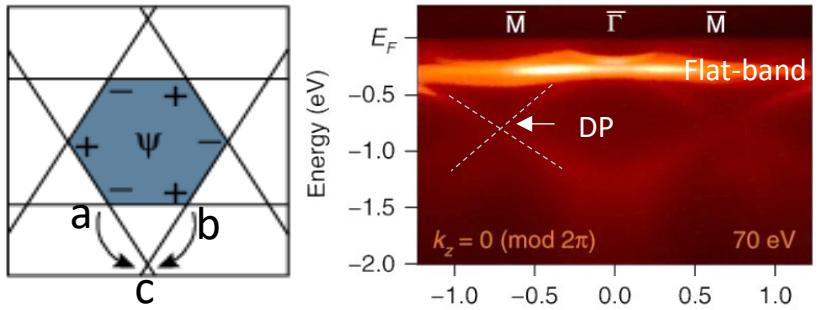
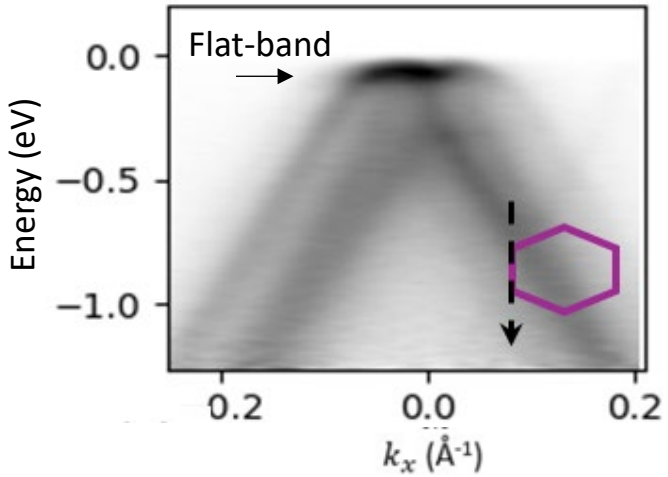
Orbital-Driven Frustrated Electron Hopping in a 2D Lattice

- Coexistence of Dirac and flat- band. Flat-band appears from frustrated electron hopping.
  - Geometrical frustration: kagome lattice

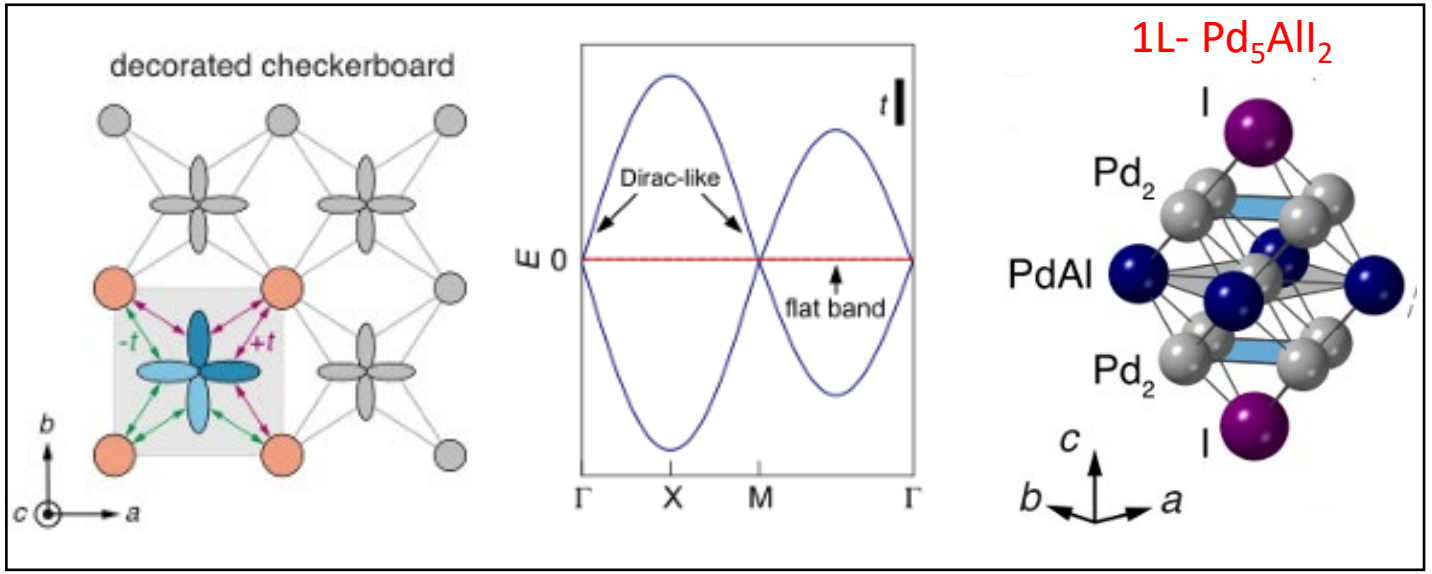


M. Kang et al., Nat. Commun. 11, 4004 (2020)

- Magic angle twisted bilayer graphene



- Why flat and Dirac bands scientifically important?
- Can we create flat and Dirac bands without geometrical lattice frustration?



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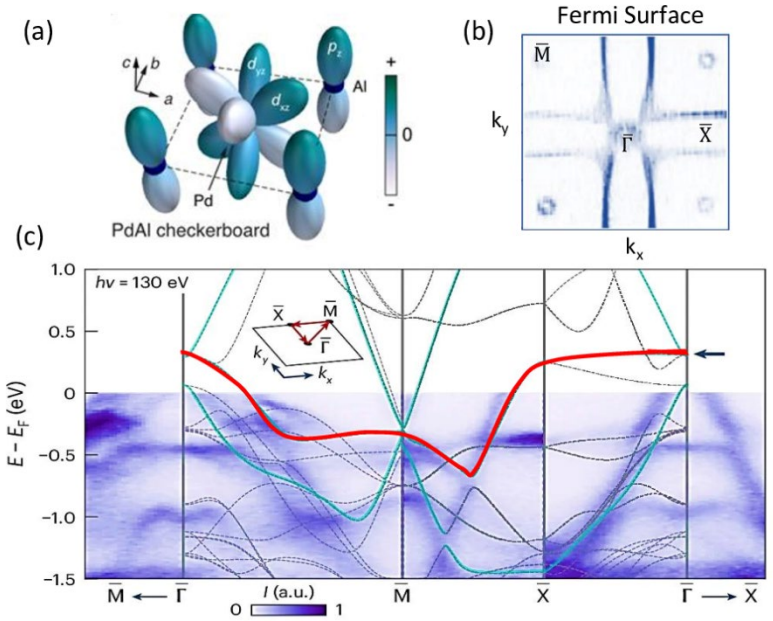

(a) Orbital orientation of PdAl layer in Pd_5AlI_2 forms a checkerboard lattice. (b & c) *ARPES Fermi surface map and band structure (blue) along the* $\overline{\Gamma}$- $\overline{M}$- $\overline{X}$- $\overline{\Gamma}$ *path (inset; red) of the surface BZ. DFT calculated band structure is overlaid on top (dashed grey) with bands linked to the decorated checkerboard model highlighted in cyan and red.*

Devarakonda, A., Koay, C.S., Chica, D.G. et al. "Frustrated electron hopping from the orbital configuration in a two-dimensional lattice." *Nat. Phys.* **21**, 1260–1266 (2025). https://doi.org/10.1038/s41567-025-02953-2

Work was performed in part at NSLS-II

Scientific Achievement

Scientists show that Pd_5AlI_2 can mimic the electronic behavior of frustrated lattices, creating both flat and Dirac-like bands from a simple square lattice.

Significance and Impact

This work reveals a new way to achieve the exotic electronic properties of frustrated lattices in simple, stable materials, opening paths to discover and design novel quantum materials.

Research Details

- Angle-resolved photoemission spectroscopy (ARPES) measurements at NSLS-II Beamline 21-ID showed Dirac-like bands that were intersected by a flat band.
- These findings confirmed the hallmark features of Lieb- and dice-lattice physics in a stable solid-state system.

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