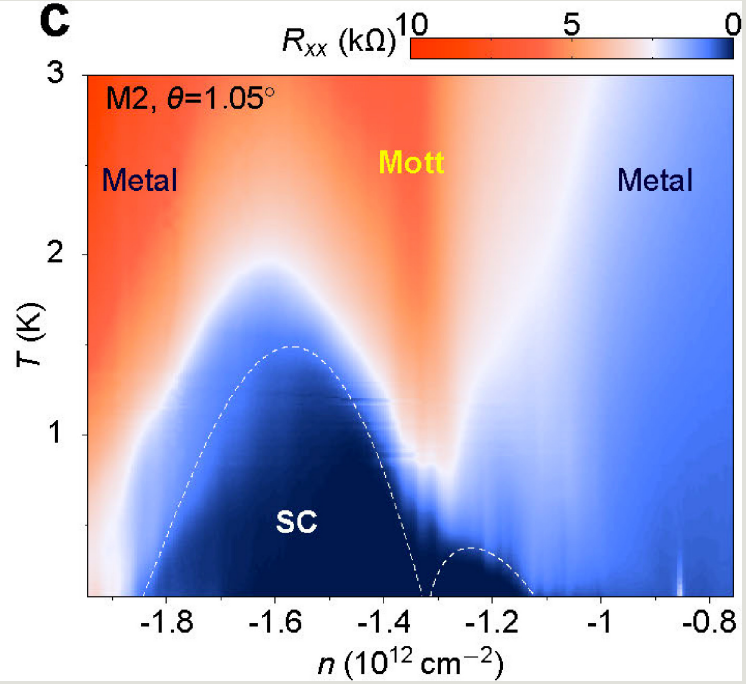
The ν=-2 state in Twisted Bilayer Graphene:



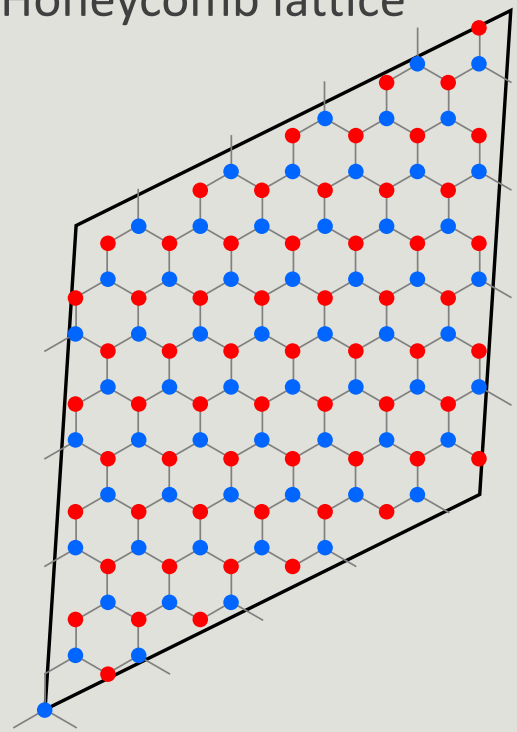
a Bad Mott Insulator?

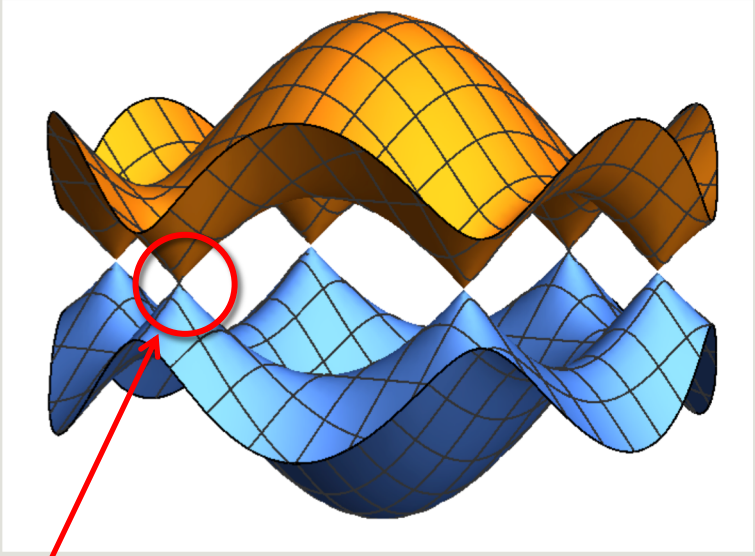
LOUK RADEMAKER, 22 AUGUST 2019, TDLI, SHANGHAI

Graphene

Single atomic layer of carbon atoms

Honeycomb lattice

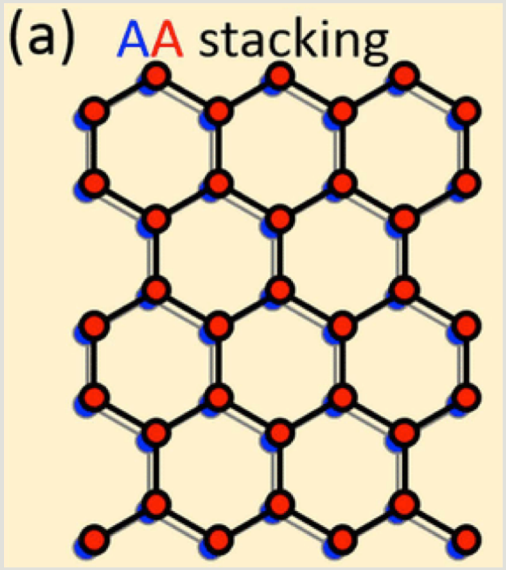


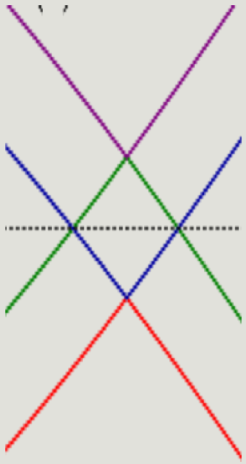


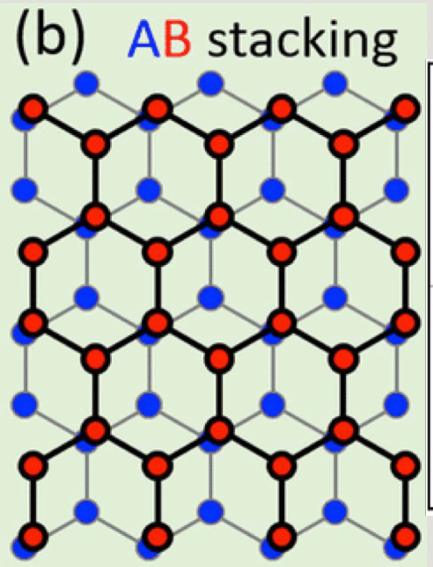
$$H = v_F \vec{\sigma} \cdot \vec{k}$$

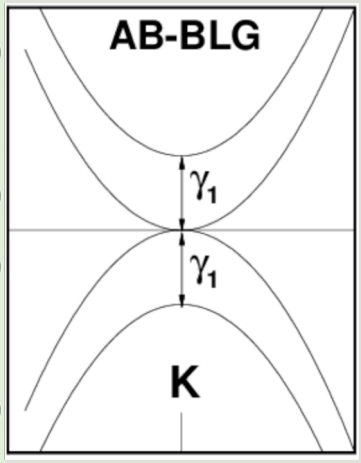
Effective massless Dirac fermions
at K and K' points in Brillouin zone

Bilayer Graphene









Atoms directly above each other

Dirac cones **shifted up/down**

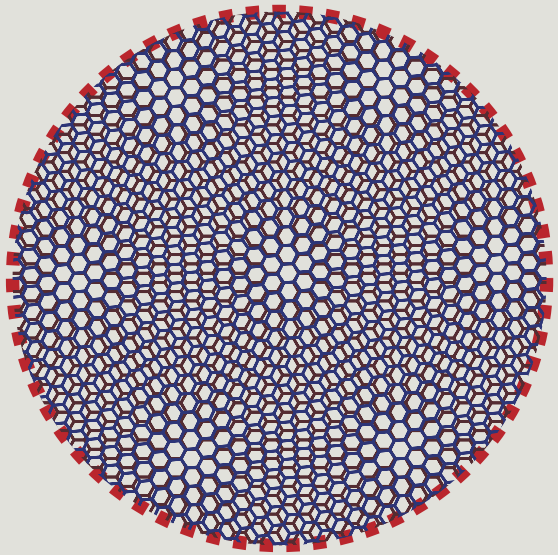
A-sites in one layer on top of B-sites of second layer

One Dirac cone **gapped**
Other Dirac cone becomes **quadratic**

Twisted Bilayer Graphene

At small angles, you get a **Moiré** pattern

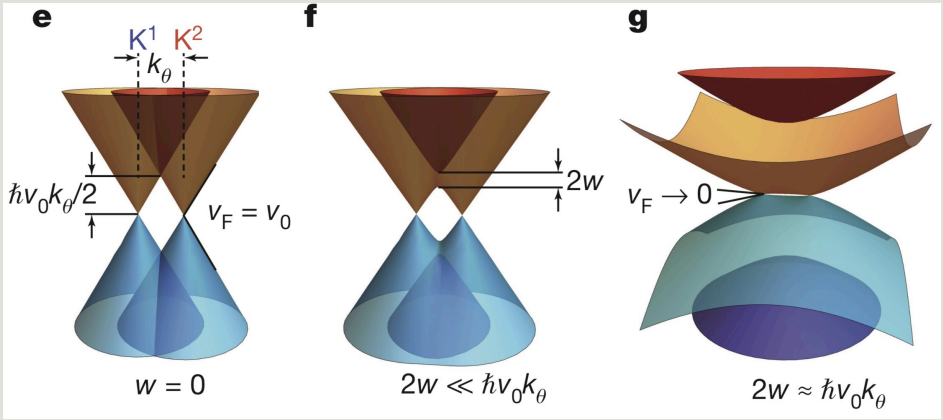
with **enlarged** unit cell



And therefore a **mini-Brillouin zone**

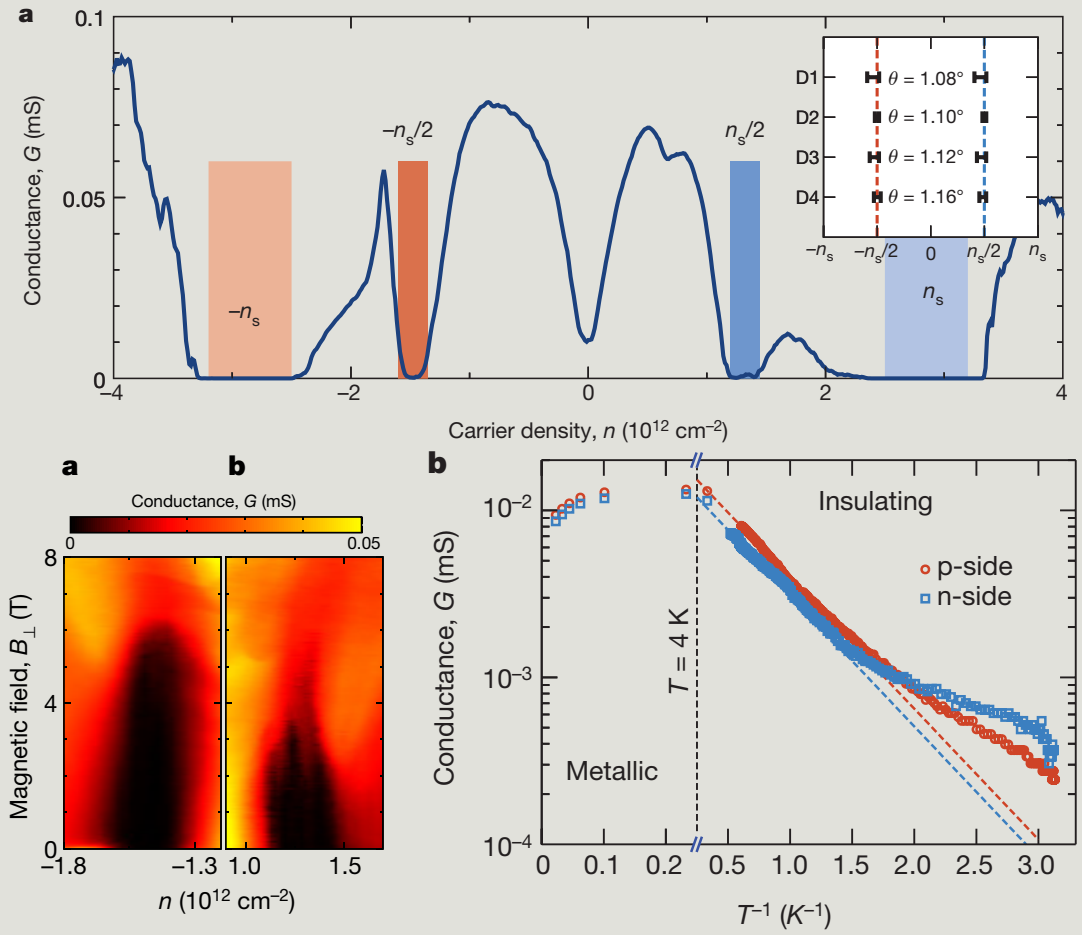
The K points of both layers are close

Including interlayer hopping leads to level repulsion,
which leads to a **reduced Fermi velocity**



Ref: Cao et al, Nature 2018 (two papers); Bistritzer PNAS 2011

Bad Mott insulator



At $|\nu|=2$, conductance suddenly **drops** below T=4K

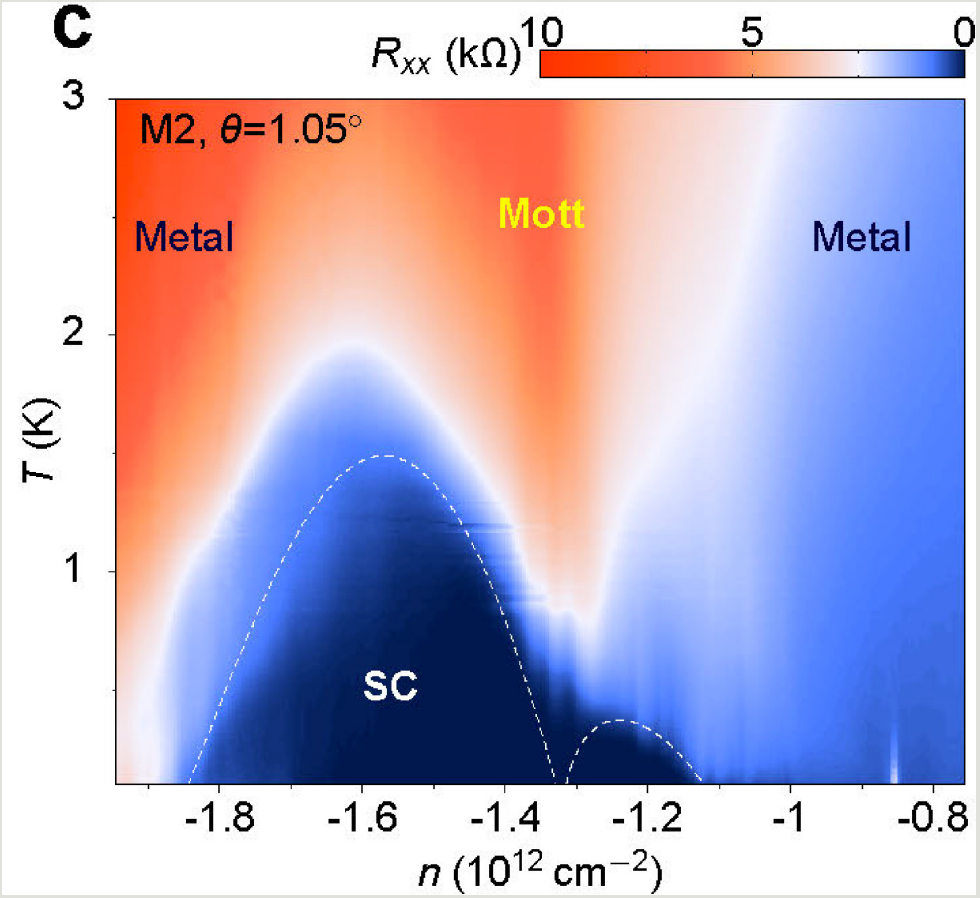
Commensurate density suggests **Mott** physics

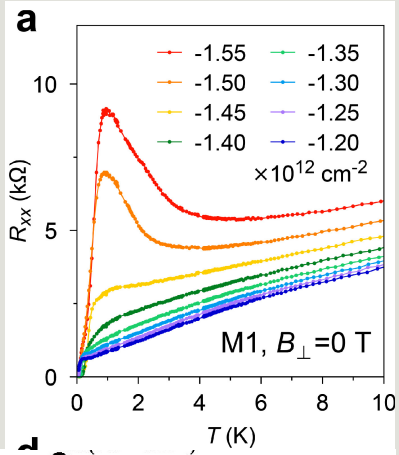
But… system only insulating at low T, easily destroyed by field, at lower T becomes SC…

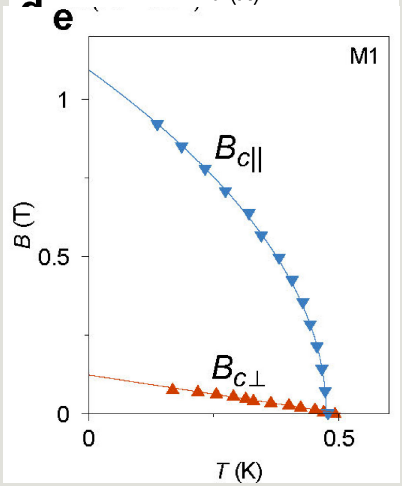
A **Bad Mott insulator?**

Ref: Cao et al, Nature 2018 (two papers)

Superconductivity







Ref: Cao et al, Nature 2018 (two papers)

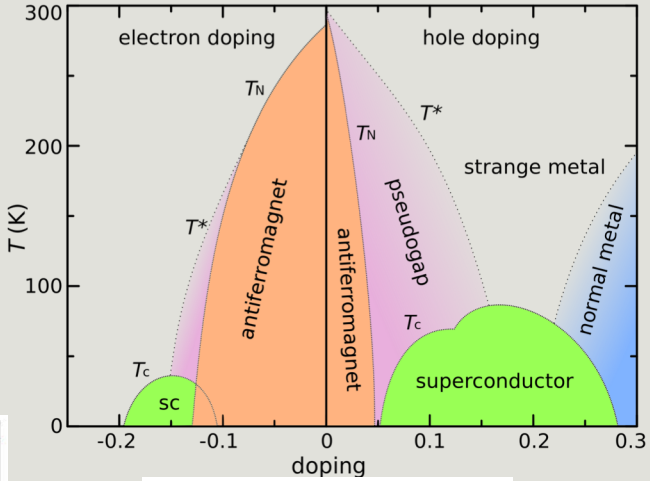
Why is it so exciting?

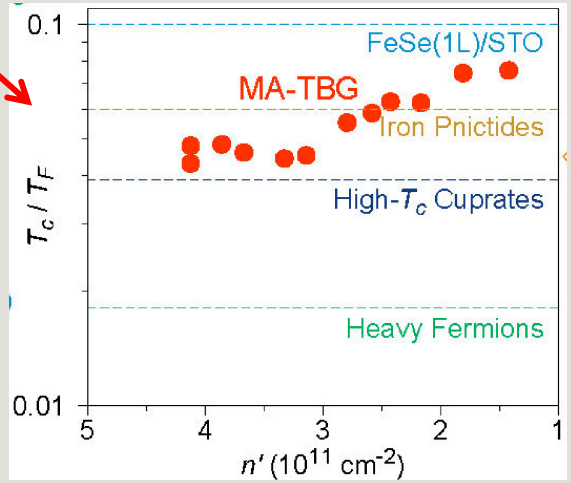
A “**clean**” system with **strong correlations**

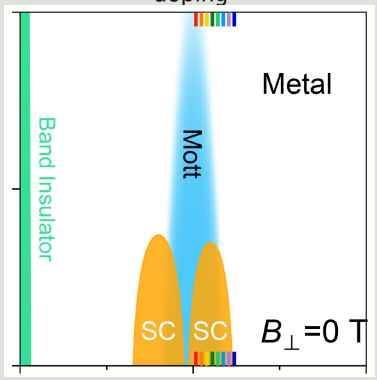
Easily **tunable** by gating

Comparison to **cuprates**

‘**High**’ T_c

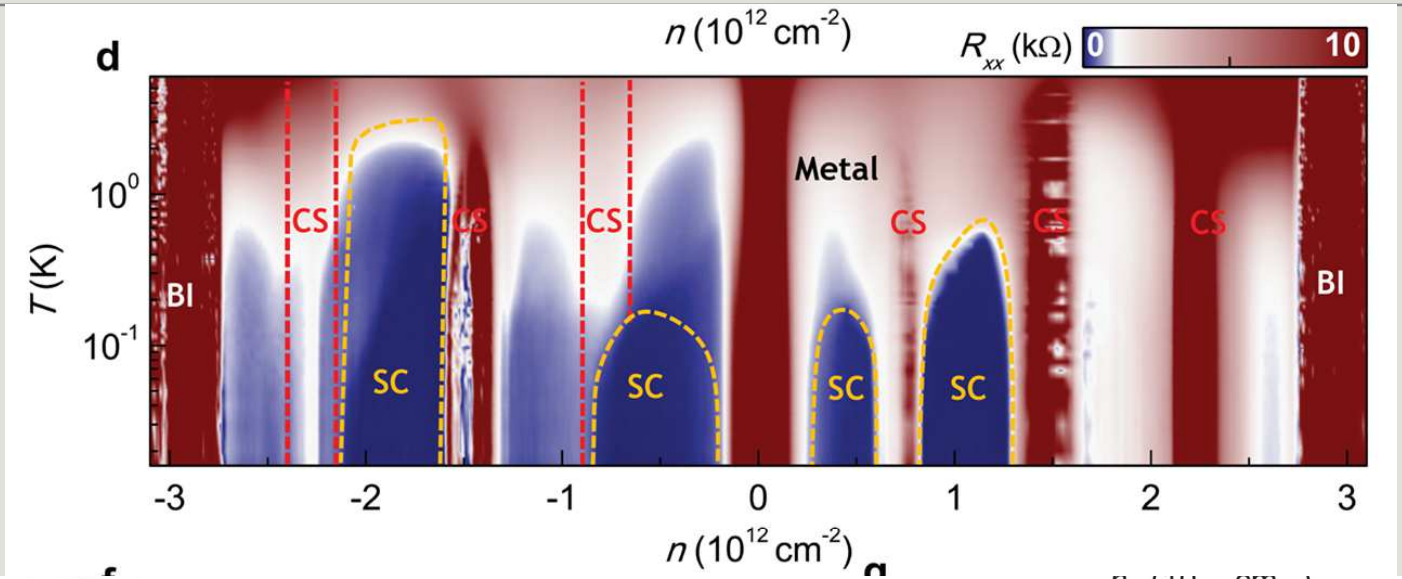


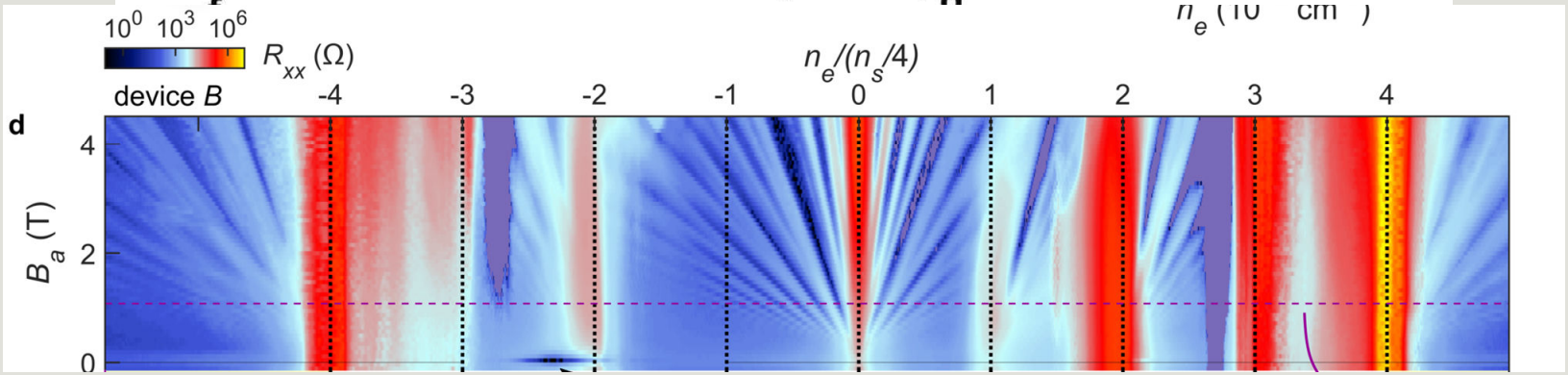




Ref: Cao et al, Nature 2018 (two papers)

2019: More Domes & Fans





Ref: Lu, 1903.06513; Uri, 1908.04595

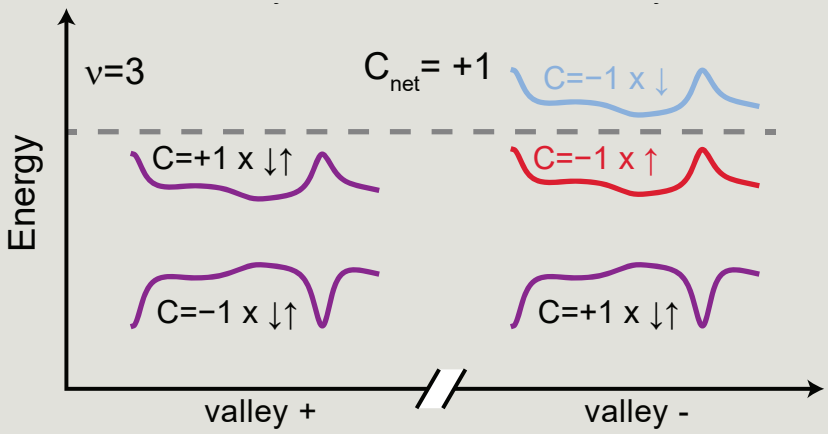
Quantum Anomalous Hall Effect

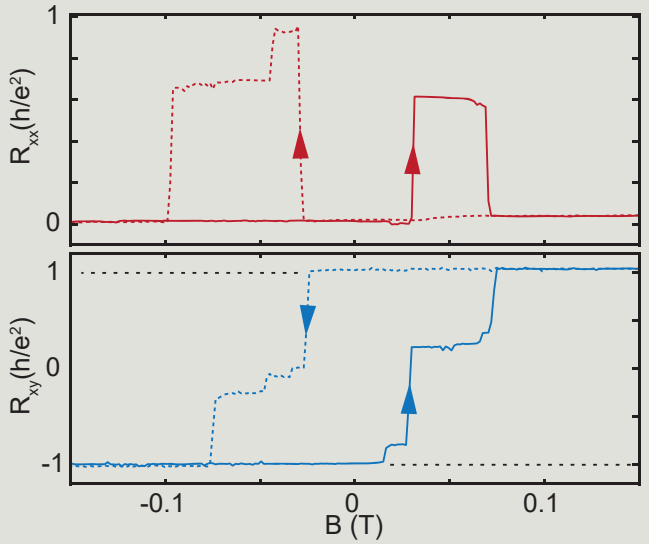
In samples where the hBN substrate is **aligned** with the graphene, the substrate **opens up a gap at charge neutrality**.

The **resulting band structure** has opposite Chern numbers for different Dirac 'valleys'

At ν=3, interactions then cause **ferromagnetic state**

FM + Topology = QAH

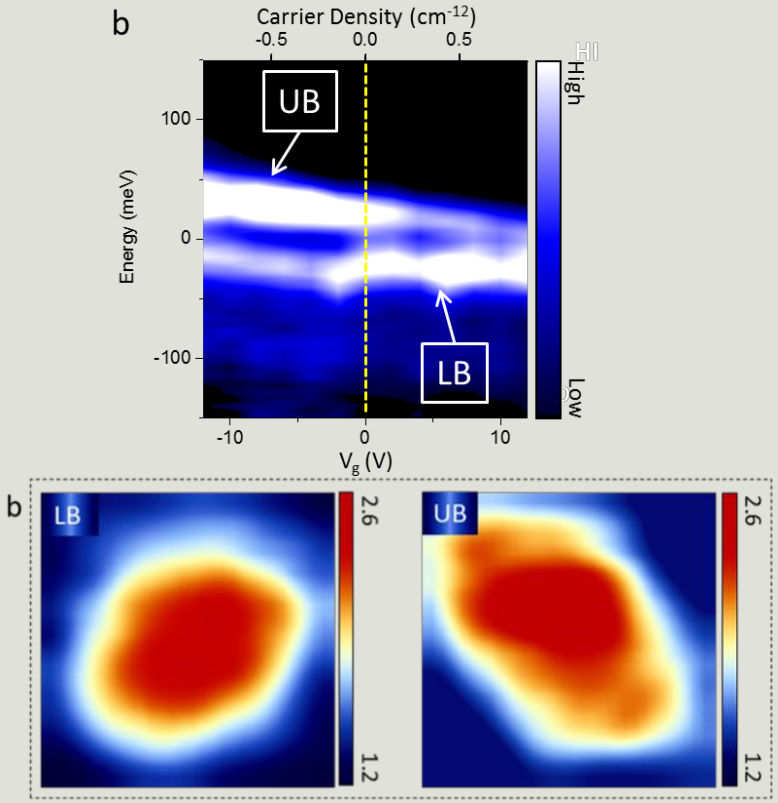


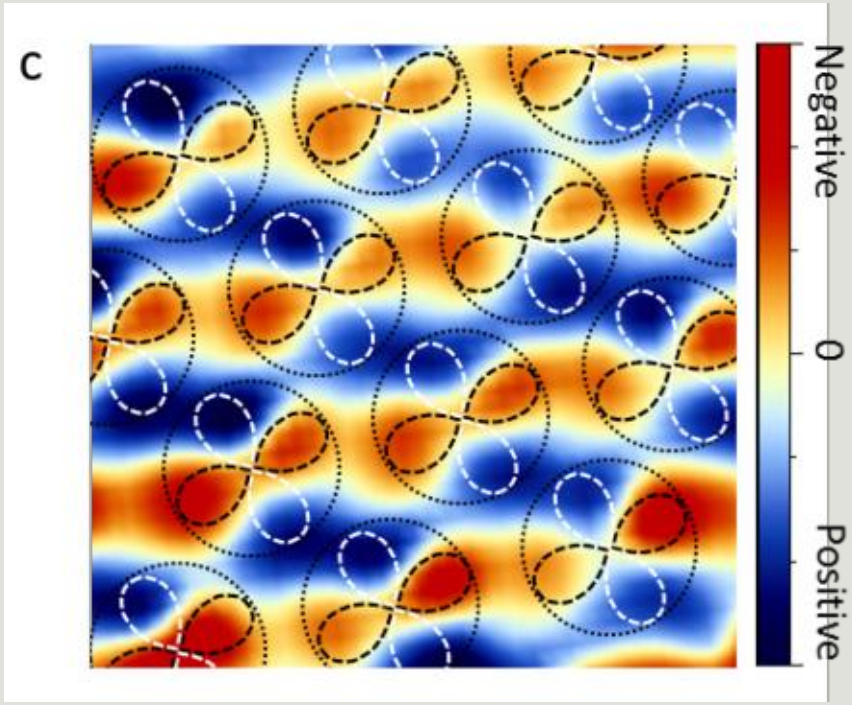


Ref: Serlin, 1907.00261; Sharpe, 1901.03520; Bultinck, 1901.08110

Nematicity

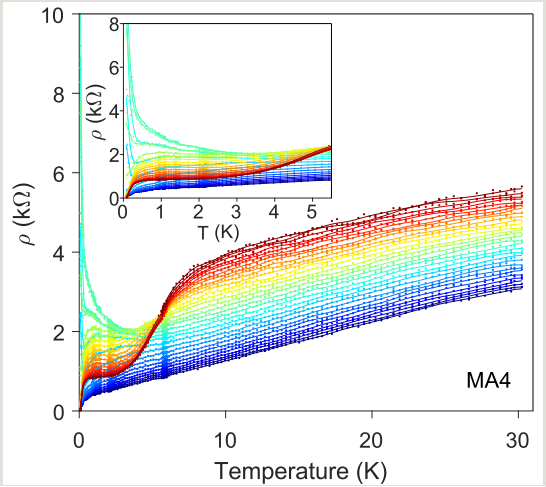
Can locally measure the charge density by integrating STS spectra

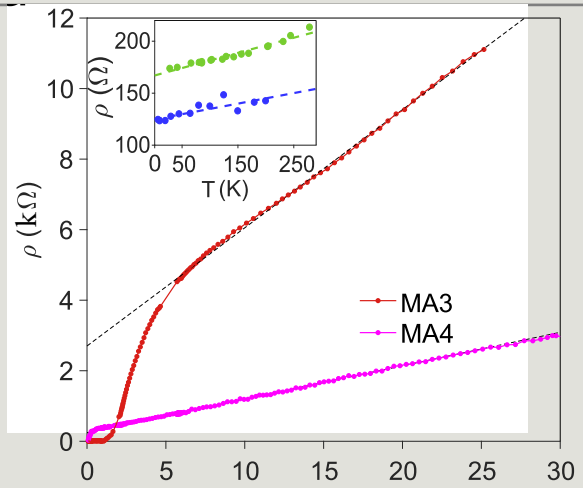


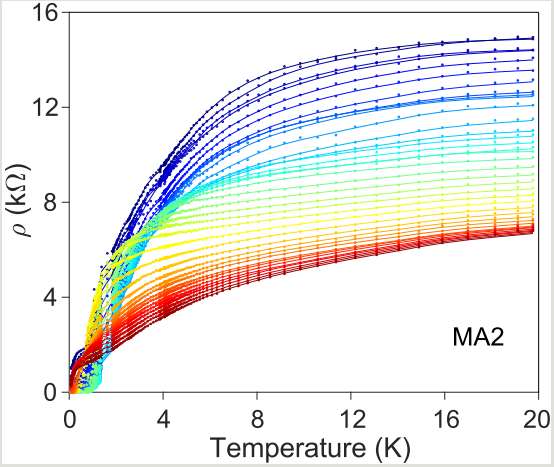


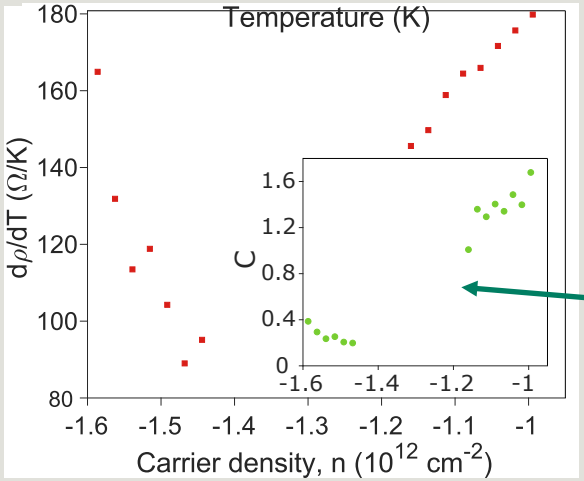
Ref: Jiang, 1904.10153

Planckian dissipation









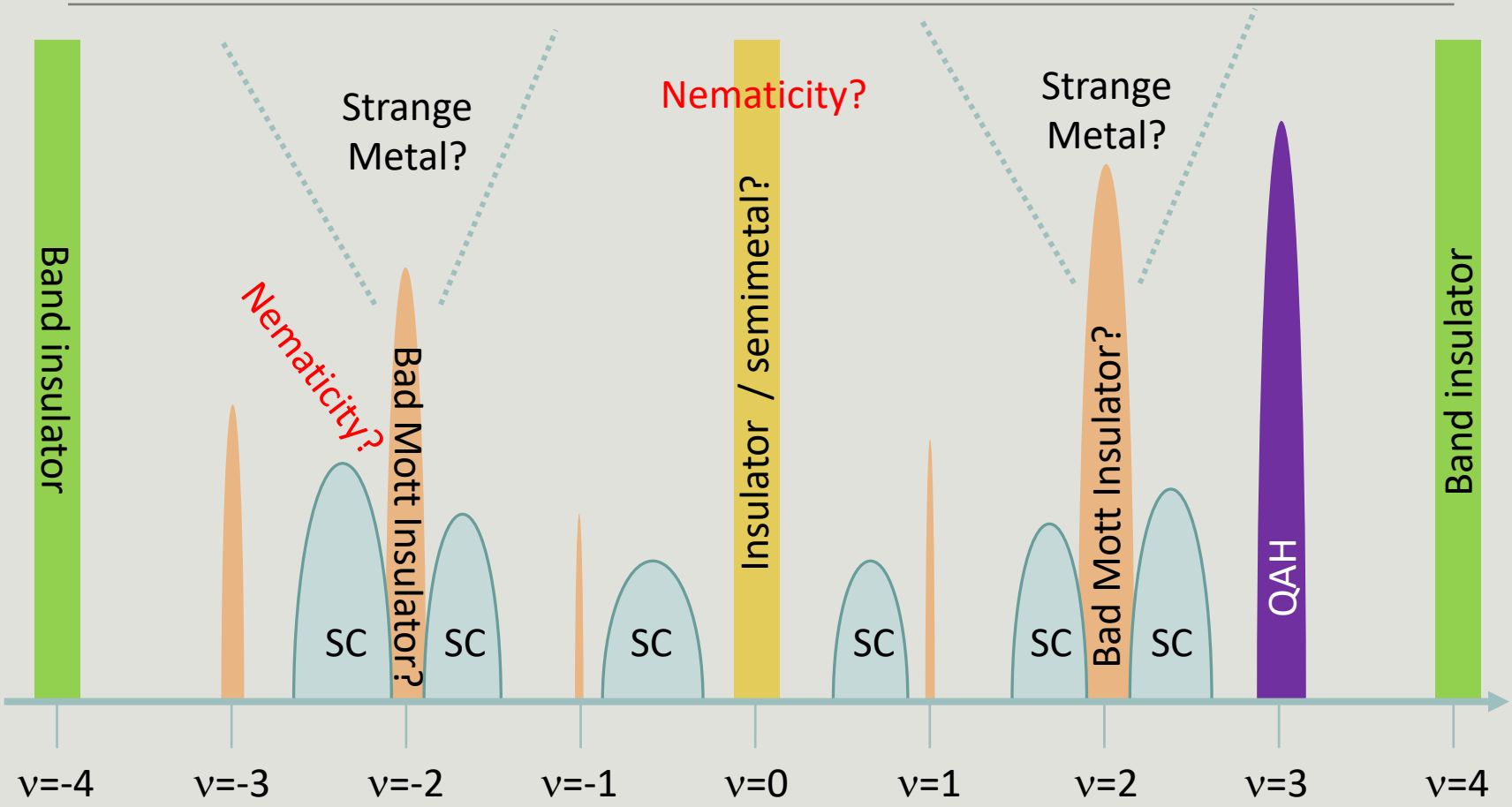
At $|\nu|=2$, the temperature regime **above** the Bad Mott insulator displays **linear T resistivity**

Prefactor of relaxation time is order one, is it **Planckian dissipation**?

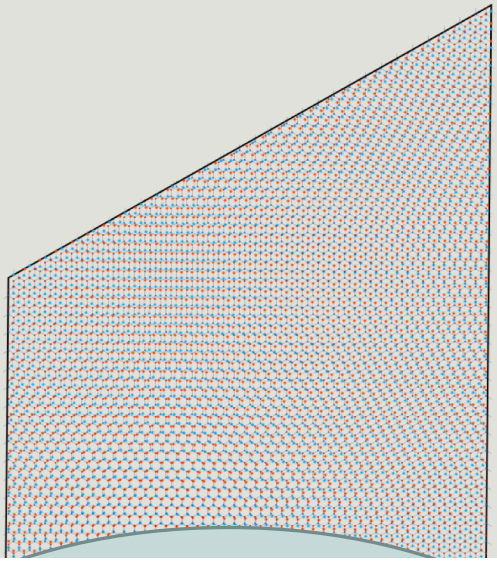
$$\tau = \frac{\hbar}{\alpha k_B T}$$

Ref: Cao, arXiv:1901.03710

Experimental conclusion



Goal: a simple model

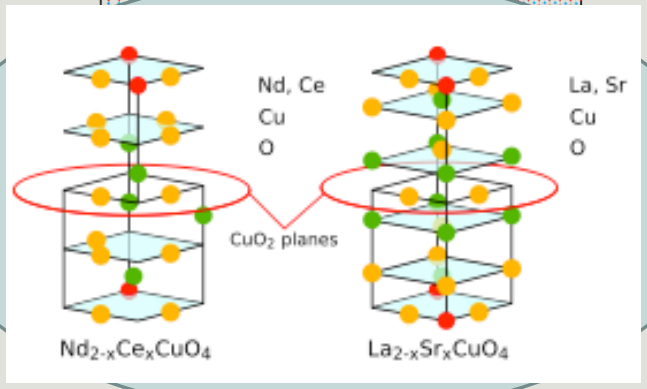


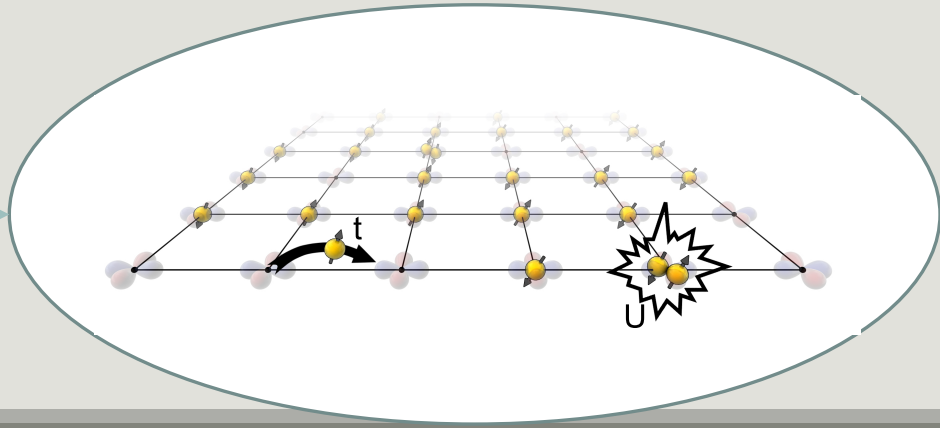
Full lattice model is **challenging**: >11,000 bands

To include interactions, need a **simplified model** of **local Wannier orbitals**

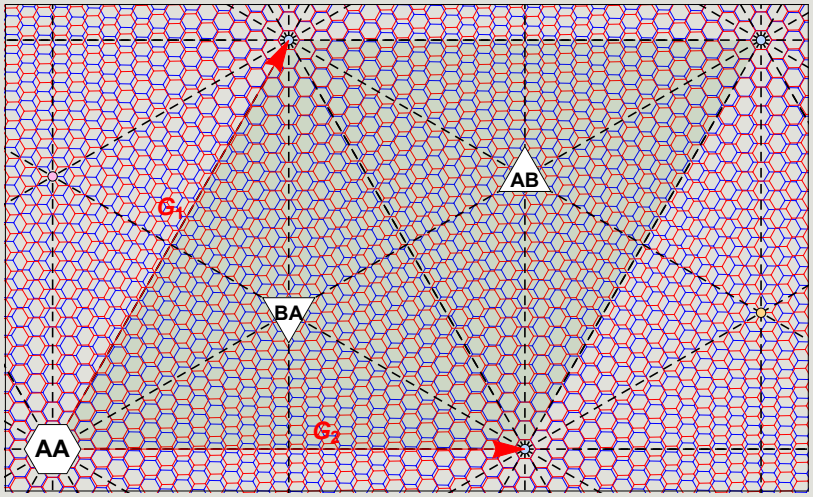
$$w_m(\mathbf{r}) = \int_{\mathrm{BZ}} d\mathbf{k}\; U^{\mathbf{k}}_{mn}\; \psi_{n\mathbf{k}}(\mathbf{r})$$

Compare to getting square lattice Hubbard model out of the **cuprates**

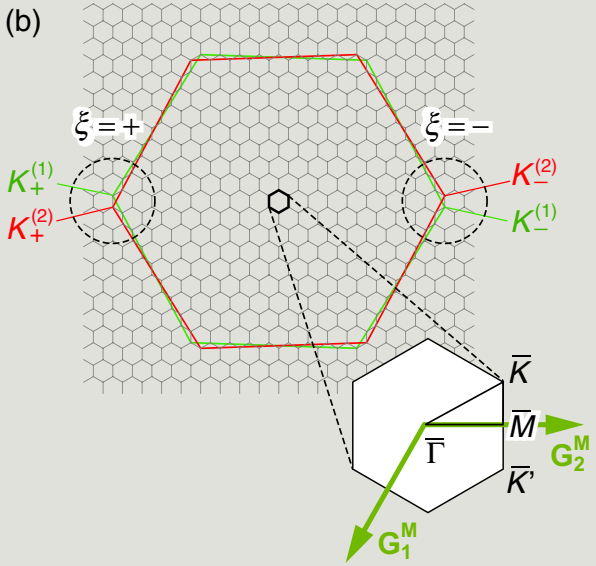




Symmetries



Start with **AA stacked bilayer** and rotate in hexagon center: D6, D3, C2 symmetries



Less symmetry if rotating somewhere else

Wei's question

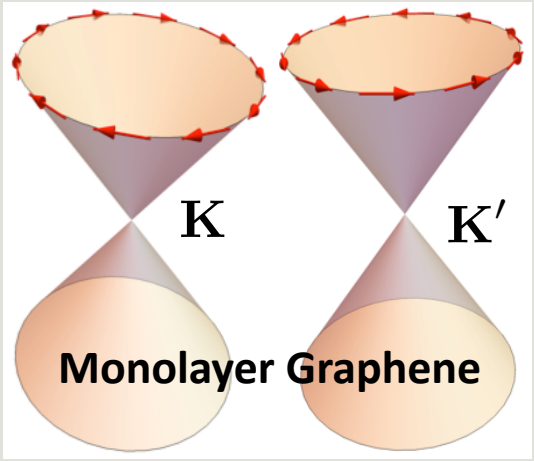
More symmetry in continuum model:
in particular **Valley symmetry**

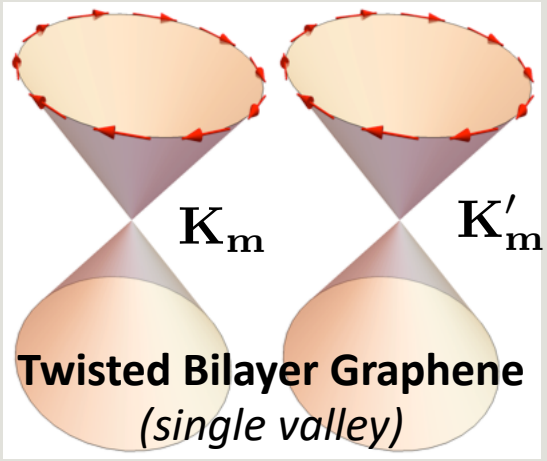
Ref: Zou, 1806.07873; Koshino PRX 2018

“Fragile” topology

Topological insulator cannot be transformed into an **atomic insulator**

In monolayer graphene, Dirac cone have **sublattice chirality**





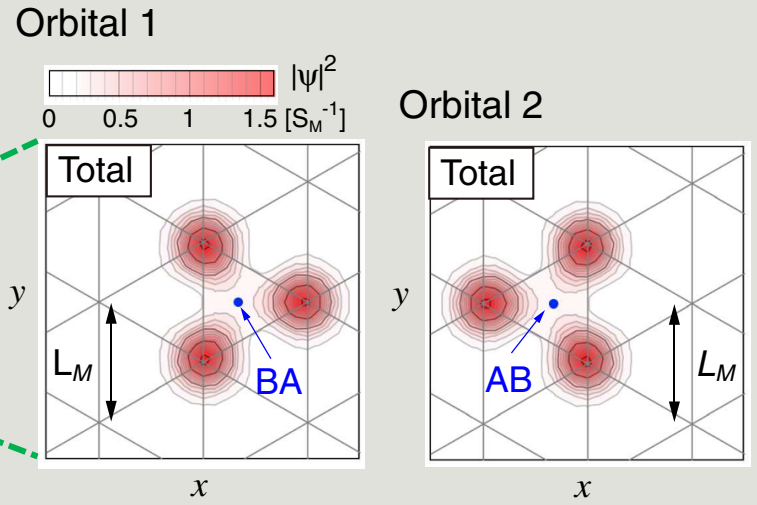
In **single valley** in **twisted bilayers** both cones have the **same chirality**!

It **cannot be described by an atomic orbitals**, even though it doesn’t have a topological index

Ref: Zou, 1806.07873; Po, 1709.06551

Way out: nonlocal orbitals

Construct Wannier orbitals that are **non-local: 'fidget spinners'**



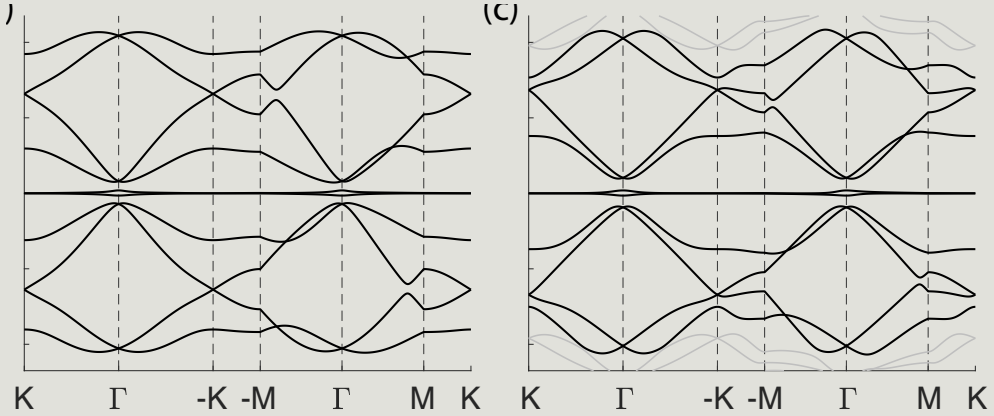
But **interactions are insane**:
up to 5th nearest neighbor are comparable in energy!

n	0	1	2	3	4	5
V_n	1.857	1.533	1.145	1.068	0.697	0.614
$V_n^{(\mathrm{approx})}$	1.857	1.524	1.136	1.081	0.679	0.610
J_n	N/A	0.376	0.0645	0.010	0.014	0.001

Ref: Koshino, PRX 2018; Kang, PRX 2018

Way out: more orbitals

You can also include **more orbitals** to circumvent the non-locality of the Wannier functions



Note: for Mott localization some **symmetry agnosticism** is useful
Band symmetries are not necessarily respected by the Mott state!

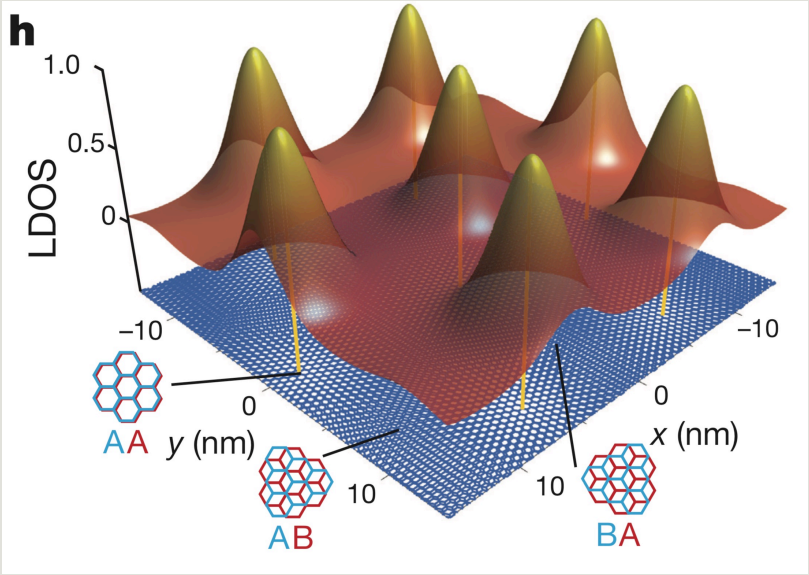
Ref: Po, 1808.02482; Haule, 1901.09852

Real-space structure

The main question is:

What is the real-space structure of the orbitals?

First observation: density of states at charge-neutrality is peaked at **AA**



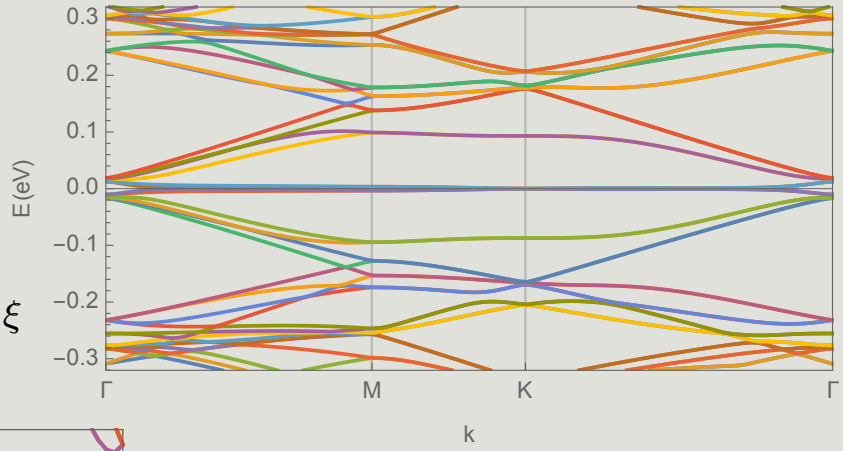
Flat bands

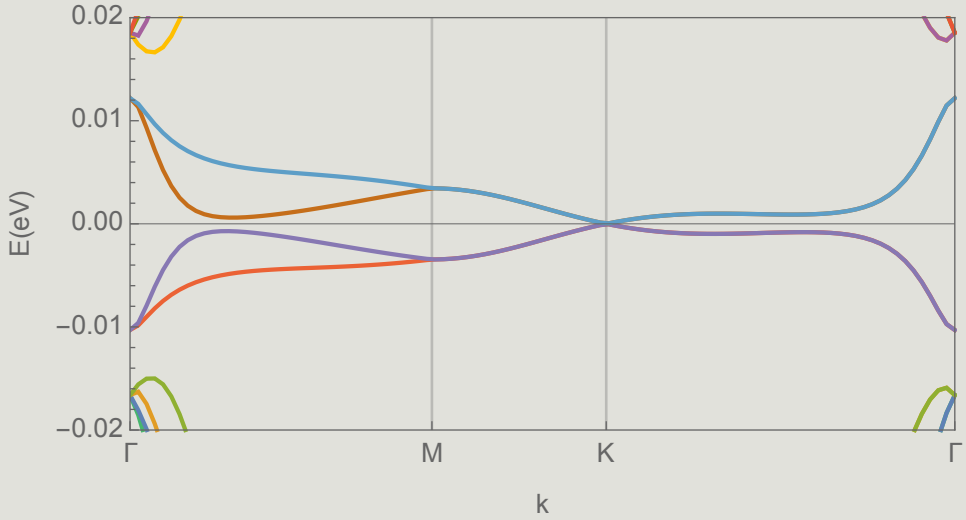
Look at the whole band structure

Using **tight-binding** model

In-plane: nearest neighbor hopping

Interlayer hopping $t_\perp(\mathbf{r}) = t_{\perp 0} e^{-|\mathbf{r}|/\xi}$





Zoom-in around charge neutrality:

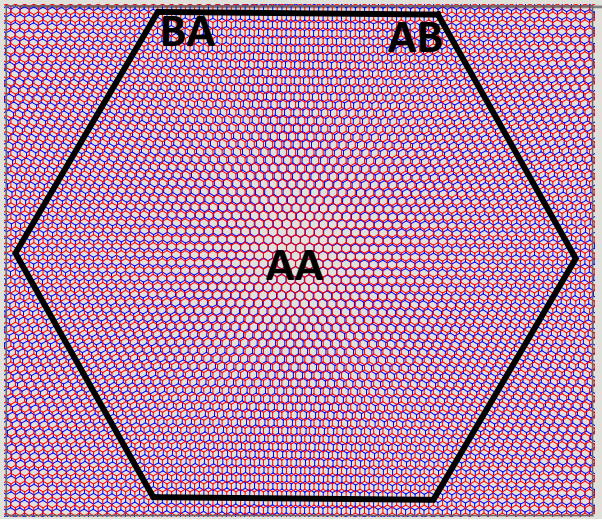
Bandwidth of 11.25 meV

Double **degenerate** at *K*

Almost double degenerate at *M* and *Γ*

Bandgap towards other bands

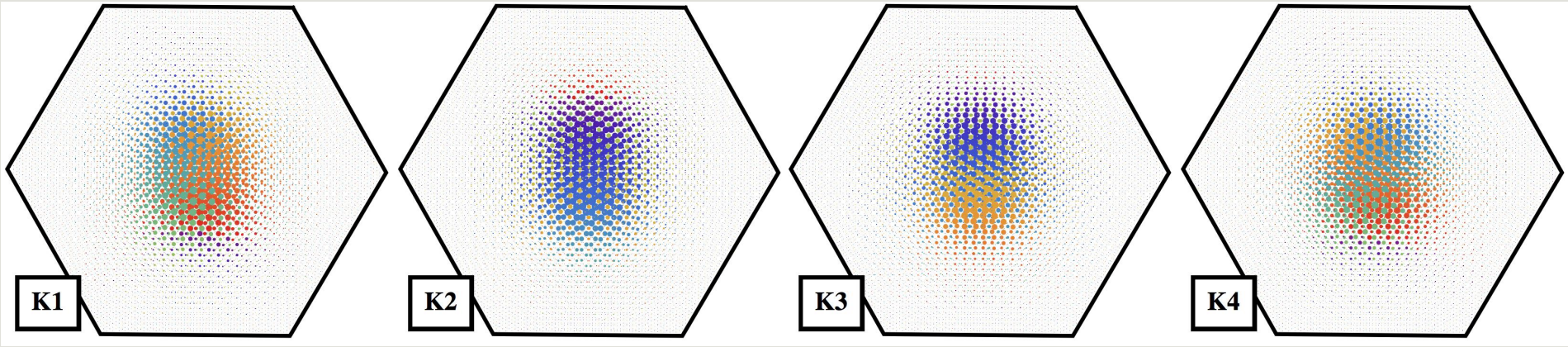
States at charge neutrality



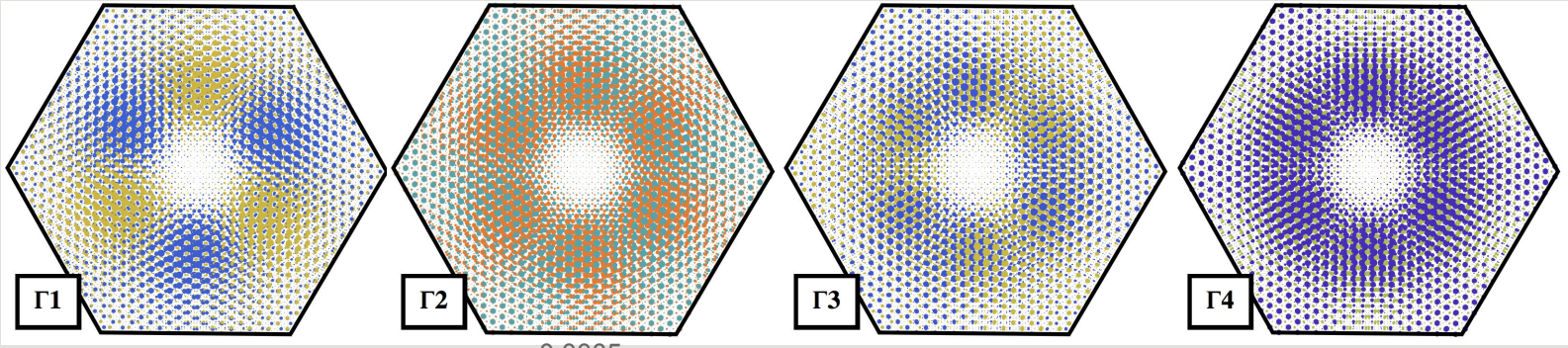
The states at *K* and *K'* are localized at

AA stacking centers of the unit cell

Notice that there are **4 'center' orbitals**

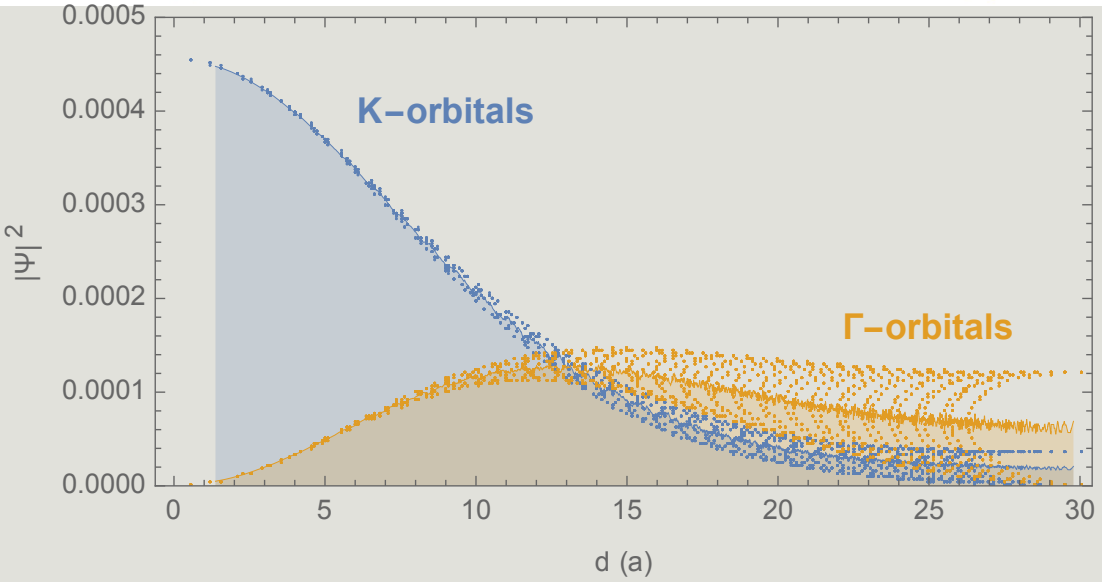


States at the flat band edge

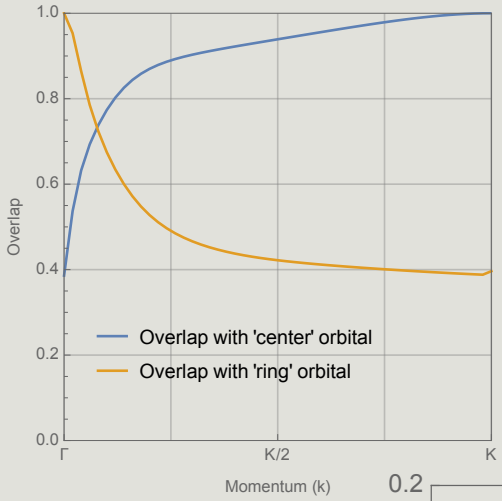


However, at the Gamma point, the wavefunctions **vanish** at the AA centers.

They form a **ring-like structure**!



Mixed-orbital flat bands



Effective model should include this **hybridization**

'Center' orbitals hop on **honeycomb** lattice

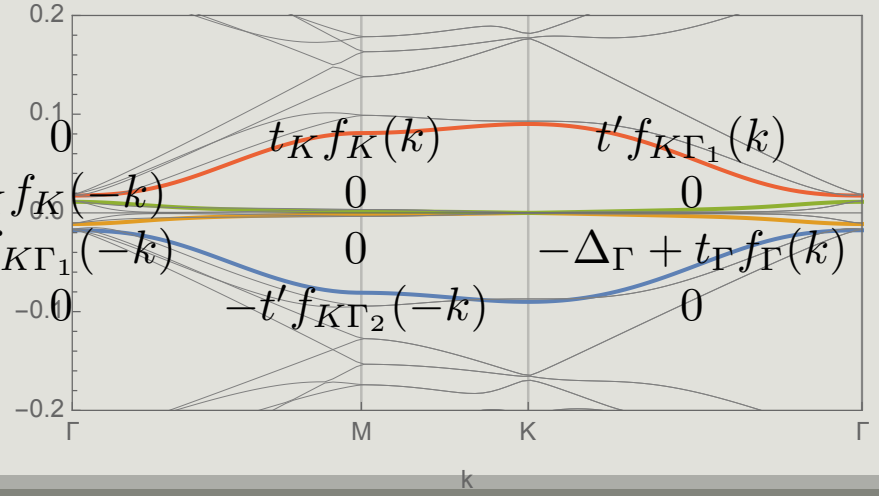
$$f_K(\mathbf{k}) = 1 + e^{i\mathbf{a}_1\cdot\mathbf{k}} + e^{i\mathbf{a}_2\cdot\mathbf{k}}$$

'Ring' orbitals hop on **triangular** lattice

$$f_\Gamma(\mathbf{k}) = 2\left(\cos\mathbf{a}_1\cdot\mathbf{k} + \cos\mathbf{a}_2\cdot\mathbf{k} + \cos\mathbf{a}_3\cdot\mathbf{k}\right)$$

$$H_4(k) = \begin{pmatrix} 0 & t_K f_K(k) & t' f_{K\Gamma_1}(k) & 0 \\ t_K f_K(k) & 0 & 0 & -t' f_{K\Gamma_2}(k) \\ t' f_{K\Gamma_1}(-k) & 0 & -\Delta_\Gamma + t_\Gamma f_\Gamma(k) & 0 \\ 0 & -t' f_{K\Gamma_2}(-k) & 0 & \Delta_\Gamma - t_\Gamma f_\Gamma(k) \end{pmatrix}$$

$t_{K\Gamma} = 4.7\,\mathrm{meV}$



x 2

Coulomb interactions

Coulomb repulsion is **long-range** and **quite strong** in graphene

$$V(\mathbf{r}_i - \mathbf{r}_j) = \frac{1.438}{0.116 + |\mathbf{r}_i - \mathbf{r}_j|}\ \mathrm{eV}$$

(Wehling PRL 2011)

Two physical effects:

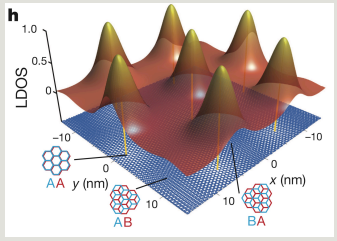
- Hubbard **U** - depends on the orbital

$$U = \int d\mathbf{r} d\mathbf{r}' |\psi(\mathbf{r})|^2\, V(\mathbf{r} - \mathbf{r}')\, |\psi(\mathbf{r}')|^2$$

490 meV for center orbital
Localization!

- **Unequal** charge distribution

$$E_{\mathrm{int}} = \int d\mathbf{r} d\mathbf{r}' \delta n(\mathbf{r})\, V(\mathbf{r} - \mathbf{r}')\, \delta n(\mathbf{r}')$$



Hartree: Set-up

The idea is to **decouple** density-density interactions

$$H_H = \sum_i \delta n(\vec{r}_i)\phi_i$$

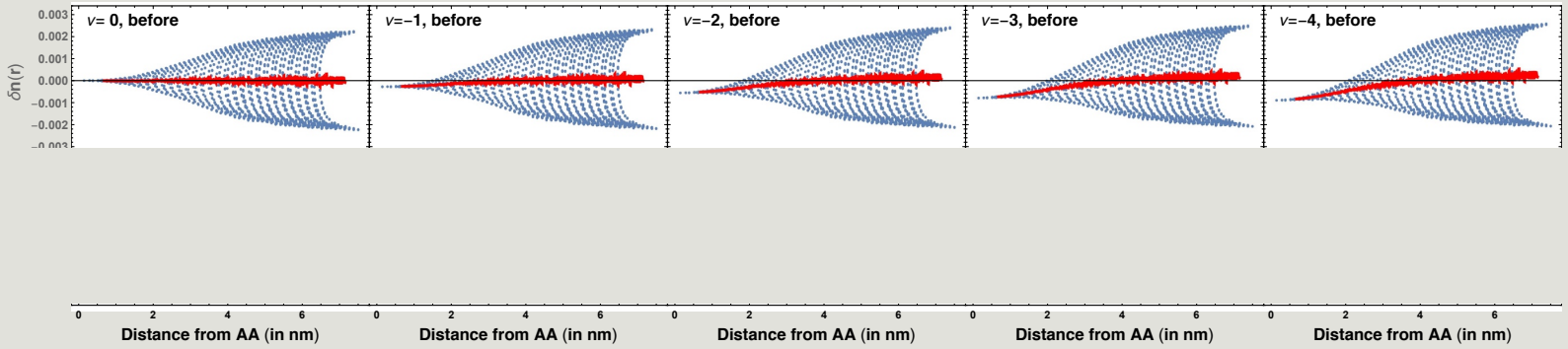
introducing **Hartree fields** ϕ

$$\phi_i = \sum_j V(\vec{r}_i - \vec{r}_j)\langle \delta n(\vec{r}_j)\rangle$$

Solved this **self-consistently** for different doping levels (from ν=-4 to 0)

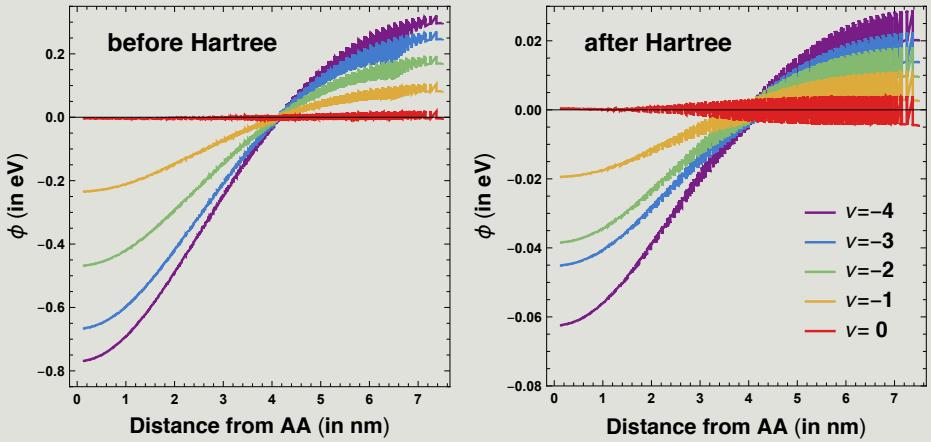
(Note that we **do not** include Fock corrections. $\langle c_j c_i^\dagger \rangle c_j^\dagger c_i$)

Charge transfer



Depending on the **electron density**, have a macroscopic charge imbalance between AA and AB/BA

Leads to **large electric fields** that are reduced by **Hartree-Fock self-energy**

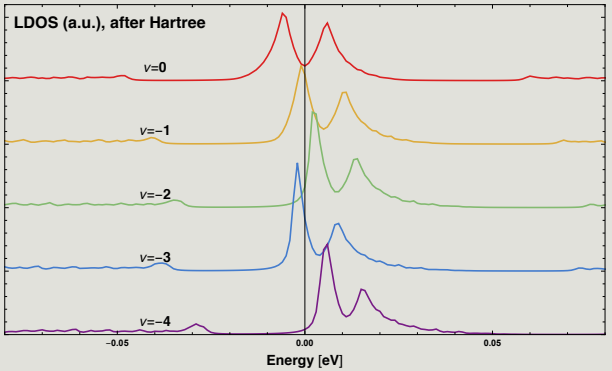


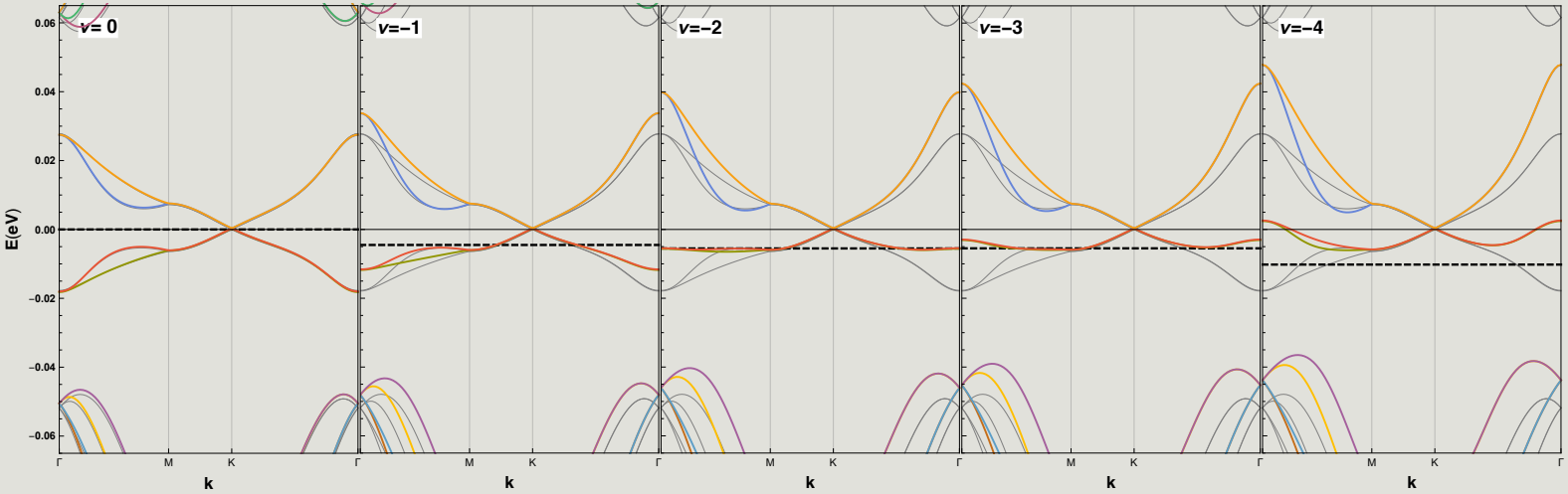
Renormalized bandstructure

Charge transfer from center to ring causes states at Γ **pushed up in energy**

Band flattening, mostly at $|\nu|=2$

And the Van Hove singularity in STS is **pinned** to Fermi level

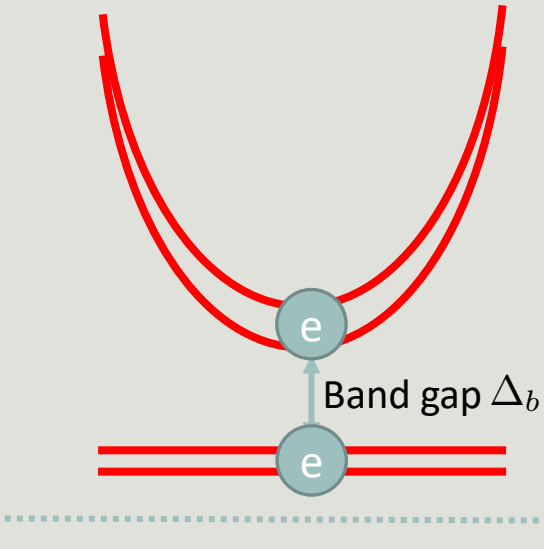




Speculations on ν=2

Need to add **Hubbard U** on top of renormalized bands

But… U is **typically on the order of or larger than band-gap!**



Two dispersive bands

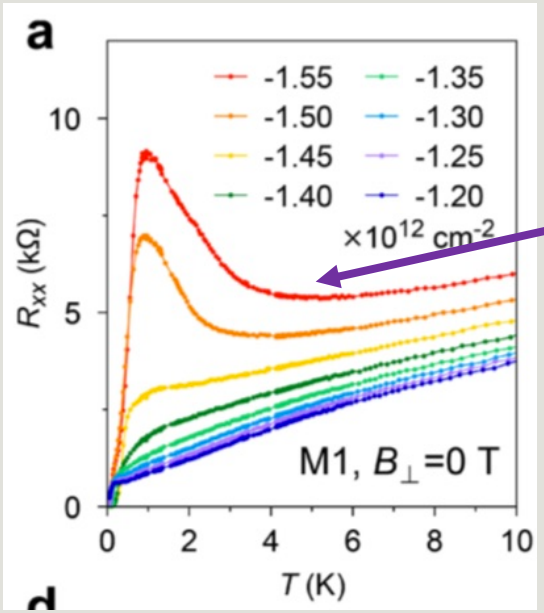
Two flat bands

Charge neutrality

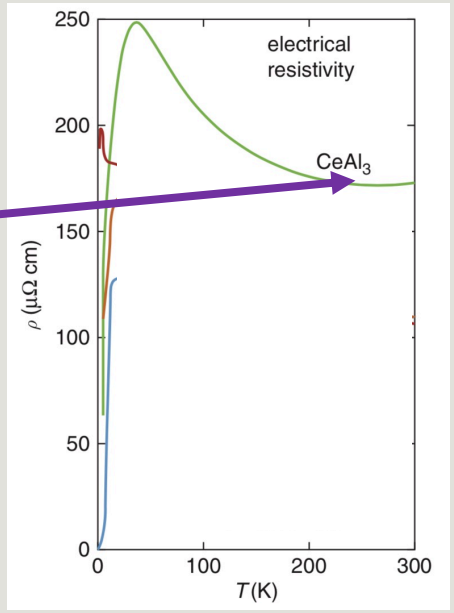
If $U > \Delta_b$,
energy is lower by
occupying one flat band
and **one dispersive band**

Speculations on ν=2 (cont.)

Localized (flat band) electrons hybridized with **conducting** (dispersive band) electrons: this is a **Kondo lattice system**!

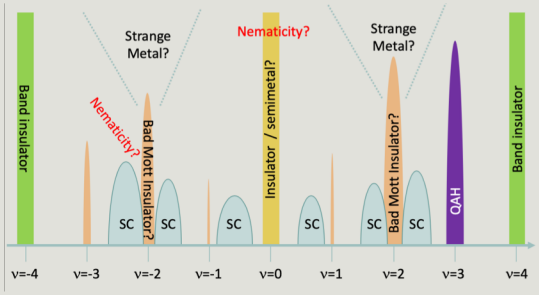


Resistivity minimum associated with formation of the **Kondo singlet**



Very low T implies **very subtle energy competition** – future work…

Summary

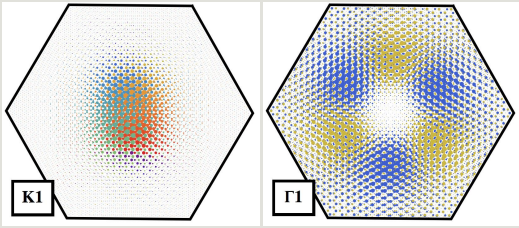


Twisted bilayer graphene is an interesting **interacting** material

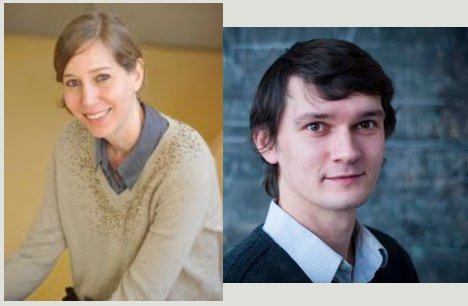
Challenge to find effective low-energy model

There are **ring** and **center** orbitals in the full tight-binding model

Interactions favor a **charge-transfer** from center to ring at Hartree-level



Renormalized band-structure still needs **Hubbard** interactions, still work in progress



In collaboration with **Paula Mellado** (Santiago, Chile) and **Dima Abanin** (Genève, Switzerland)

References: *arXiv:1805.05294 (PRB 2018), arXiv:1907.00940*