) TBLG systems.

References

[1] E. Y. Andrei and A. H. MacDonald, Nat. Mater. 19, 1265-1275 (2020). [2] R. Bistritzer and A. H. MacDonald, PNAS 108, 12233-12237 (2011); G. Tarnopolsky *et al.*, Phys. Rev. Lett. 122, 106405 (2019); Y. Ren *et al.*, *ibid.* 126, 016404 (2021). [3] Y. Cao *et al.*, Nature 556, 43-50 (2018); *ibid.* 556, 80-84 (2018). [4] A. C. Gadelha *et al.*, Nature 590, 405-409 (2021). [5] V.-H. Nguyen *et al.*, 2D Mater. 8, 035046 (2021). [6] A. Kerelsky *et al.*, Nature 572, 95-100 (2019); I. Brihuega *et al.*, Phys. Rev. Lett. 109, 196802 (2012); S. Huang *et al.*, *ibid.* 121, 037702 (2018).

Figures

Electronic bandstructure (left), total DOS and local DOS (right) of TBLG at $\sim 0.5^\circ$

