# Twistronics of rhombohedral graphite

Xiaoqian Liu [1] Yifei Guan [1] Oleg V. Yazyev [1]

[1]Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Chair of Computational Condensed Matter Physics

## Introduction

In this work, we study the topology of flat bands at surfaces and twist stacking faults in rhombohedral graphite. Unlike Bernal graphite, rhombohedral graphite hosts flat surface states near Dirac points due to intrinsic chiral symmetry, characterized by a quantized Zak phase. Twisting introduces moiré periodicity, modifying bandwidth and interface flat bands through the interplay with Zak phase topology. In the low-energy effective model, the Chern number of flat bands scales linearly with layer count [?], but even weak disorder disrupts this scaling since the bandgap exponentially decays with the number of layers. We quantify the effects of disorder, showing that the Chern number in twisted rhombohedral graphite eventually vanishes.

## Twist stacking fault in rhombohedral graphite

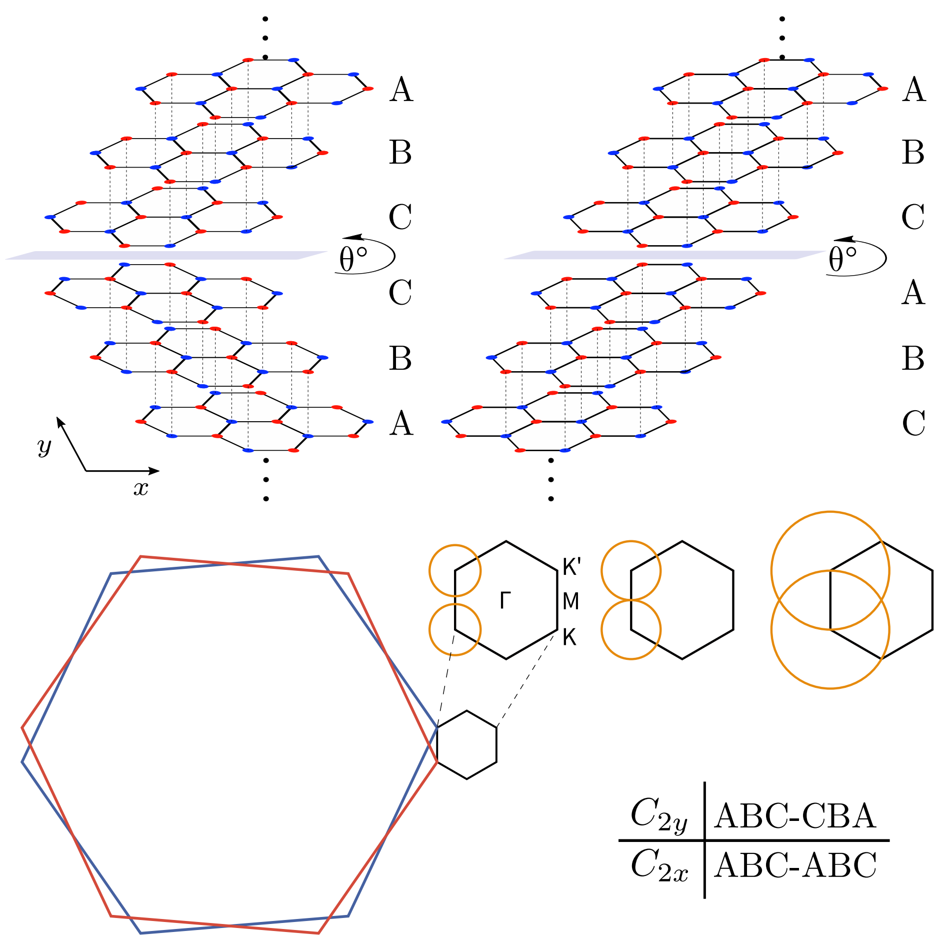


Figure 1. Twisted rhombohedral graphite structure and Brillouin zones of twisted rhombohedral graphite for different configurations. The yellow rings mark regions where the Zak phase $\mathcal{Z} = \pi$.

The chirality of rhombohedral graphite indicates the different twist stacking faults [?]. In the presented twisted rhombohedral graphite, the left configuration has $C_{2x}$ symmetry, and ABC-ABC interface; while the right configuration has $C_{2y}$ symmetry, and ABC-CBA interface.

## Modeling Approach

- **The Hamiltonian** of the system is built by tight-binding model or continuum model.
- **Recursive Green's function** is used to investigate the infinite-layer system.

$$G(E,k) = [E + i\eta - H(k) - \Sigma_{Top}(k) - \Sigma_{Bottom}(k)]^{-1}$$

$$\rho(E,k) = -\frac{1}{\pi}\mathbf{Im}[\mathbf{Tr}G(E,k)]$$

- **The Zak phase** is used to characterize the surface state.

$$\mathcal{Z}(k_x,k_y) = i\int_{k_z=0}^{2\pi} \left\langle u(\vec{k})|\partial_{k_z}|u(\vec{k})\right\rangle dk_z$$

## Rhombohedral resolved LDOS

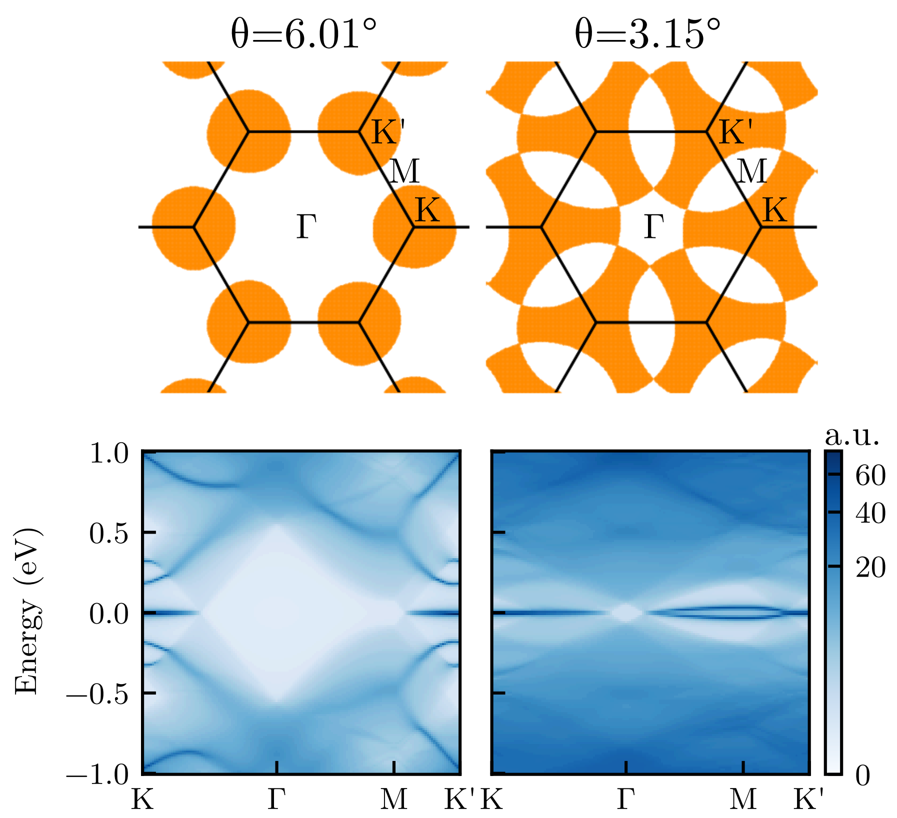


Figure 2. Schematic diagram of Zak phase and LDOS of twisted rhombohedral graphite at twist angles $\theta = 6.01°$ and $\theta = 3.15°$

The non-trivial Zak phase creates the interface flat bands, and the overlap between the Zak phases causes the bands' dispersion.

## Topological argument

Followed by Liu's result [?], the Chern number of the flat band for twisted multilayer rhombohedral graphene system scales linearly with the number of layers.

$$C^{K}_{\alpha,\alpha'} = +[\alpha(M-1) - \alpha'(N-1)]$$

$$C^{K'}_{\alpha,\alpha'} = -[\alpha(M-1) - \alpha'(N-1)]$$

However, a key question remains: does the Chern number continue to increase as the number of layers grow?

In other words, **Will the interface state and the surface state remain coherent if the number of stacking layers goes to infinity in the real situation?**

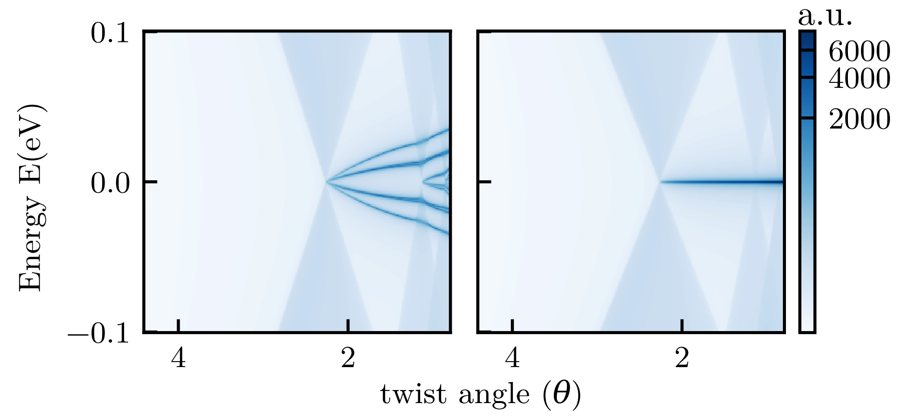


Figure 3. The bandwidth evolution of twisted rhombohedral graphene at $\Gamma$ point. left: $w_{AA} = 20\,$meV; right: $w_{AA} = 0\,$meV.

The answer is No. In real systems, disorder and quantum fluctuations would limit the coherence length, preventing it from becoming truly infinite. This gives the physical meaning of the non-chiral AA-sublattice term in the continuum model.

## Chern number evolution in the presence of disorder

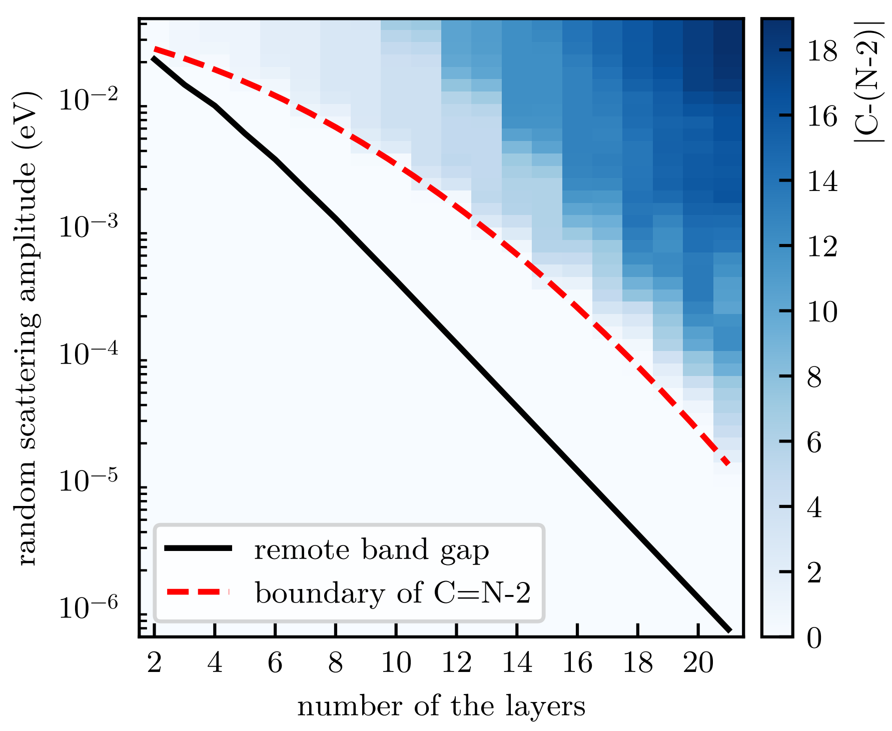


Figure 4. The evolution of Chern number with random scattering disorder

Random scattering disorder is introduced at the surface of twisted rhombohedral graphene. And the disorder affects the linear relation between the number of layers and the Chern number, let the Chern number eventually converge to 0.

## Conclusion

- **The topological flat band is decided by the interplay between the moiré periodicity and the Zak phase.** To be clear, the $\pi$ Zak phase protects the interface flat bands, and the overlap between $\pi$ Zak phases causes band dispersion.
- **In the chiral limit, twisted rhombohedral graphite could have degenerate flat bands.** The flat bands come from the surface states and interface states. After breaking the chiral symmetry, we can split these two states.
- **The Chern number of twisted rhombohedral graphite system is tunable with finite disorder at the surface.** The Chern number decreases as the disorder strength increases, and eventually vanishes.

## References

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Email: xiaoqian.liu@epfl.ch