Extended Abstract

Investigating the Unique Properties of Twisted Trilayer Graphene for Advanced Electronic Applications

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Abstract

Twisted trilayer graphene (tTLG) is a tunable platform for correlated electron physics and device concepts that emerge from moiré superlattices. Here, we theoretically examine how the twisting angles (θ_{12}, θ_{23}), rotation direction, and a perpendicular displacement field E control the low-energy band structure and density of states (DOS). Using a momentum-space continuum Hamiltonian based on the Bistritzer–MacDonald framework and a nearest-neighbor tight-binding description, we compute minibands near the moiré Brillouin zone and evaluate DOS with Gaussian broadening. We find that reducing the twist angles compresses the moiré Brillouin zone, enhances DOS at the Fermi level, and yields flat bands, thereby strengthening electronic correlations. Reversing the rotation sense of the top layer relative to the middle layer removes the near-zero-energy flat bands and opens an energy gap, highlighting a strong chirality dependence. Moreover, an external displacement field (up to $E \approx 0.1$ V/nm) reshapes sombrero-like dispersions and shifts DOS peaks, offering band engineering knobs in tTLG. These results establish design rules for achieving flat bands and tunable insulating or potentially superconducting regimes in tTLG, paving the way for next-generation electronic and quantum devices based on multilayer moiré graphene.

Keywords: Twisted Trilayer Graphene; Moire Pattern; Band Structure; Density of States.

INTRODUCTION

Twisted multilayer graphene hosts emergent moiré physics, including flat bands, correlated insulating phases, and unconventional superconductivity near magic angles [1]. While twisted bilayers have

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been widely explored, twisted trilayer graphene provides additional tuning via two independent twist angles (θ_{12}, θ_{23}) and rotation chirality (**Fig.1**), enabling richer miniband engineering and stronger correlation effects. In tTLG, the interference of two moiré lattices from the (1|2) and (2|3) interfaces can create highly compressed moiré Brillouin zones (MBZ) and density-of-states amplification near the Fermi level when angles approach the magic-angle hierarchy.

Recent theory and experiments indicate tunable superconductivity, correlated insulators, and ferromagnetism across moiré graphene systems, motivating systematic control of bands via geometry and fields. Here we address, within a continuum momentum-space Hamiltonian, how (i) the twist angles, (ii) the rotation direction (clockwise vs. counterclockwise) of the outer layers relative to the middle one, and (iii) a perpendicular displacement field reshape the low-energy spectrum and DOS. By focusing on parameter sets close to experimentally relevant angles ($\theta_{12} = -2^\circ$, $\theta_{23} = 2.1^\circ$) and fields up to E ≈ 0.1 V/nm, we provide compact design principles to obtain flat bands or open gaps in tTLG, bridging fundamental insights with device-level band engineering.

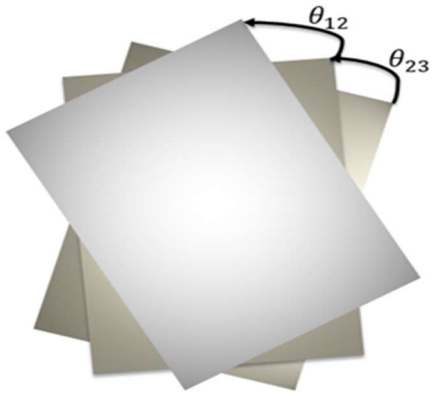


Figure1. A schematic illustration of twisted trilayer graphene (tTLG), where
denotes the rotation angle between Layer 1 and Layer, and
is the rotation angle between Layer2 and Layer 3

MATERIALS AND METHODS

We adopt a low-energy momentum-space continuum Hamiltonian[2] for tTLG, where the middle layer is fixed and the top/bottom layers are rotated by θ_{12} and θ_{23} **(Fig.1**). Interlayer tunneling matrices include AA/BB and AB/BA channels with effective couplings ($\omega_{ab} \approx 0.11$–0.2 eV) calibrated to prior tight-binding and ab initio studies. The moiré reciprocal lattice vectors are constructed from rotated graphene Bravais lattices; shrinking twist angles enlarge the real-space moiré cell and compress the MBZ.

For each (θ_{12}, θ_{23}), we diagonalize the k·p Hamiltonian on an MBZ grid around K-points to obtain minibands near charge neutrality. The displacement field E is introduced as a layer-dependent potential offset. DOS is computed from eigenvalues using Gaussian broadening with full-width-at-half-maximum. Angles close to the "magic-angle hierarchy" and representative coupling strengths are examined: (i) $\theta_{12} = -2^\circ, \theta_{23} = 2.1^\circ$; (ii) same magnitudes with reversed rotation direction; (iii) displacement fields E = 0, 0.05, 0.1 V/nm; and interlayer coupling cases ω_{ab} = 0.11 and 0.2 eV [3].

RESULTS AND DISCUSSION

Effect Of Angle

Decreasing |θ| compresses the MBZ and brings minibands closer near zero energy, enhancing DOS and forming flat bands around the Fermi level, consistent with moiré-induced correlation amplification. For $\theta_{12} = -2^\circ$, $\theta_{23} = 2.1^\circ$, pronounced near-zero-energy flat features are observed (**Fig.2 (a,b)**).

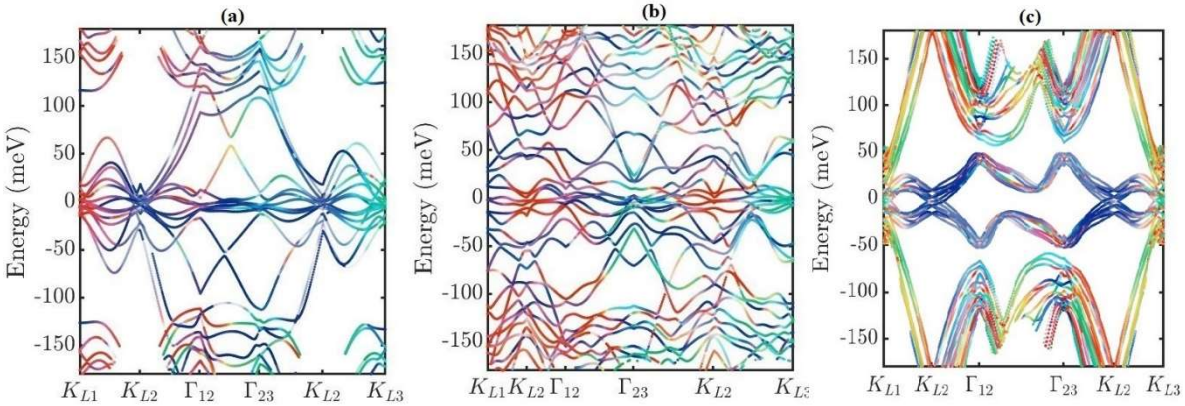


Figure 2. Twisted trilayer graphene, $\omega_{ab} = 0.11(eV)$, (a) $\theta_{12} = -2^\circ$, $\theta_{23} = 2.1^\circ$, (b) $\theta_{12} = -1.02^\circ, \theta_{23} = 2.1^\circ$, (c) $\theta_{12} = 2^\circ, \theta_{23} = 2.1^\circ$

Role of Rotation Direction

Keeping angle magnitudes fixed but reversing the rotation sense of the top layer relative to the middle layer eliminates these flat bands and opens a gap around neutrality. This chirality control provides a distinct handle to toggle between flat and gapped regimes without changing |θ| (**Fig.2 (a,c)).**

Displacement-Field Tuning

A perpendicular field up to E ≈ 0.1 V/nm reshapes sombrero-like dispersions and shifts DOS peaks, enabling band-edge control and correlated-state engineering similar to field-tunable gaps in bilayer-based moiré systems. Increasing E redistributes DOS and can suppress or enhance near-Fermi peaks (**Fig.3**).

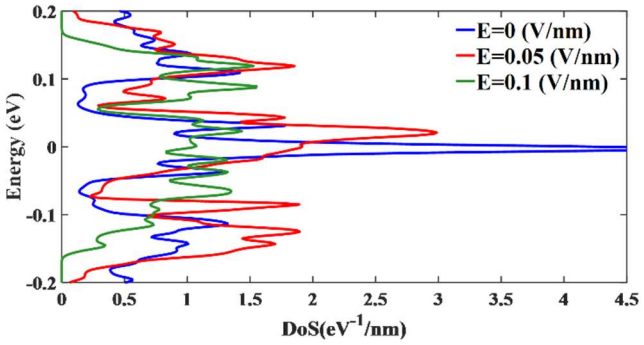


Figure 3. Density of State for $\omega_{ab} = 0.11(eV)$, $\theta_{12} = -1.02^{\circ}, \theta_{23} = 2.1^{\circ}$

CONCLUSION

Twisted trilayer graphene provides versatile control of electronic minibands through twist angles, rotation chirality, and displacement fields. Reducing twist angles generates flat bands, while reversing rotation direction opens an energy gap. Applying a vertical field further tunes band dispersion and DOS peaks. These findings establish design rules for engineering correlated and superconducting phases in tTLG-based quantum devices. Future work will focus on extending the model to include electron–phonon coupling and many-body interactions to predict experimentally observable superconducting behavior.

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