Electronic localization in small-angle twisted bilayer graphene

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ABSTRACT:

Owning to the outstanding and nicely tunable properties, twisted bilayer graphene (TBLG) systems display many fascinating features, especially, related to the electronic flat bands and the corresponding strong electronic localization observed when the twist angle is close to magic angles. 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". In such context, a comprehensive and accurate understanding of the intrinsic electronic properties of TBLG is very mandatory. However, while the electronic properties of large-angle TBLG at large twist angles down to ~1.1° have been well clarified, there are still discrepancies between theoretical explorations and experimental observations for small-angle TBLGs. In particular, the recent studies [2] have theoretically predicted a recurrent series of magic angles $\lesssim$ 1.1°. However, only the first magic angle at ~1.1° 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 ~ 1.1° 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 (i.e., as illustrated in Fig. 1). For large twist angles > 1.1°, low-energy Dirac fermions are preserved. For small-angles ($\lesssim$ 1.1°), TBLG systems present common features such as large spatial variation and strong electron localization in the AA stacking regions. The global electronic localization (maximum at ~1.1°) is shown to monotonically 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° as previously reported, and on the other hand, provide a more comprehensive and accurate understanding of the electronic properties of small-angle ($\lesssim$ 1.1°) TBLG systems.

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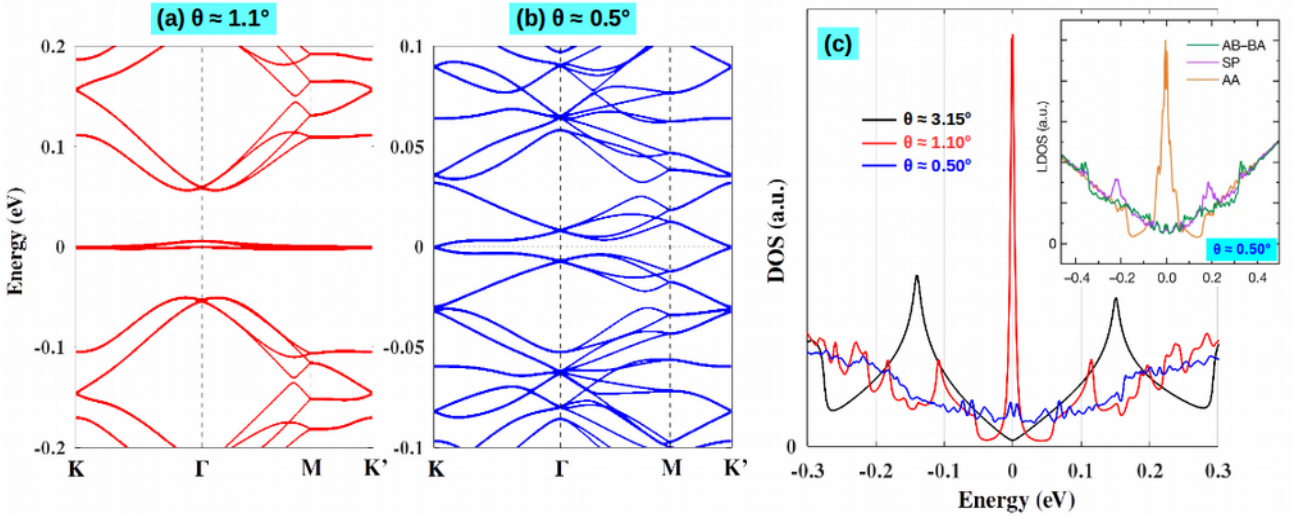

Fig.1: Electronic bandstructure of TBLG at 1.1° (a) and 0.5° (b) predicted in [2] to be the first and second magic angles, respectively. (c) Density of electronic states (DOS) at different twist angles and local DOS at 0.5° in different stacking regions (see the inset).