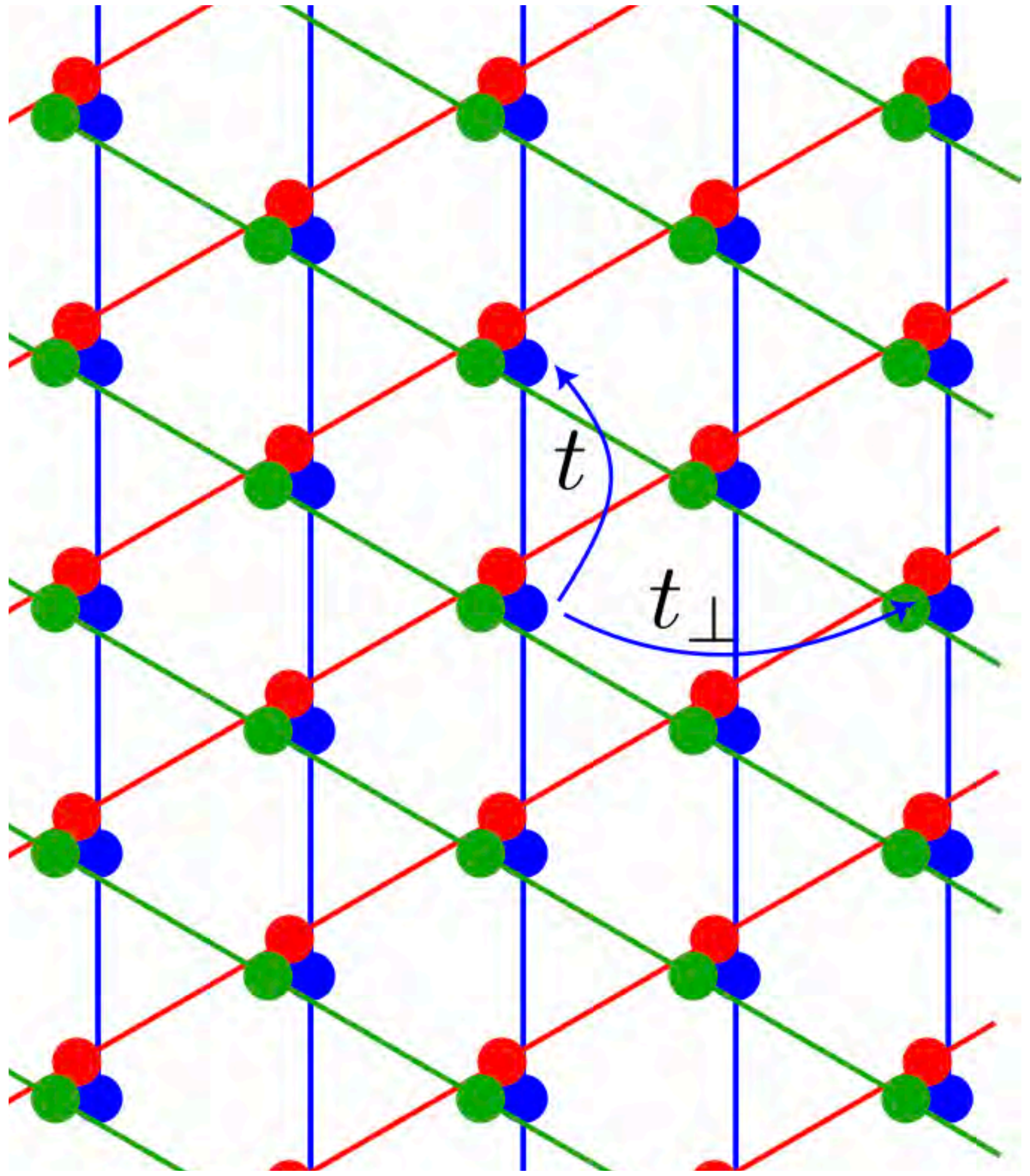
M-Point Moiré Materials I:
Symmetries, Continuum Models, and Bandstructures



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Theory Winter School, NHMFL, January 12-16, 2026

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UKRI Engineering and Physical Sciences Research Council

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Dumitru Călugăru Konstantinos Vasiliou

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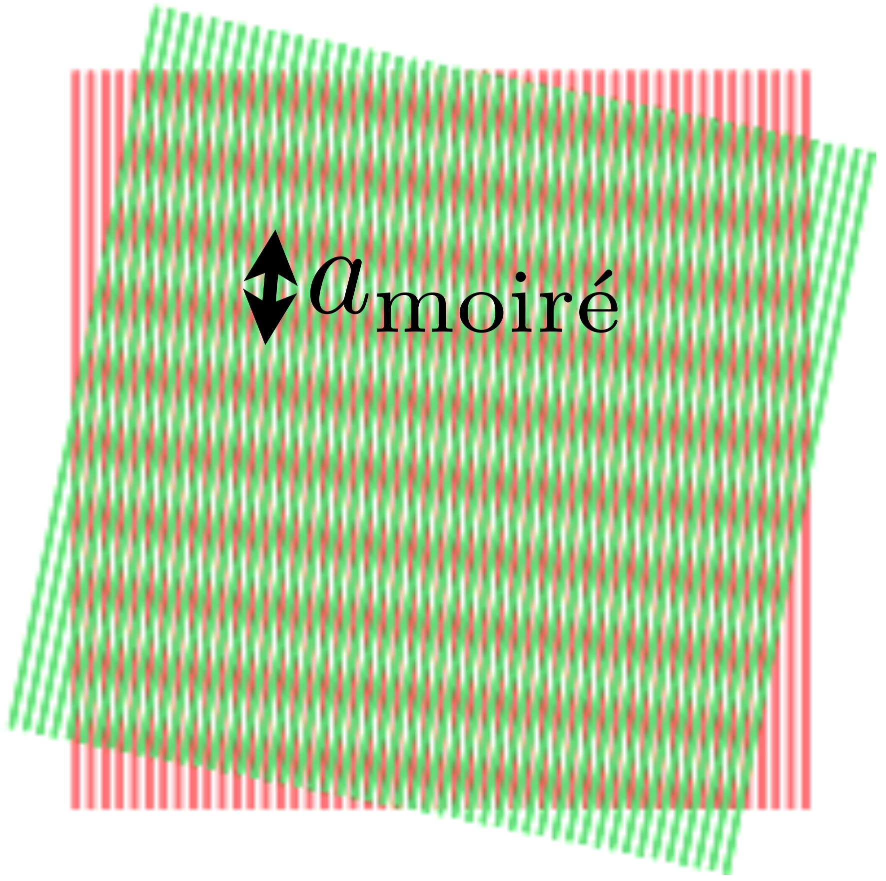
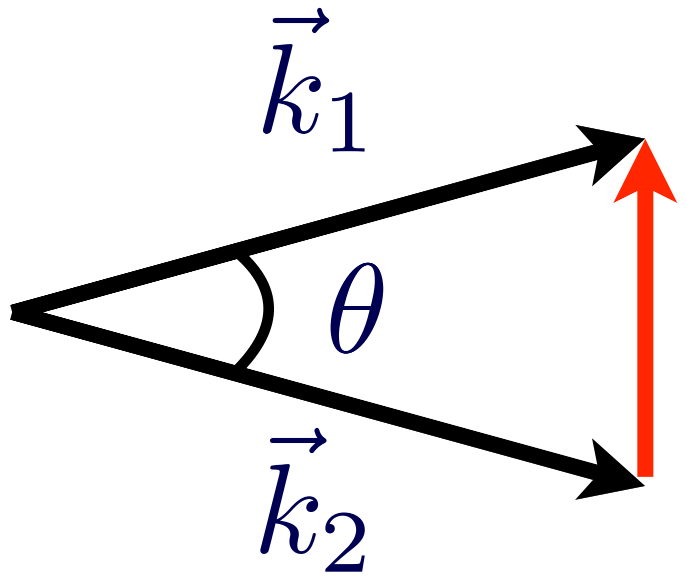
+discussions with **Haoyu Hu, Andrei Bernevig**

Moiré Materials

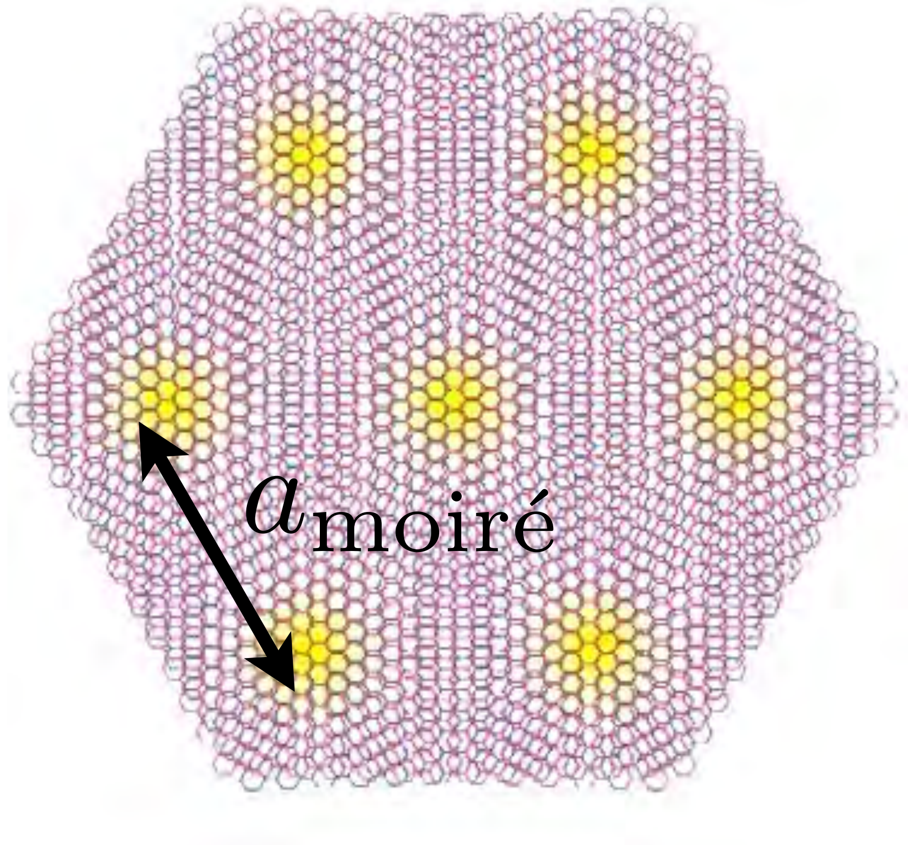
2D materials (graphene, TMDs,…) held together by van der Waals forces



$$V_i(x) \sim \cos(\vec{k}_i \cdot \vec{x})$$



$$\delta = |\vec{k}_1 - \vec{k}_2| \sim 2|\vec{k}_i| \sin\frac{\theta}{2} \approx |\vec{k}_i|\theta$$



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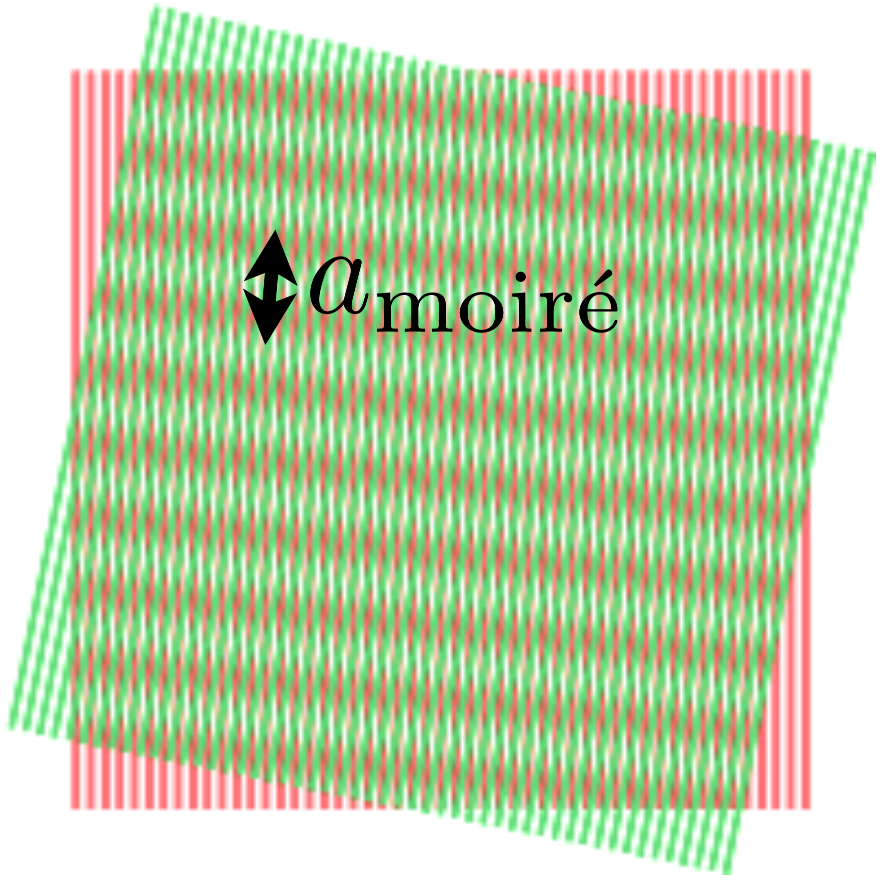

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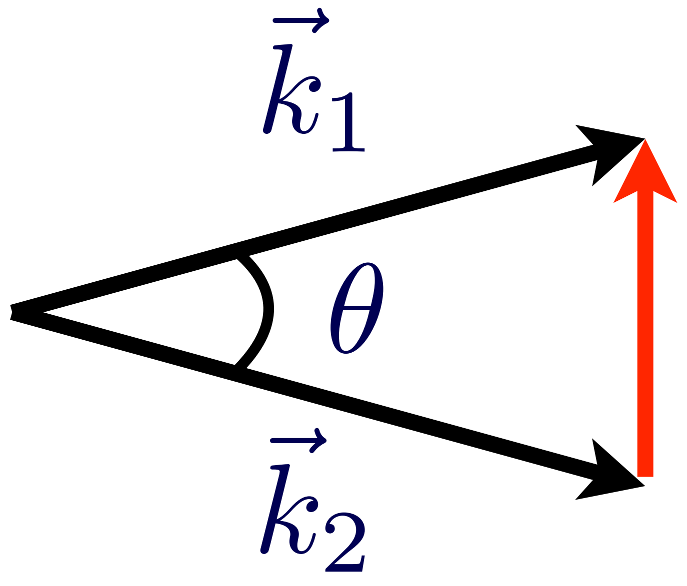

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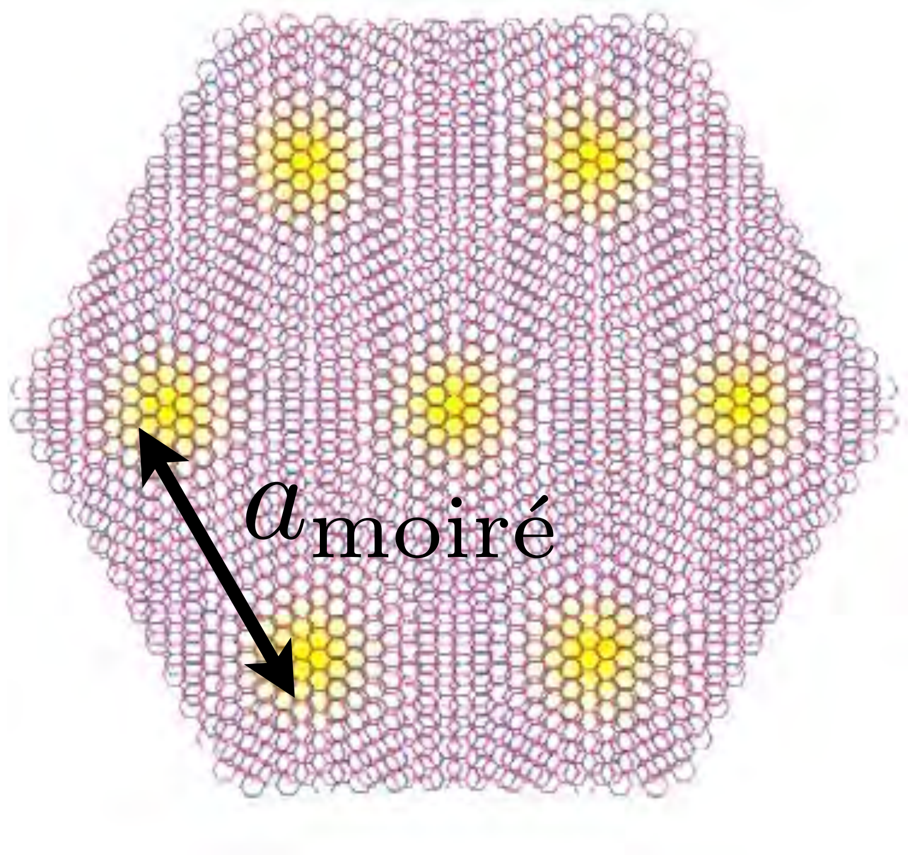

using $|\vec{k}_i| \sim \dfrac{2\pi}{a_{\text{lattice}}}$

$$a_{\text{lattice}} \sim 0.3 \text{ nm}$$

$$\theta \sim 1.5^\circ$$

$$a_{\text{moiré}} = \frac{2\pi}{\delta} \sim \frac{a_{\text{lattice}}}{\theta} \sim 10 \text{ nm}$$

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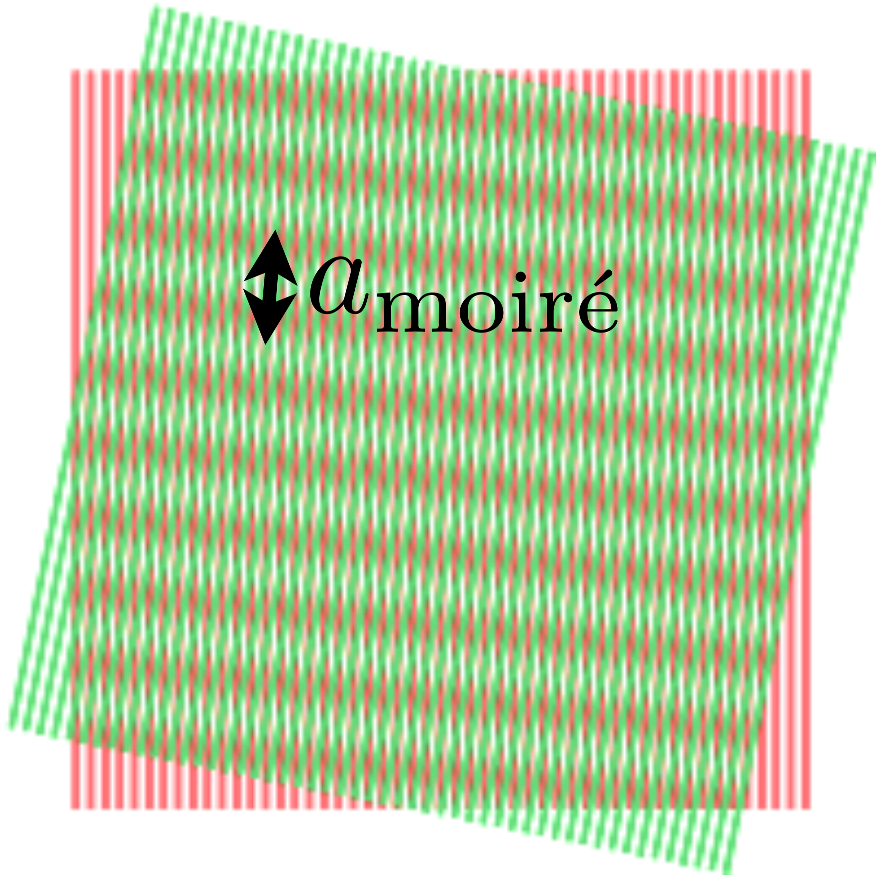

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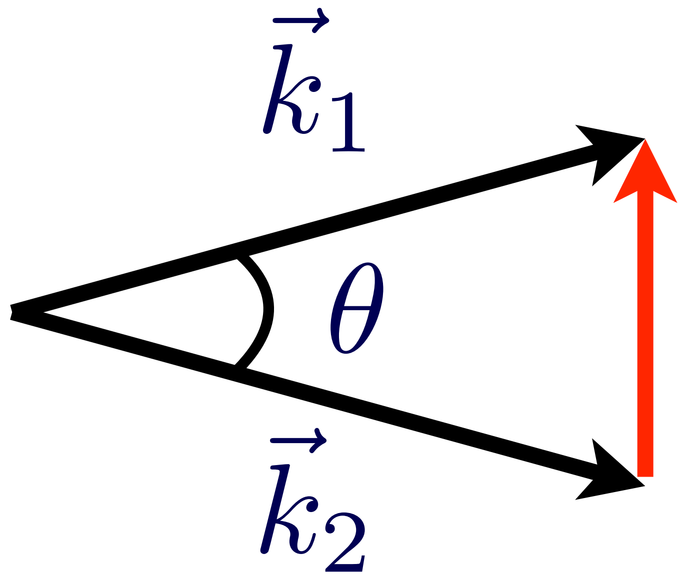

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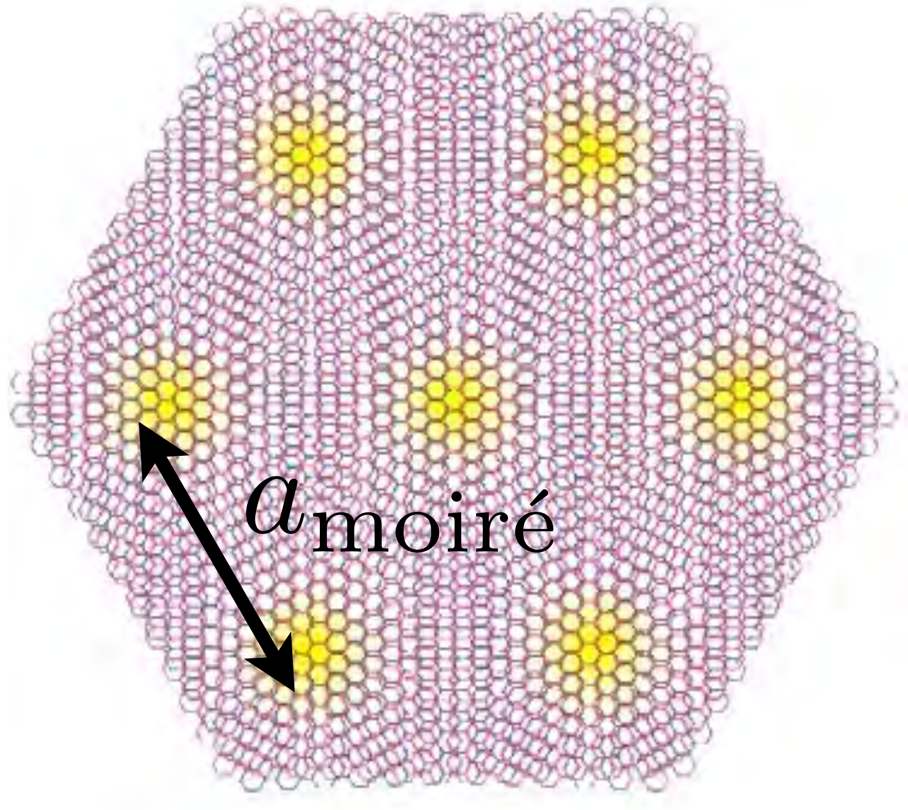

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<u>Bonus</u>: just as magnetic field modifies kinetic energy of free electrons, moiré modifies ε(k)

⇒ "flat" bands w/ small kinetic energy ⇒ strong correlations

Many possible combinations & parameters — routes to new physics!

Moiré-Scale Electrostatics & Charge Doping

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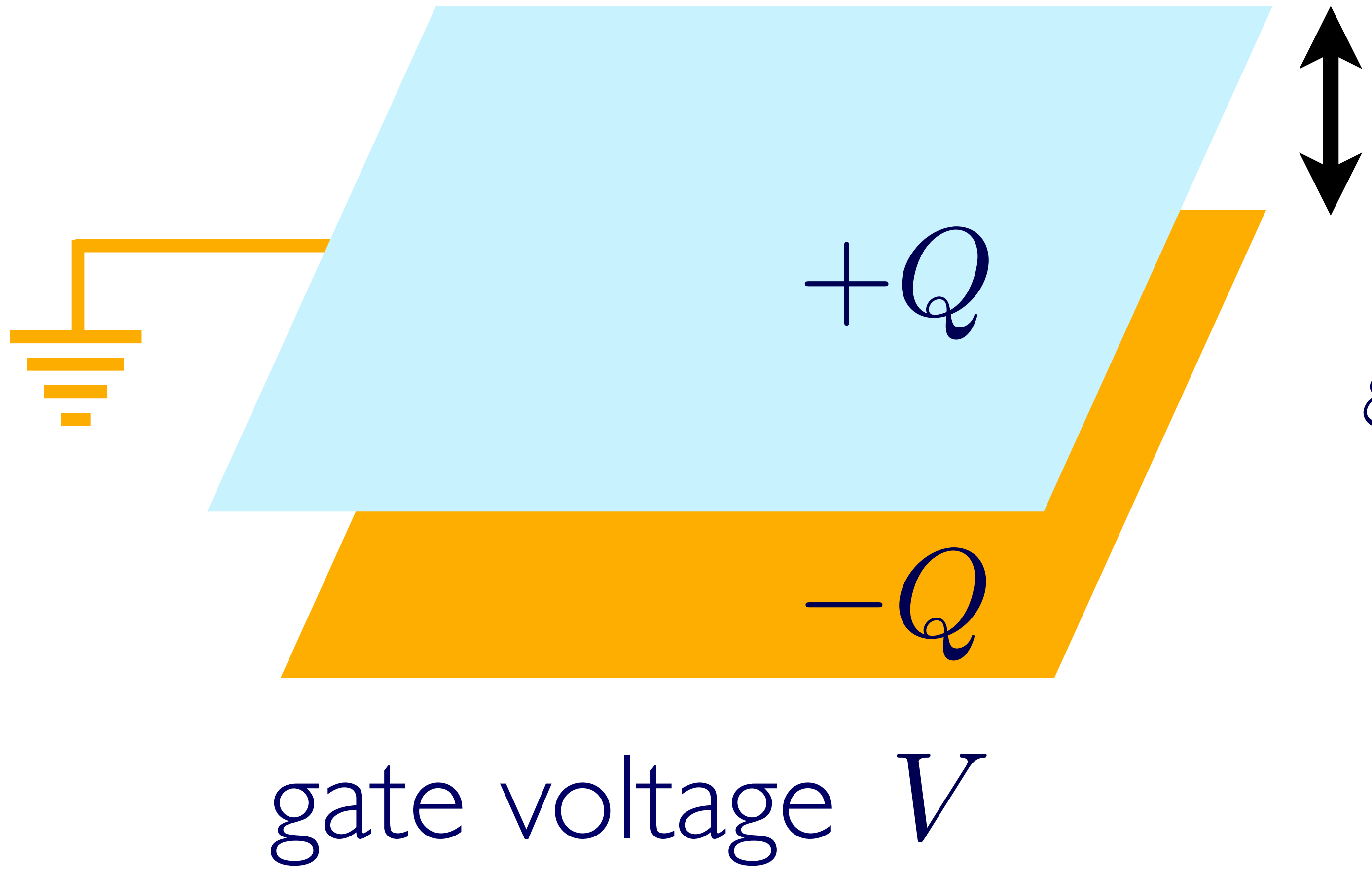
- 2D systems — electrostatic gating



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$\varepsilon_r \sim 10$

$V \sim 1$ Volt

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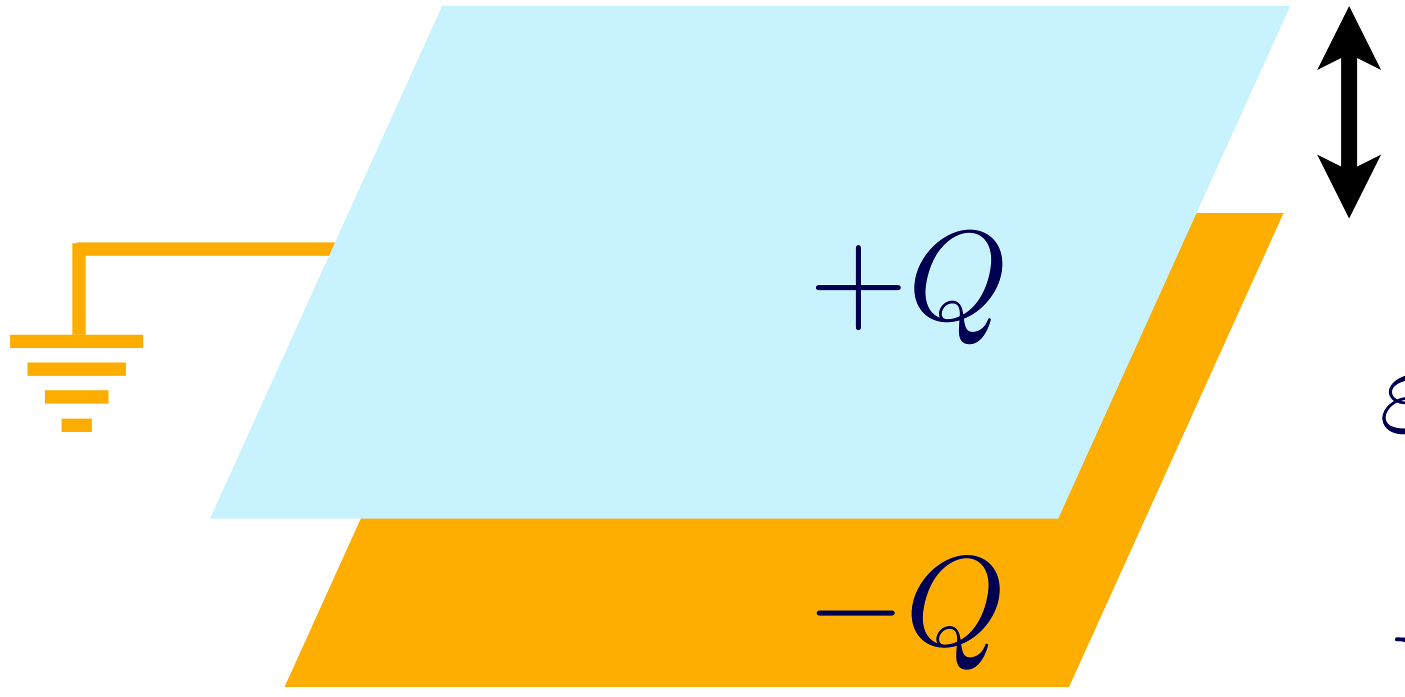

gate voltage V

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Charge density:

$$ne = \frac{Q}{A} = \frac{CV}{A} = \frac{\varepsilon V}{d}$$

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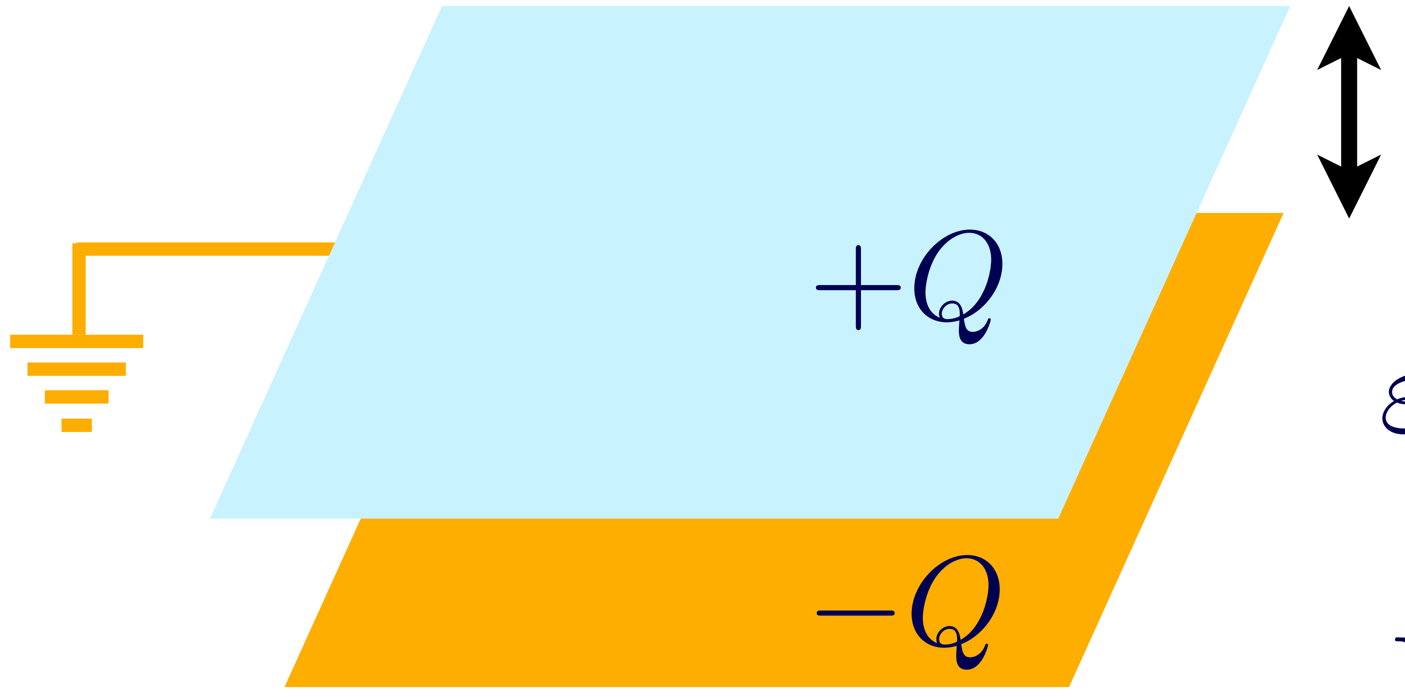

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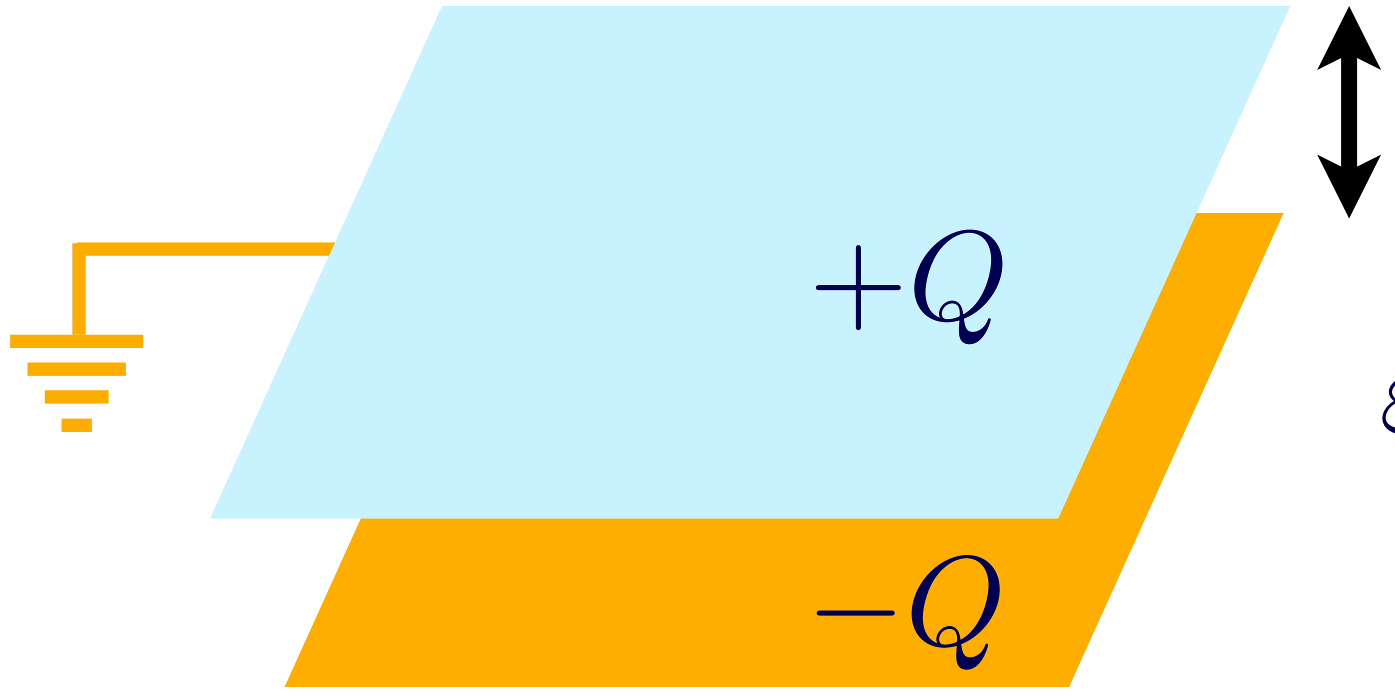

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⇒ Can "fill" or "empty" moiré bands (doping electrons/holes) just by gating

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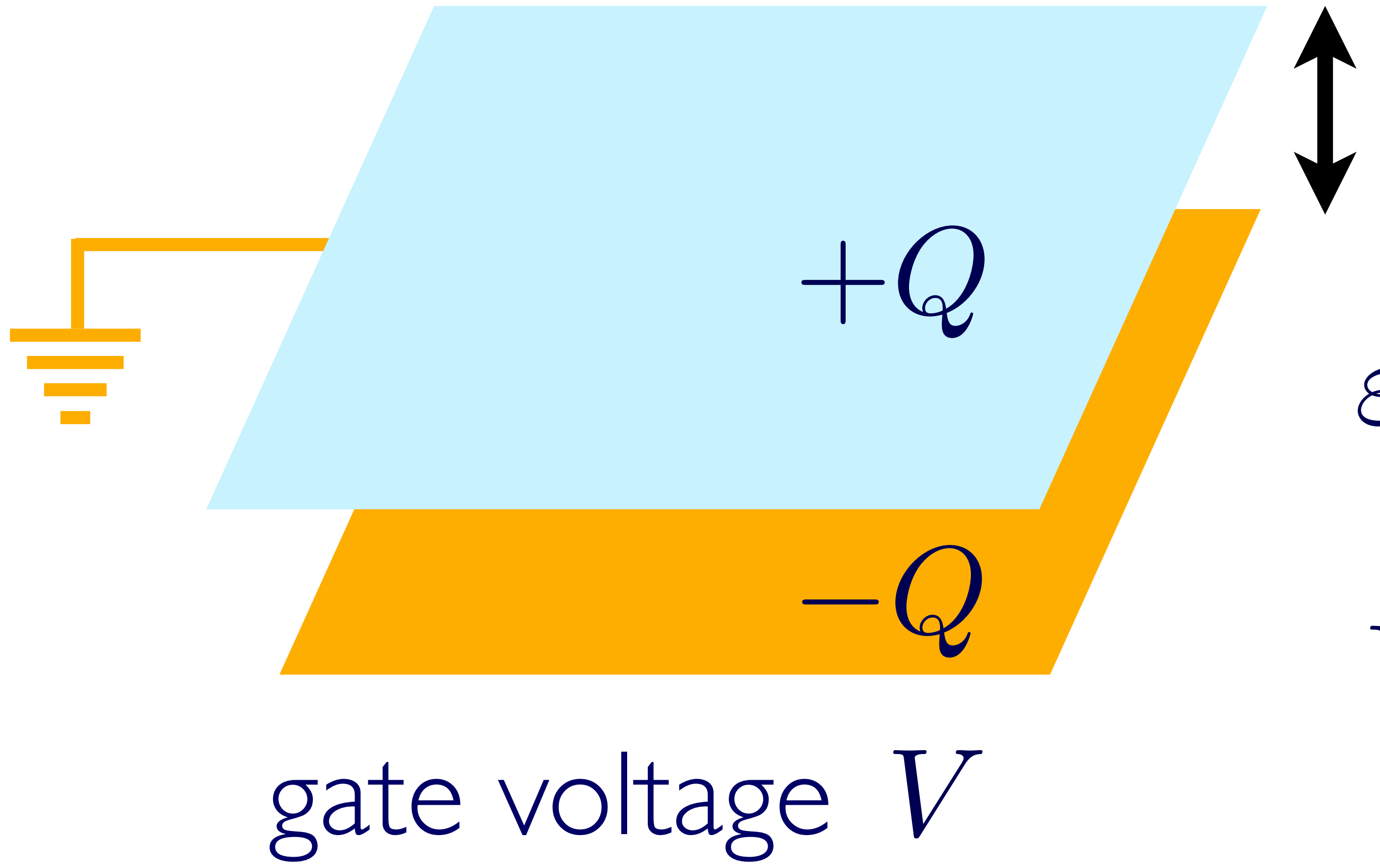

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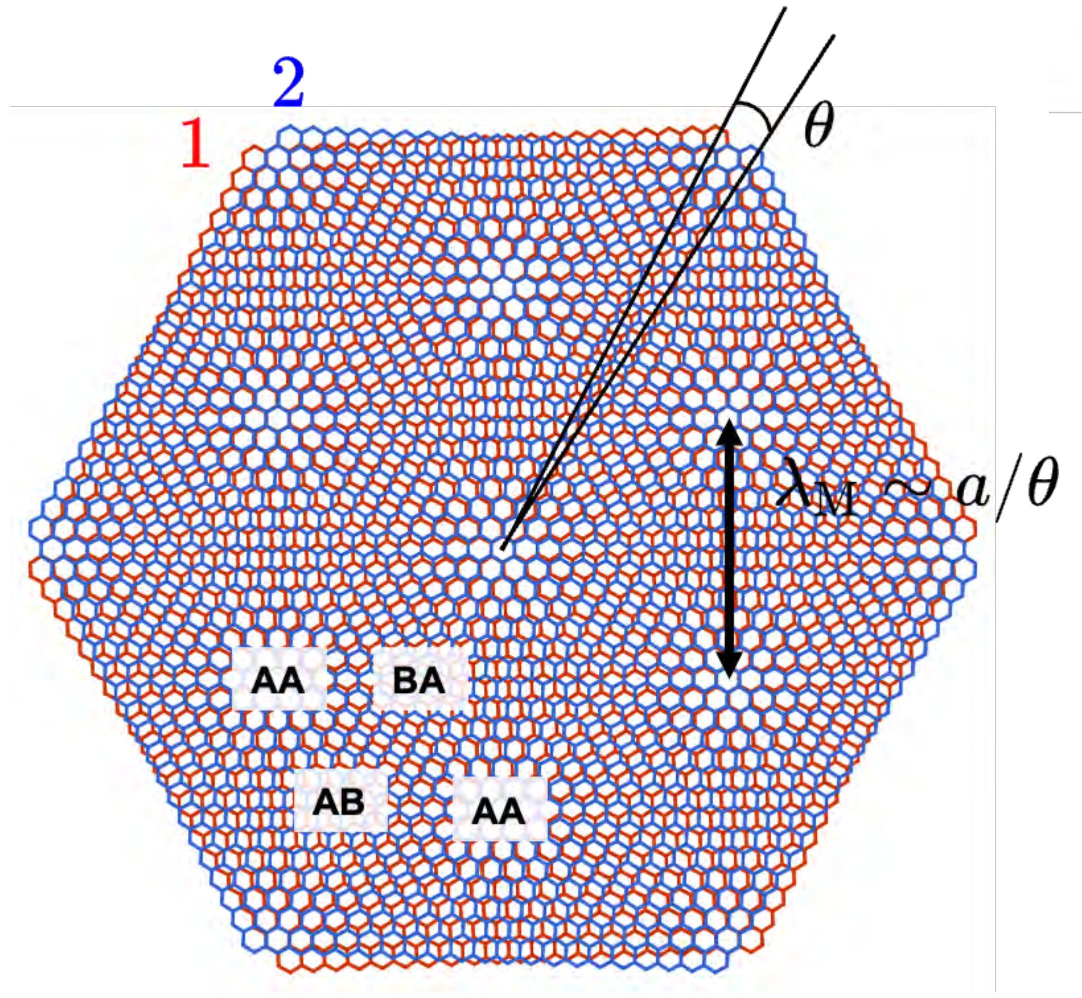
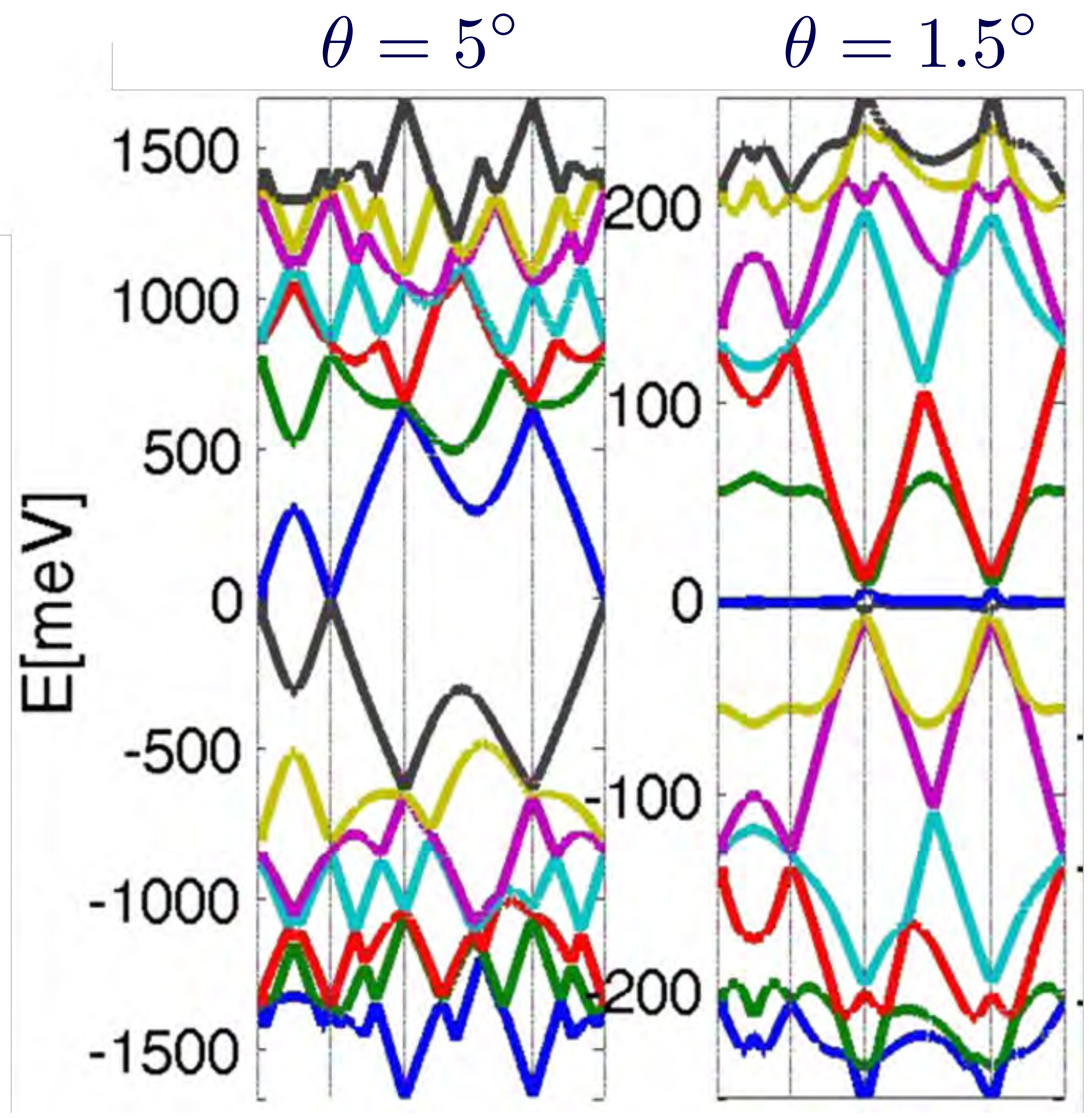
- Moiré bands: weakly dispersive + nontrivial "winding" ⇒ **correlations + topology + tunability**

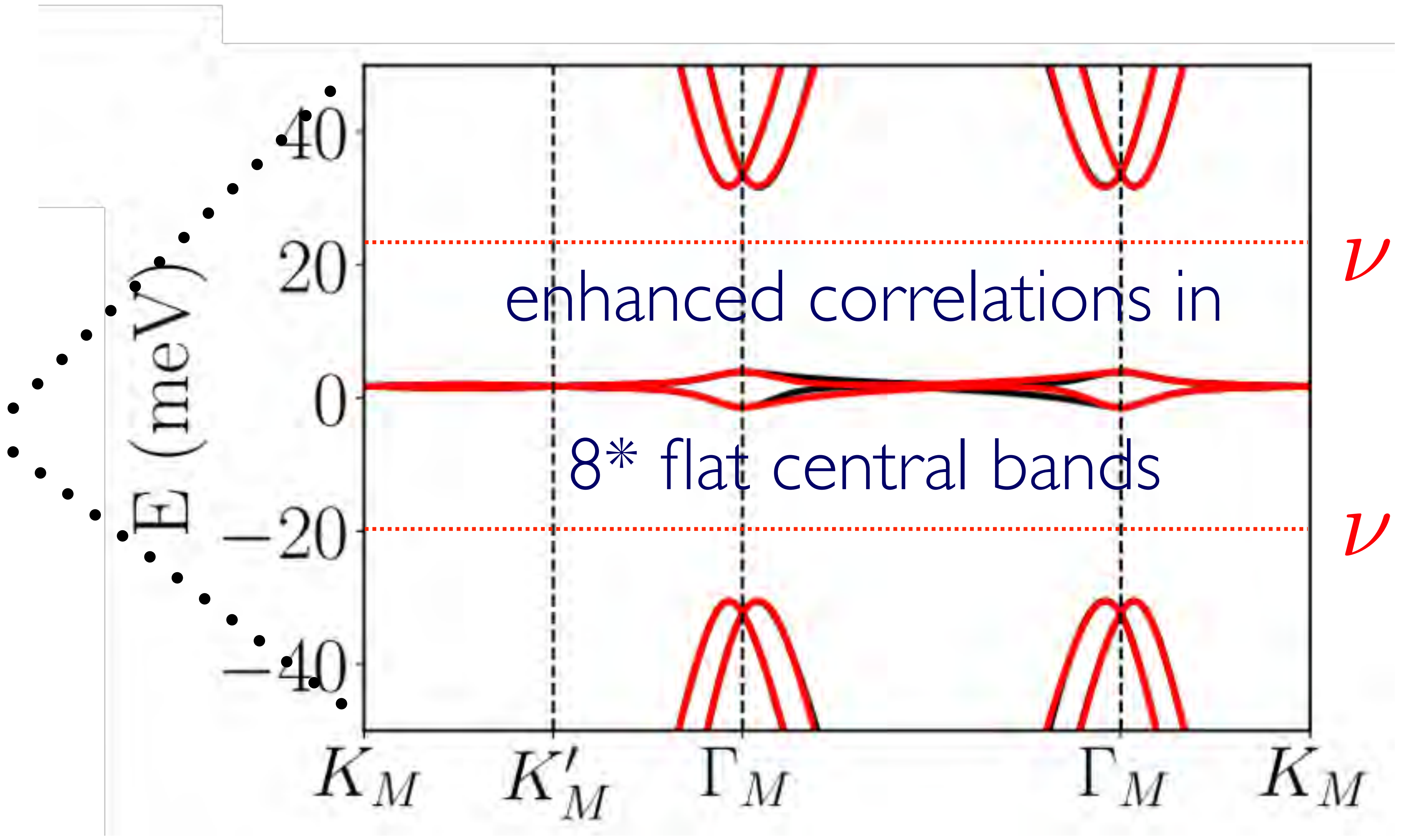
"Hydrogen Atom" of Moiré Materials: Twisted Bilayer Graphene

Linear "Dirac" dispersion gives special structure to twisted moiré multilayers of graphene

moiré-reconstructed TBG bands **almost perfectly flat** near "magic" twist angle $\theta \sim 1.05°$



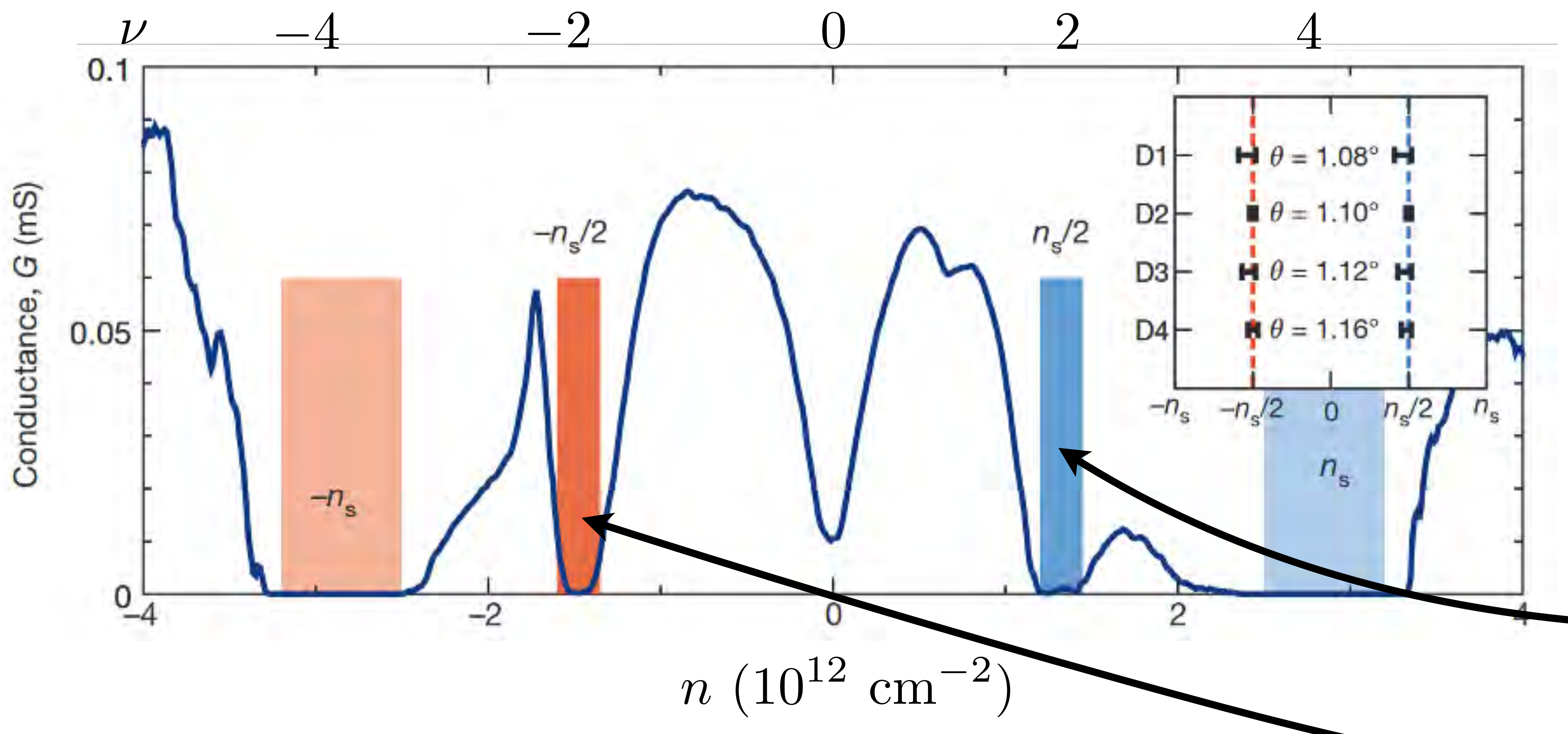




[Bistritzer & Macdonald, PNAS **128**, 12233 (2011)]

*8 electron "flavors" - 2 spin × 2 "valley" × 2 "sublattice"

TBG: Status Report



Puzzle #1

"correlated insulators"

(band theory predicts metal)

[Cao *et al* Nature **556**, 80 (2018)]

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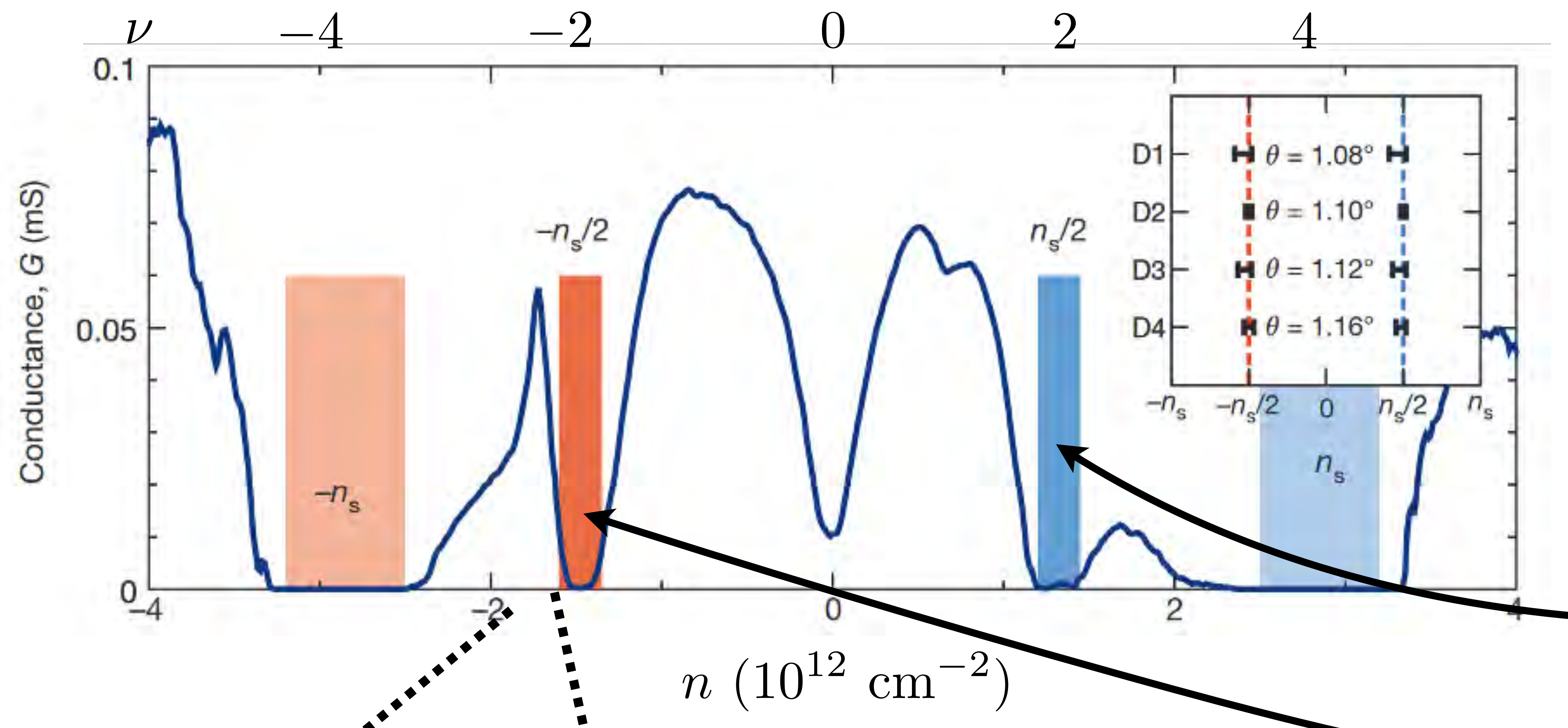

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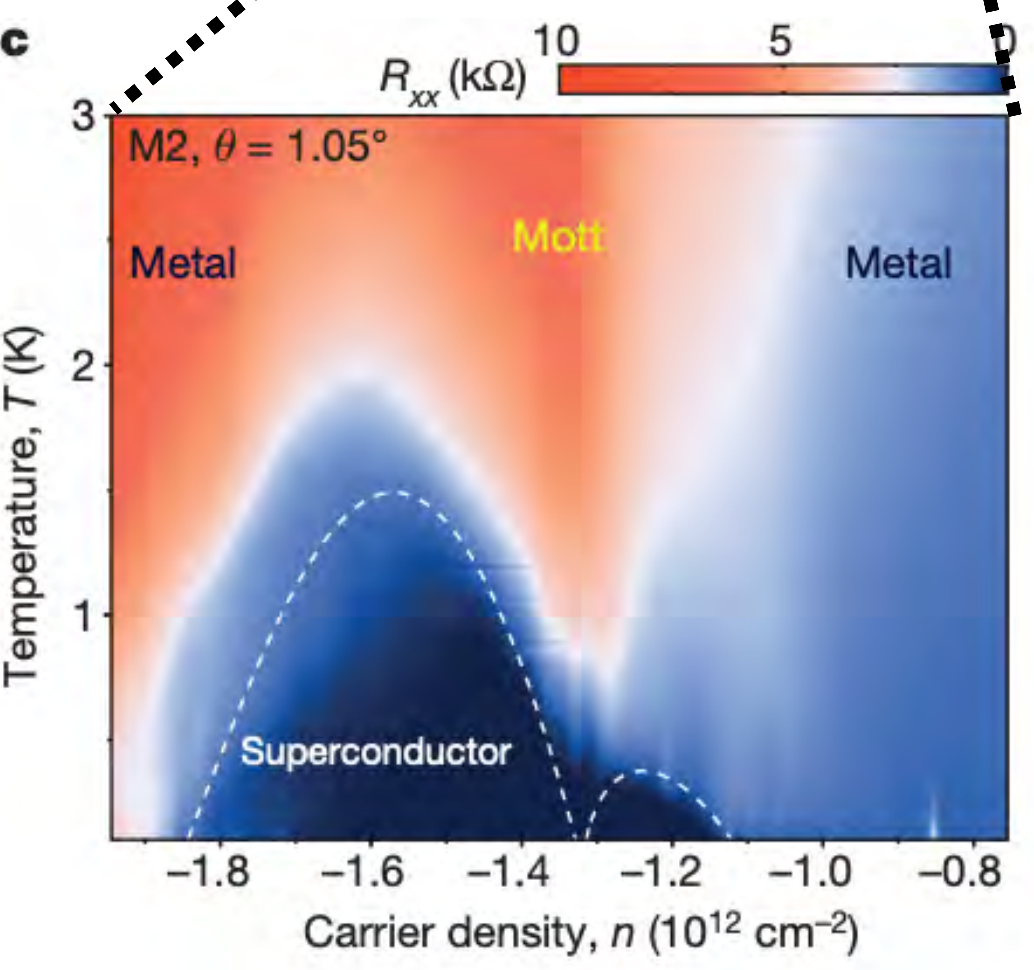

Puzzle #2
gate-tunable
superconductivity
[Cao *et al* Nature **556**, 43 (2018)]

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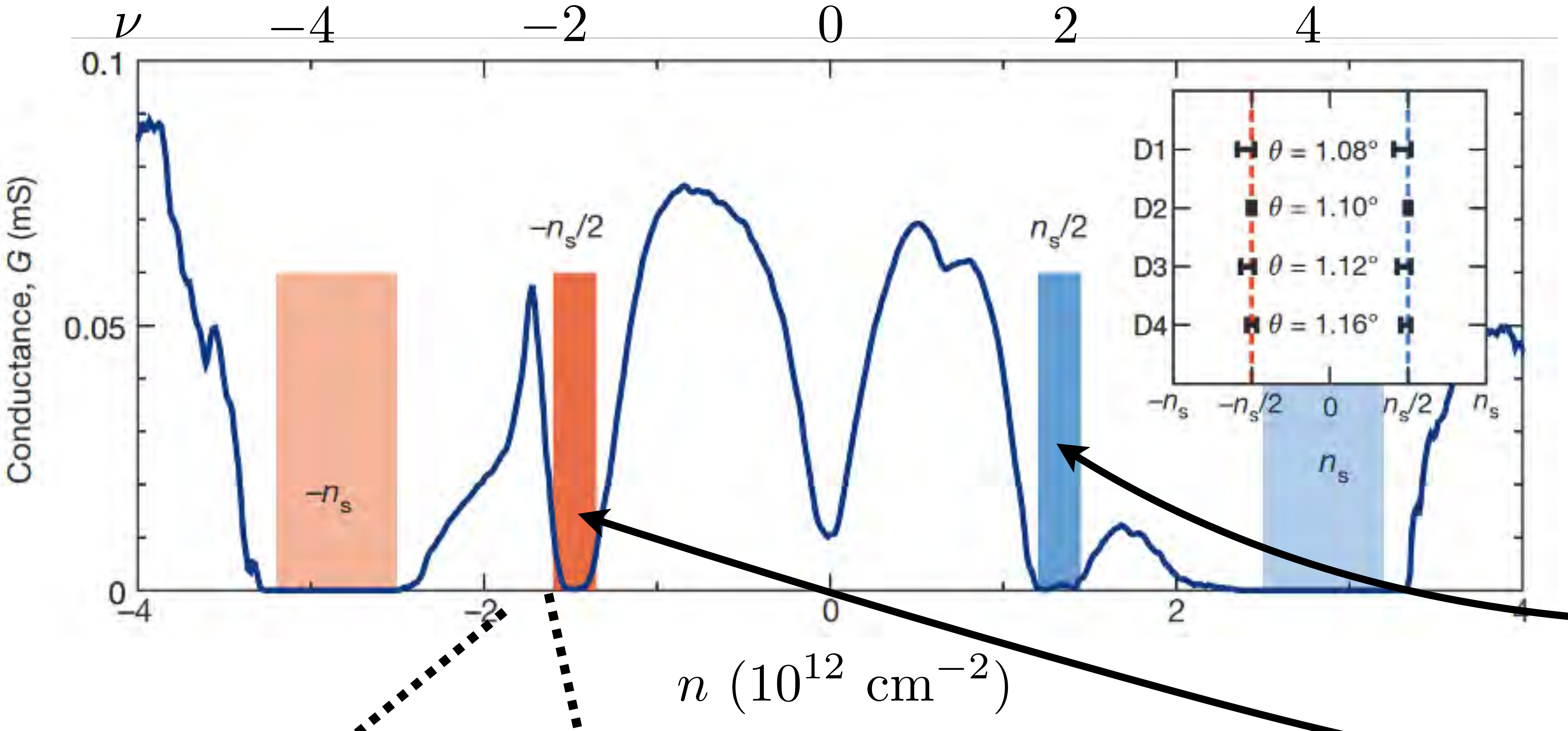

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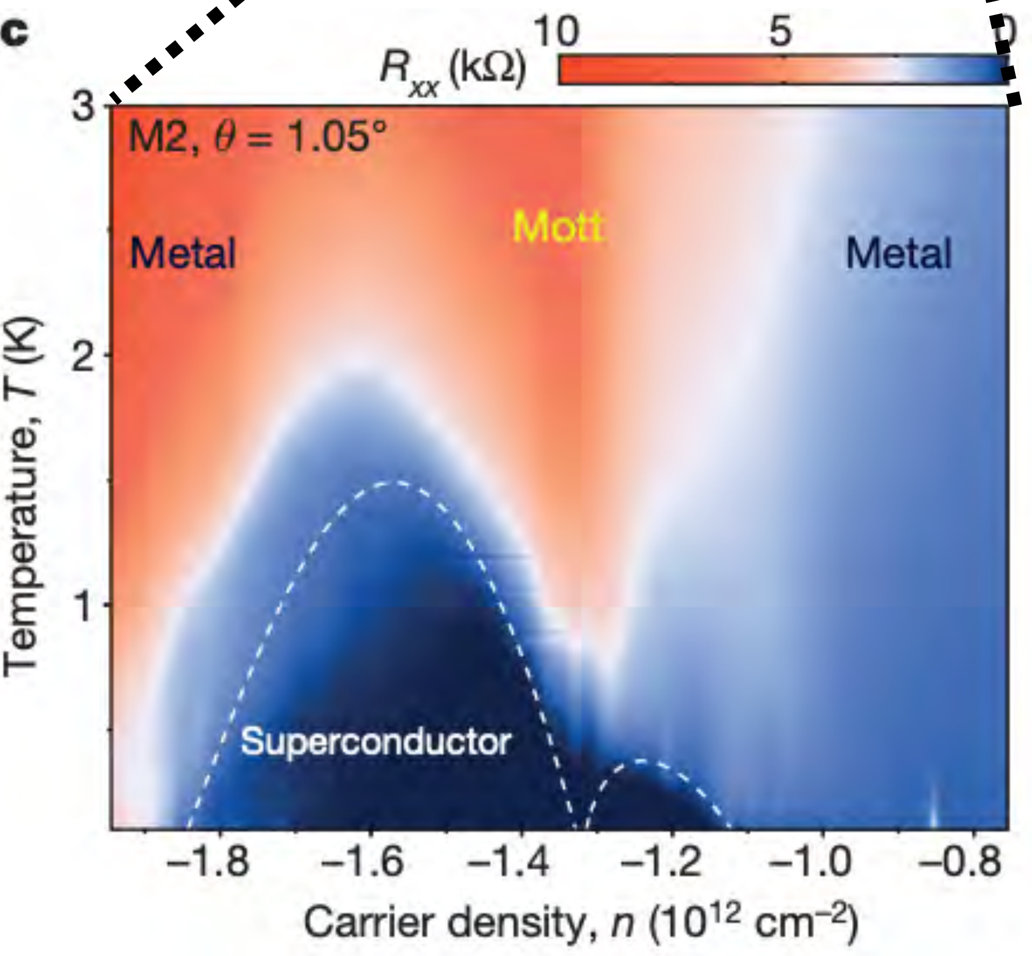

Puzzle #2

gate-tunable superconductivity

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Wide range of other related phenomena: unconventional SCs, "strange metallicity", "mixed valent" behaviour, fractional Chern insulators w/ small *B*…

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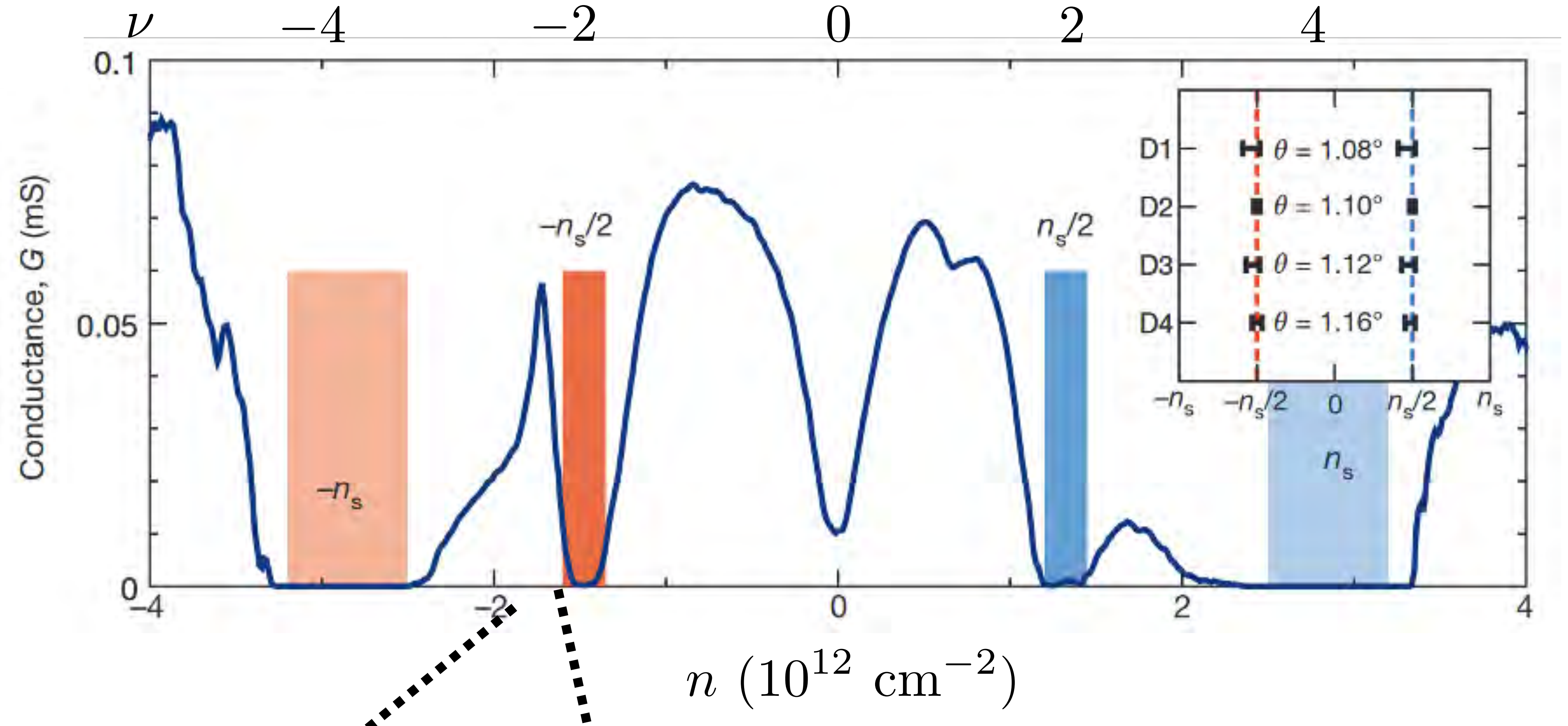

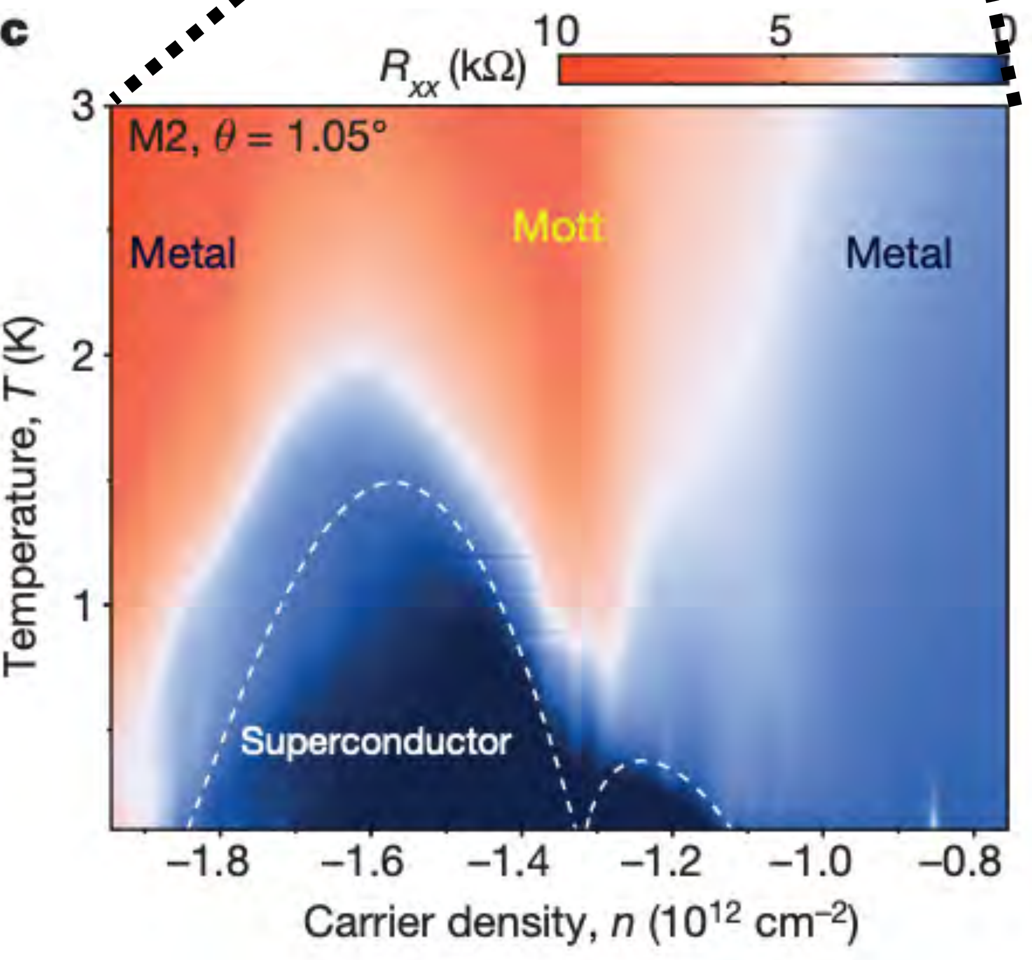

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Puzzle #1 has been *mostly* resolved

Topology + symmetry of moiré bands forces approach linked to **quantum Hall ferromagnetism**

Bultinck et al PRX **10** 031034 (2020)

"Generic" correlated insulator: "**incommensurate Kekule spiral**" predicted theoretically and seen in STM (other states in special cases)

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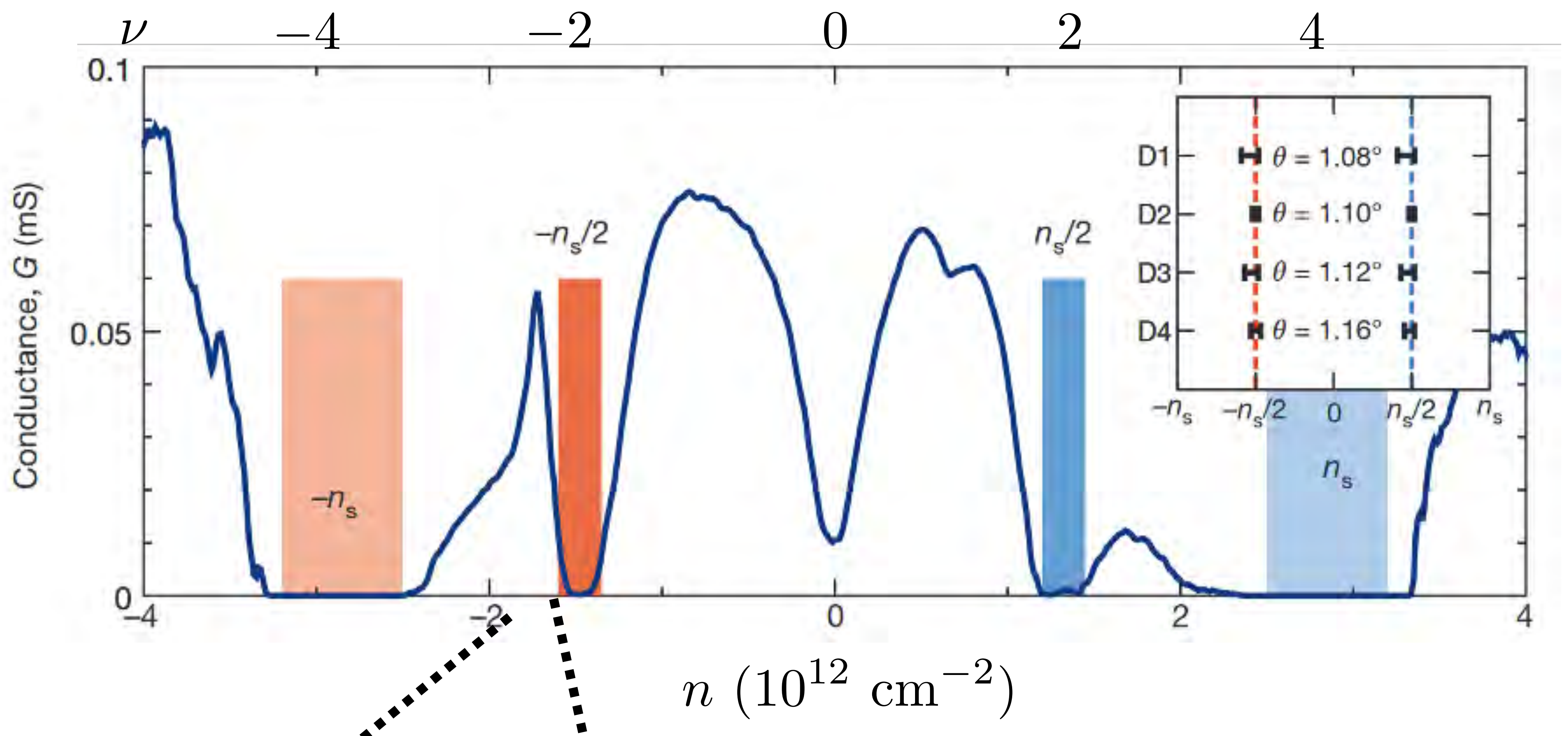

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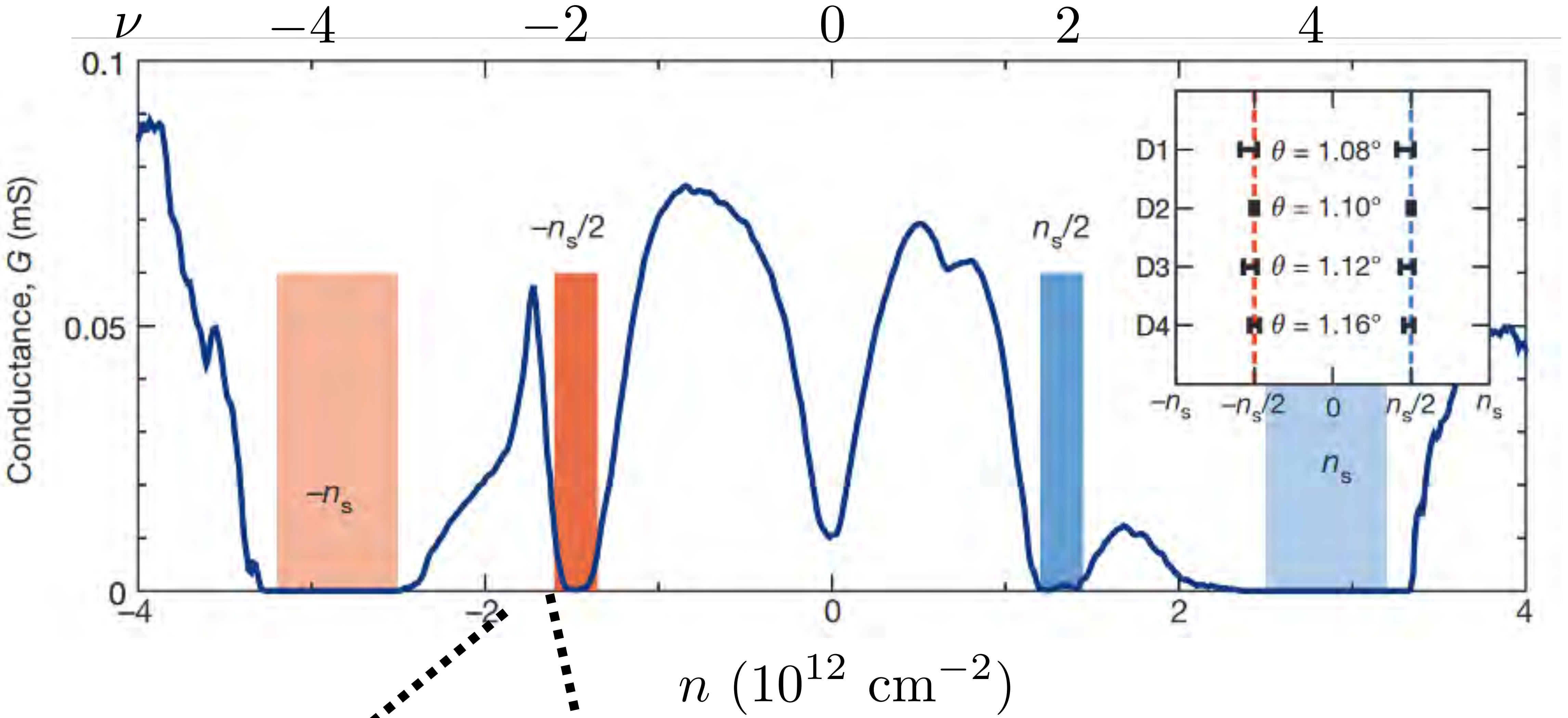

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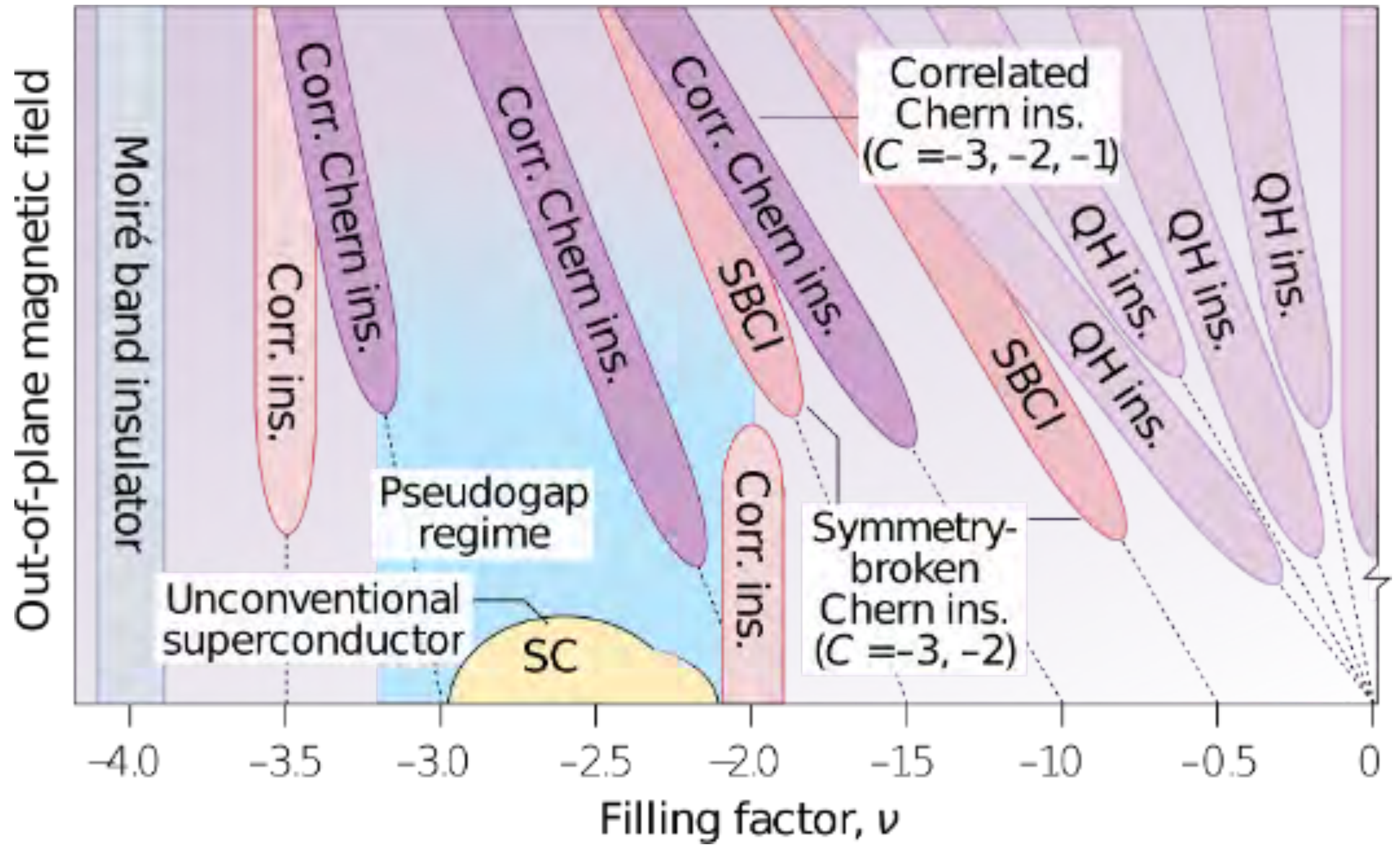
These Lectures: (theoretical) steps towards a new class of moiré systems

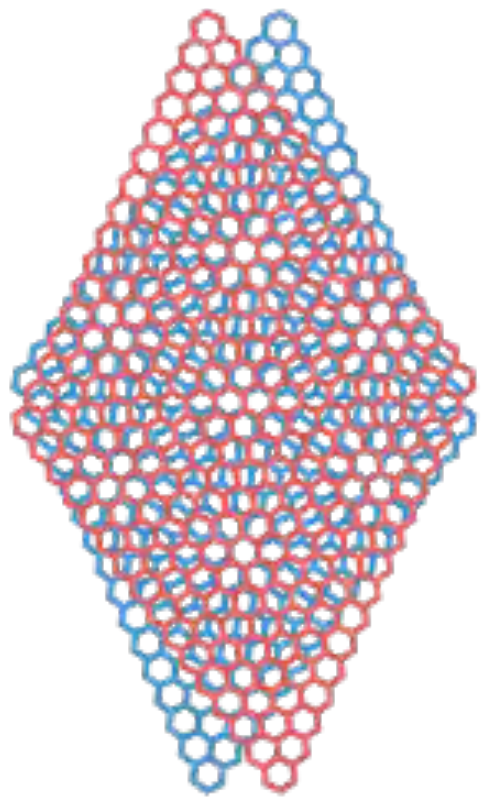
Beyond TBG: A Moiré Materials Universe

MATBG



twist

homobilayers



e.g. MAT*n*G,
tWSe2, tMoTe2

[Nuckolls & Yazdani, *Nat. Rev. Mater.* **9**, 460 (2024)]

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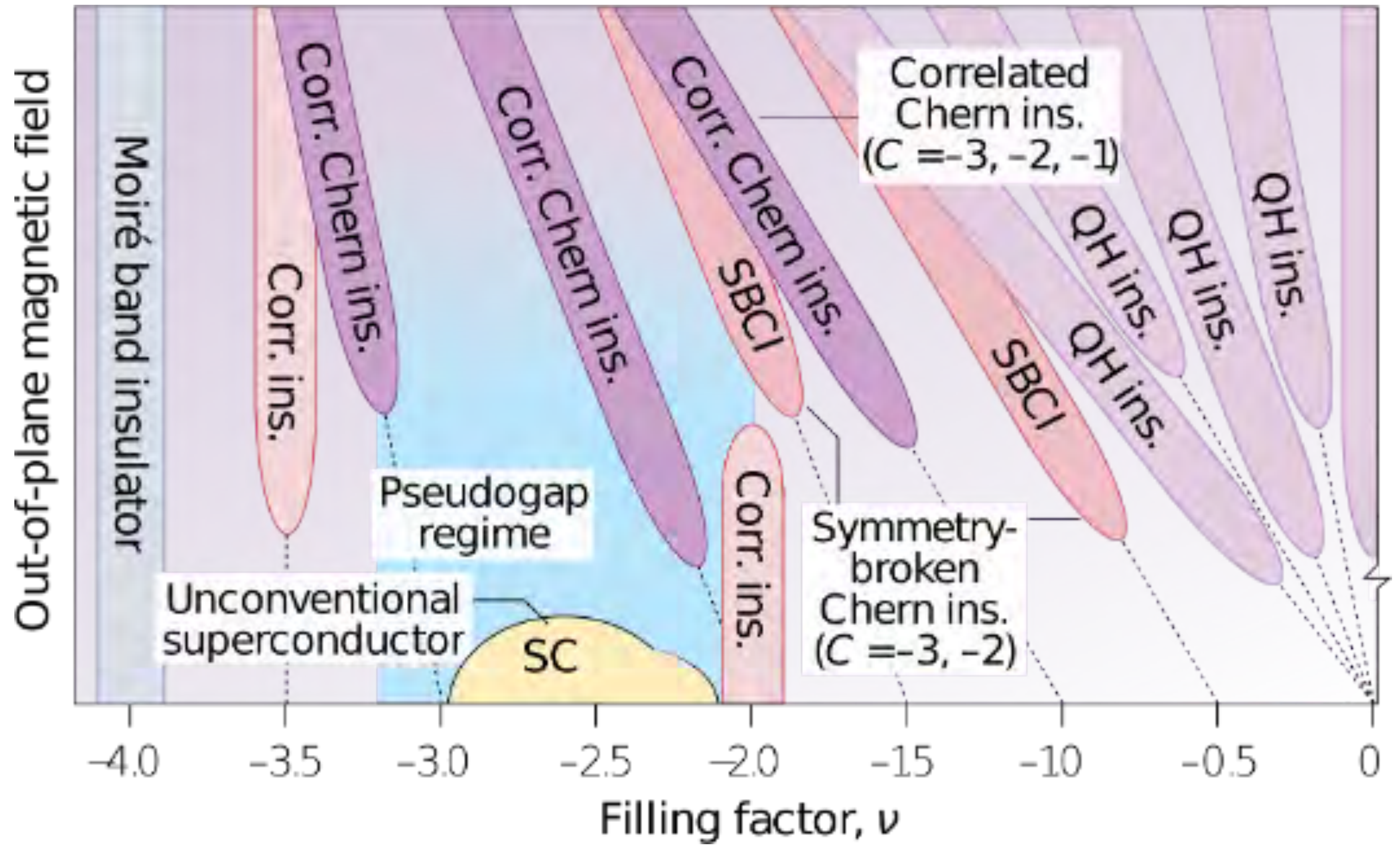
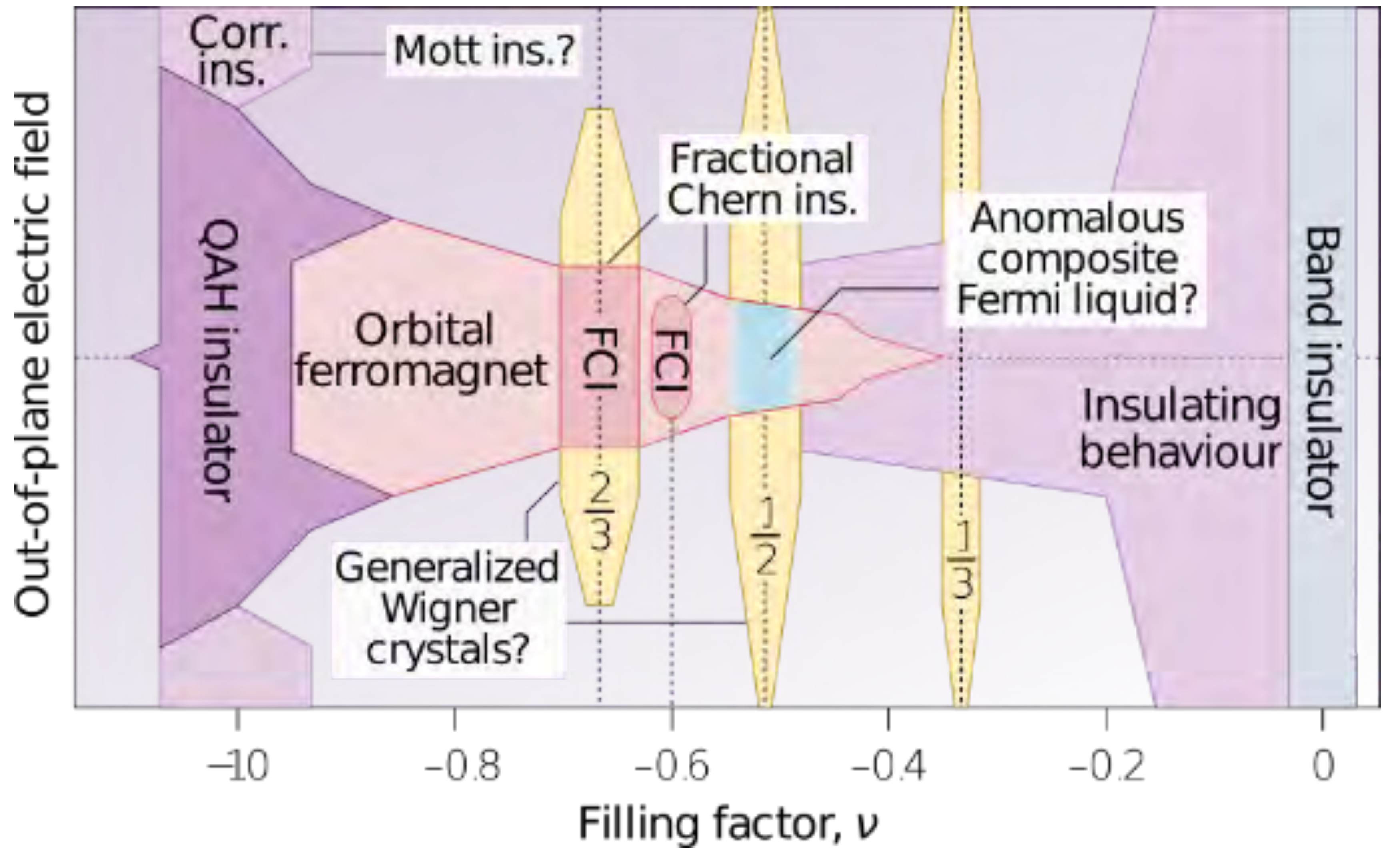


tMoTe$_2$



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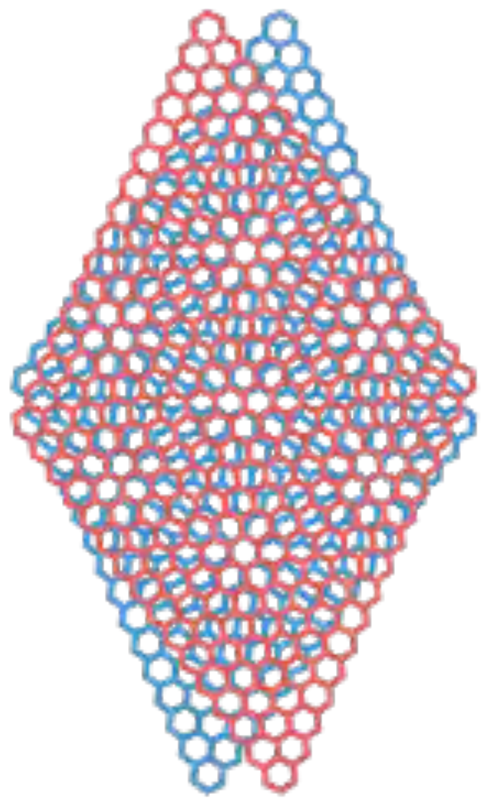

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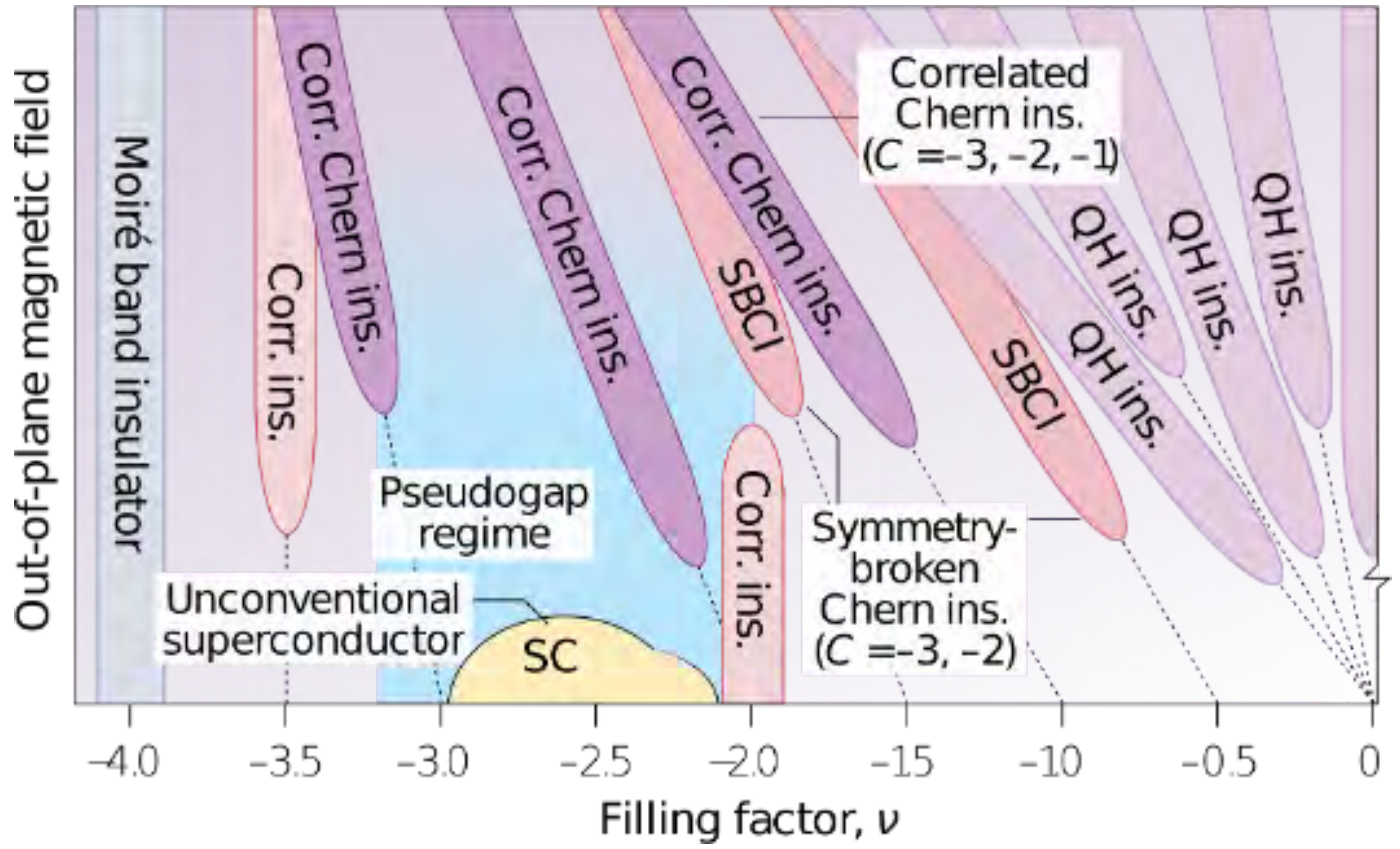
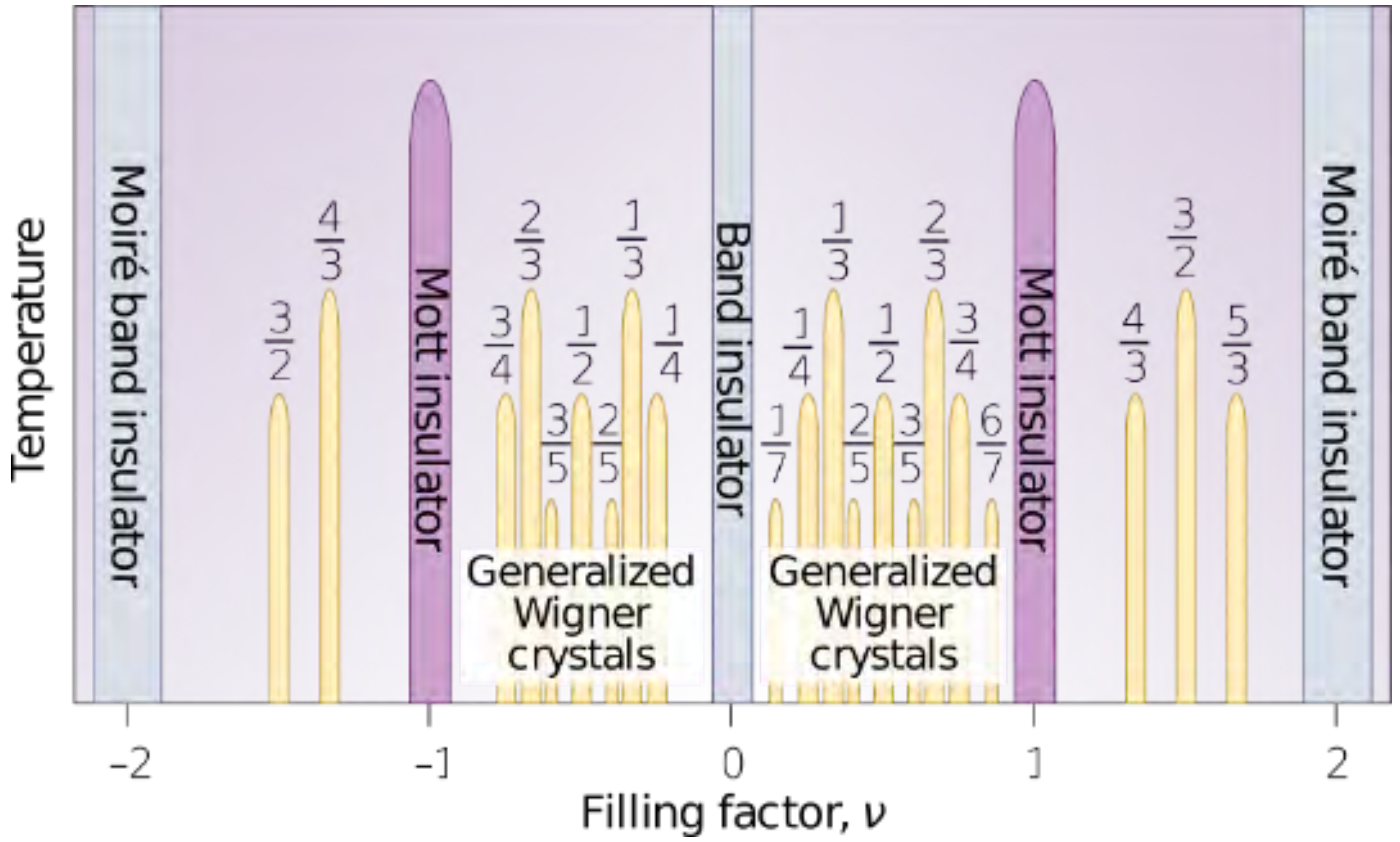


WSe$_2$/WS$_2$



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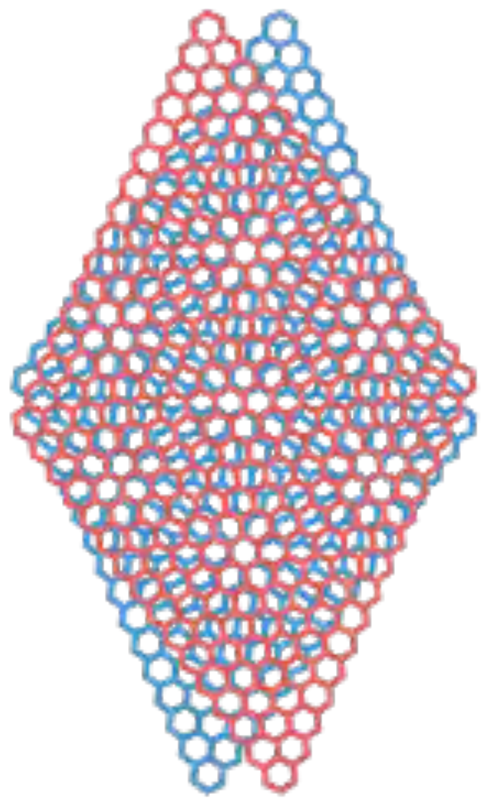
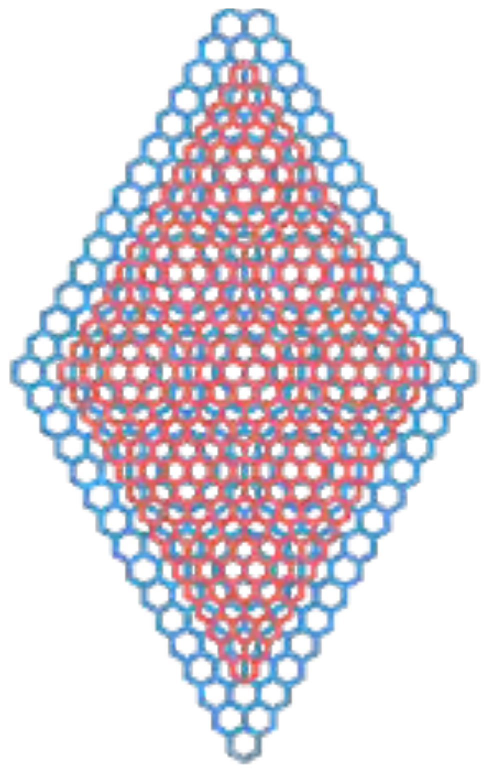


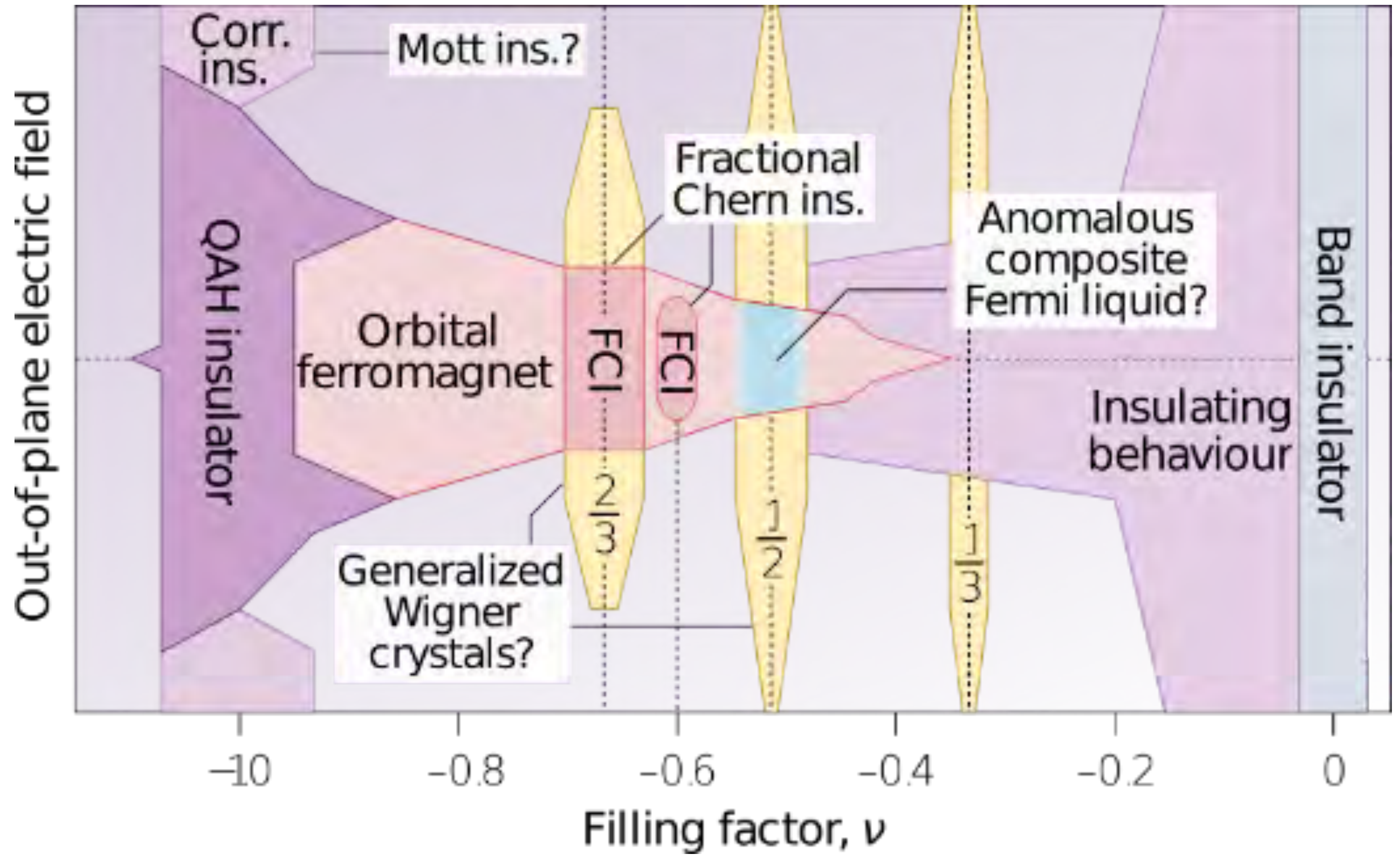
e.g. MATnG, tWSe2, tMoTe2

stack
heterobilayers

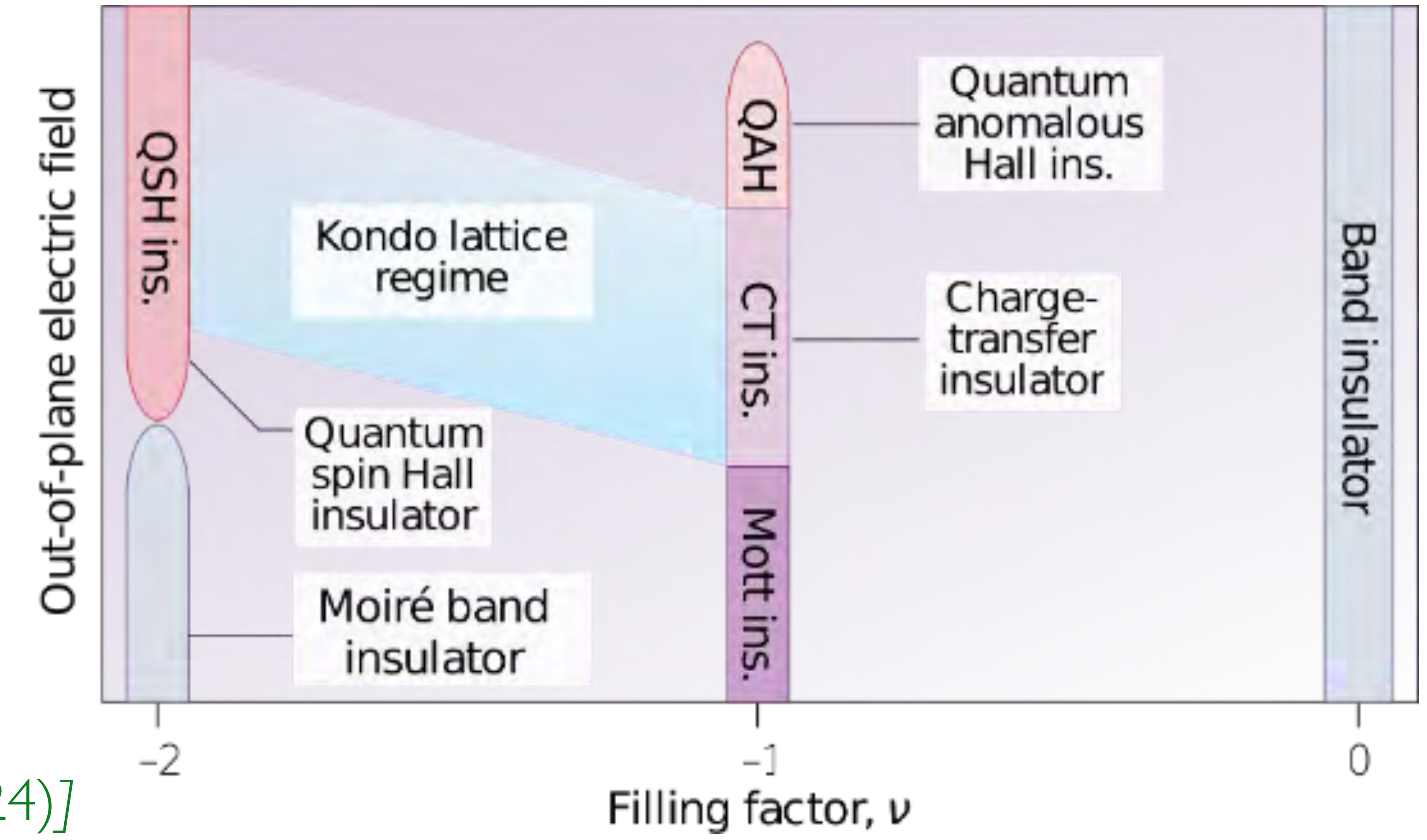


e.g. graphene/hBN, TMD1/TMD2

tMoTe$_2$



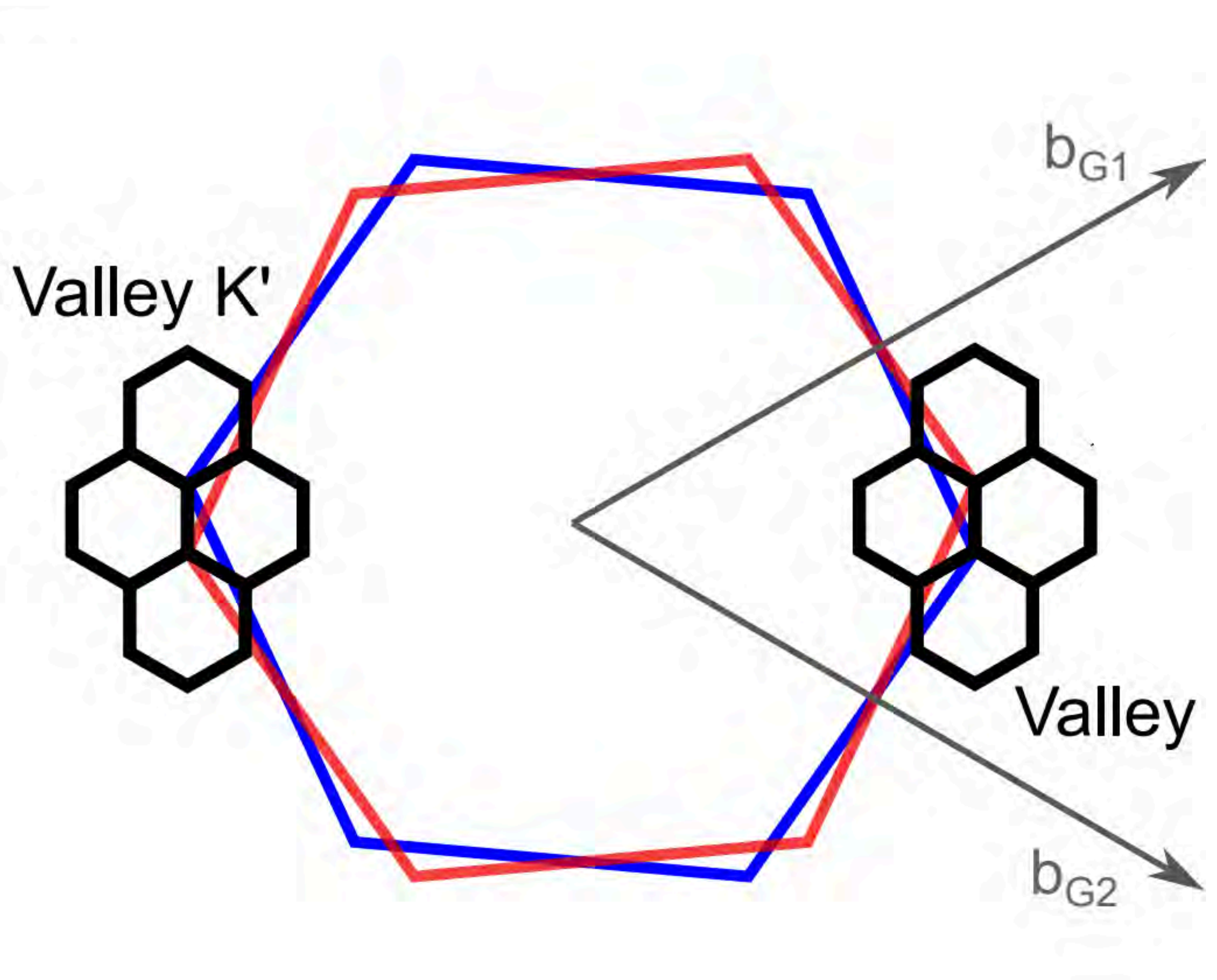
MoTe$_2$/WSe$_2$



[Nuckolls & Yazdani, *Nat. Rev. Mater.* **9**, 460 (2024)]

Moiré Beyond "K"-Theory?

Graphene/most TMDs: each layer has low-energy states near *K* points of BZ



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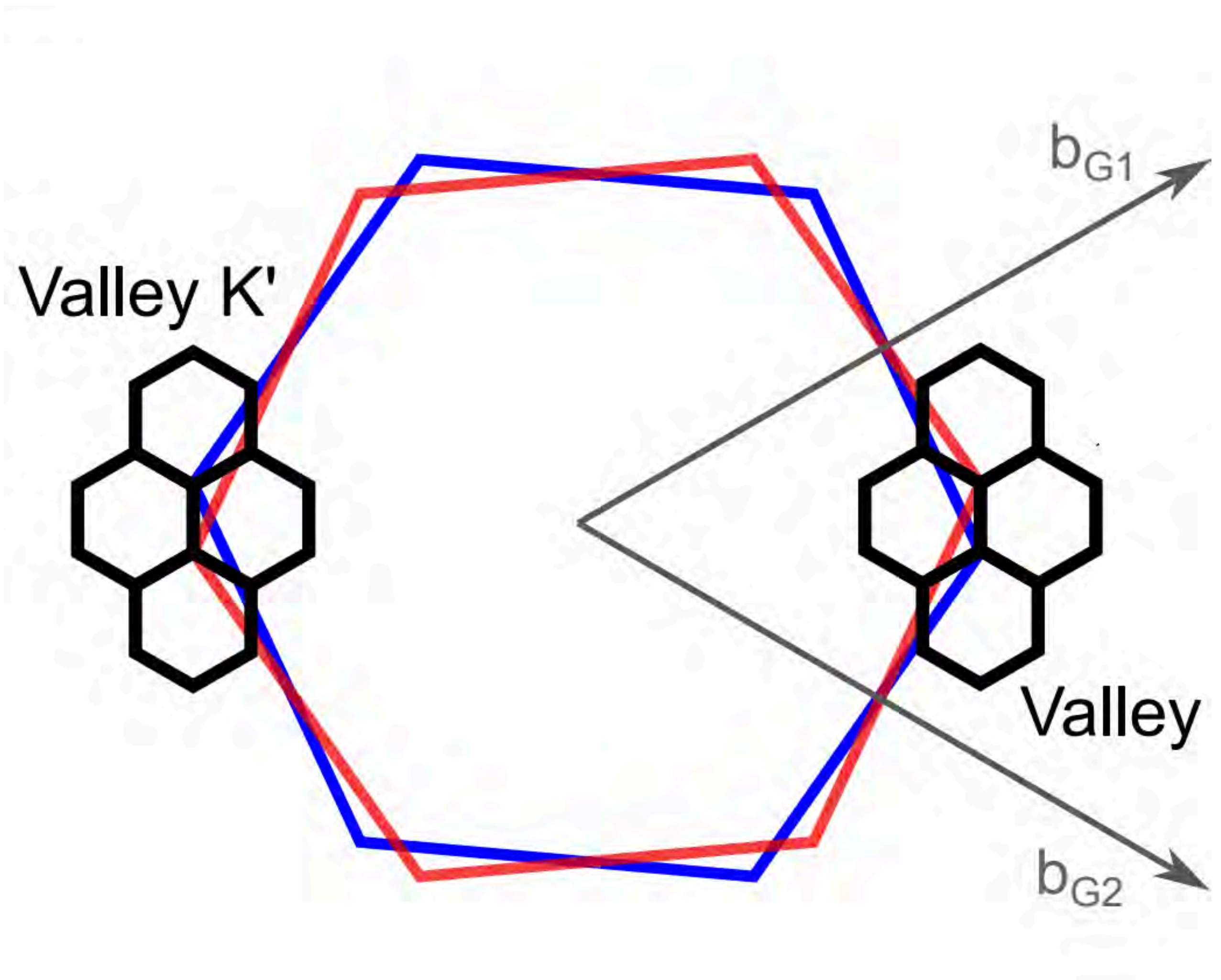

2 valleys (internal states)
w/ 2D dispersion in each valley

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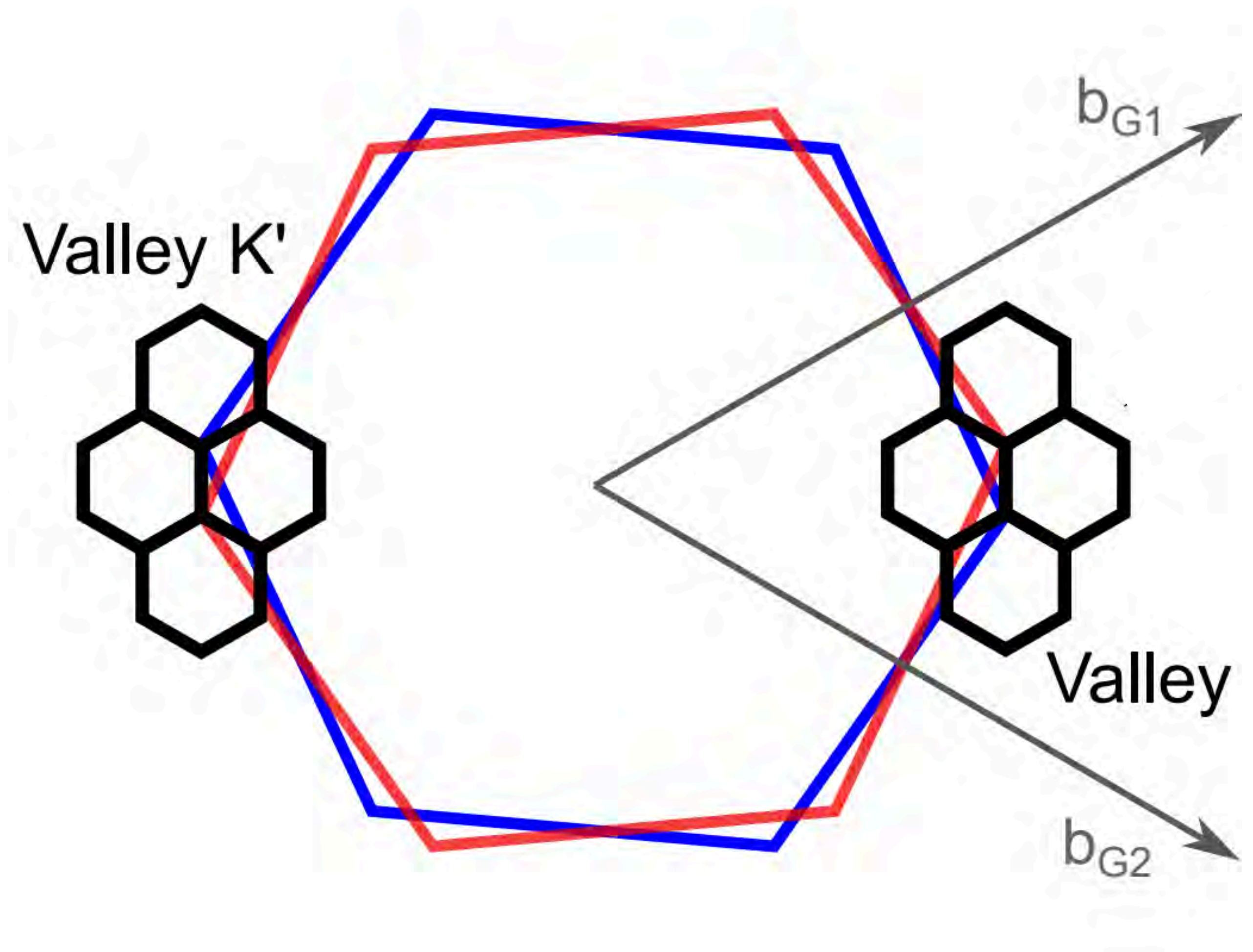
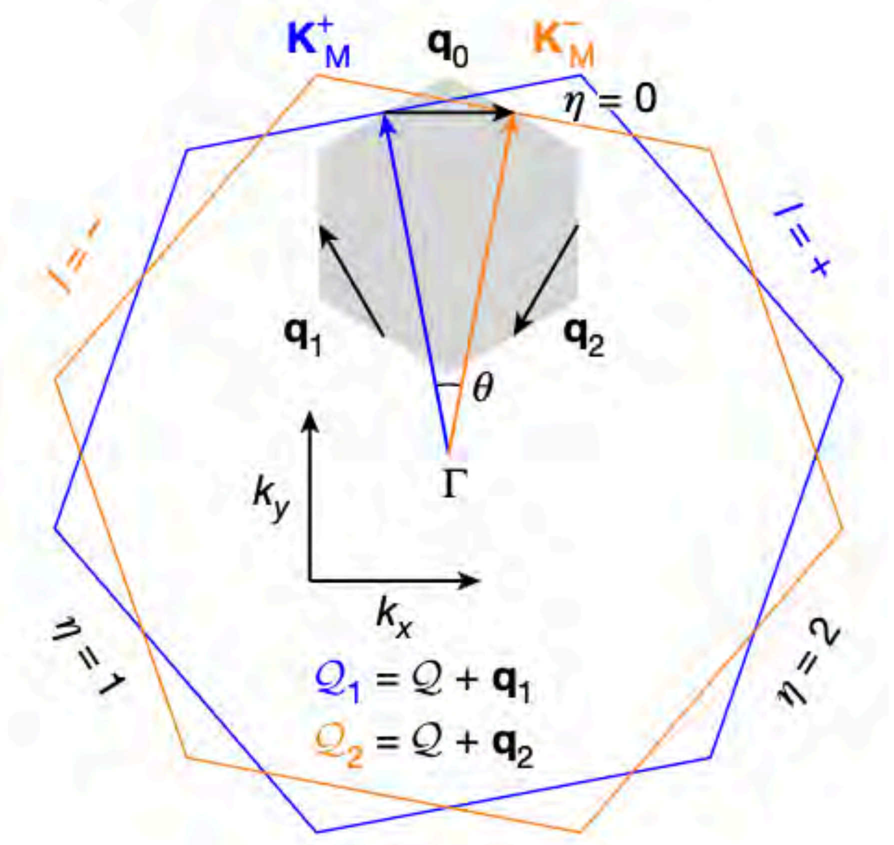


moiré reconstruction →

2 valleys (internal states)
w/ 2D dispersion in each valley

Can also twist layers whose low-energy states are other points e.g. *M*-points



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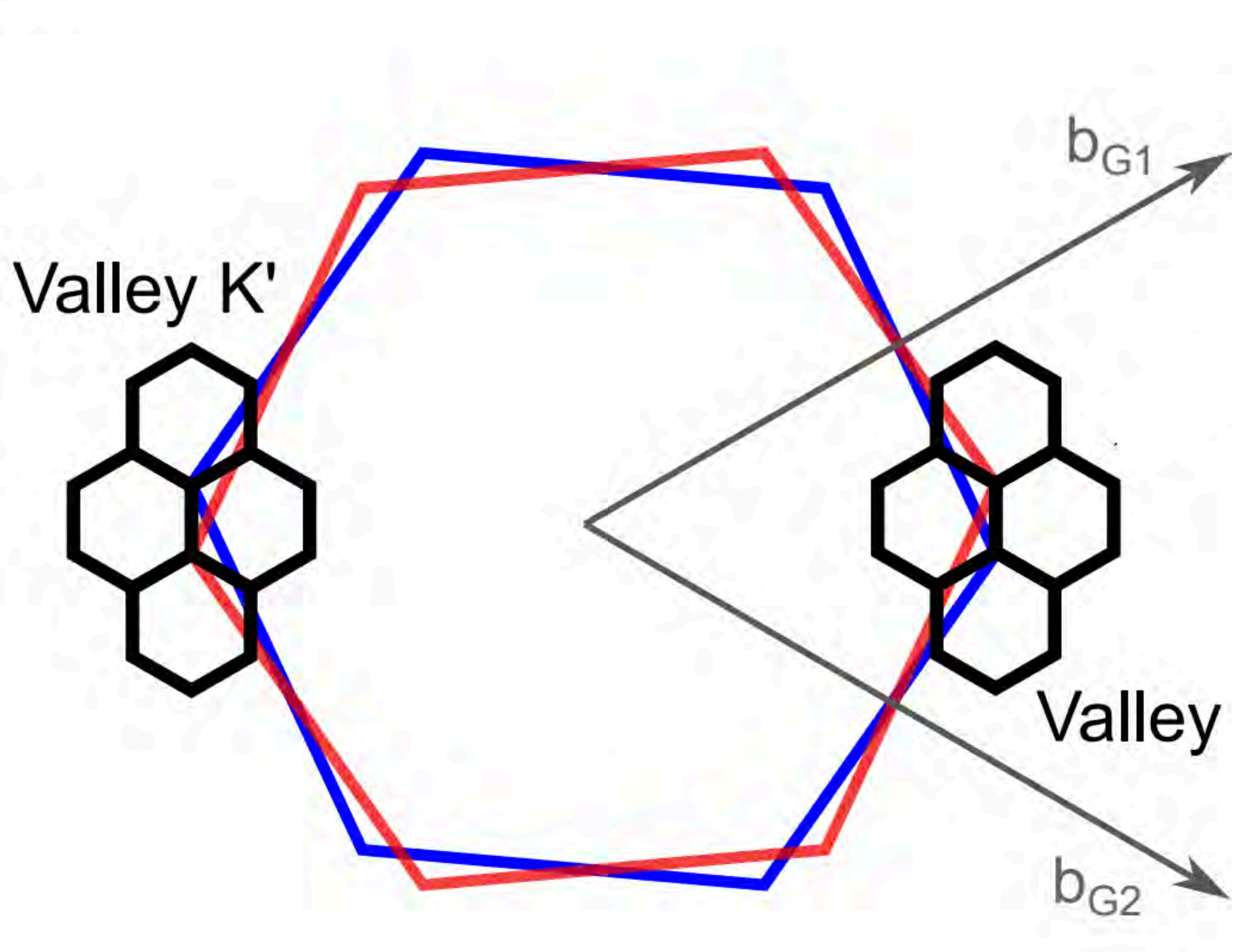

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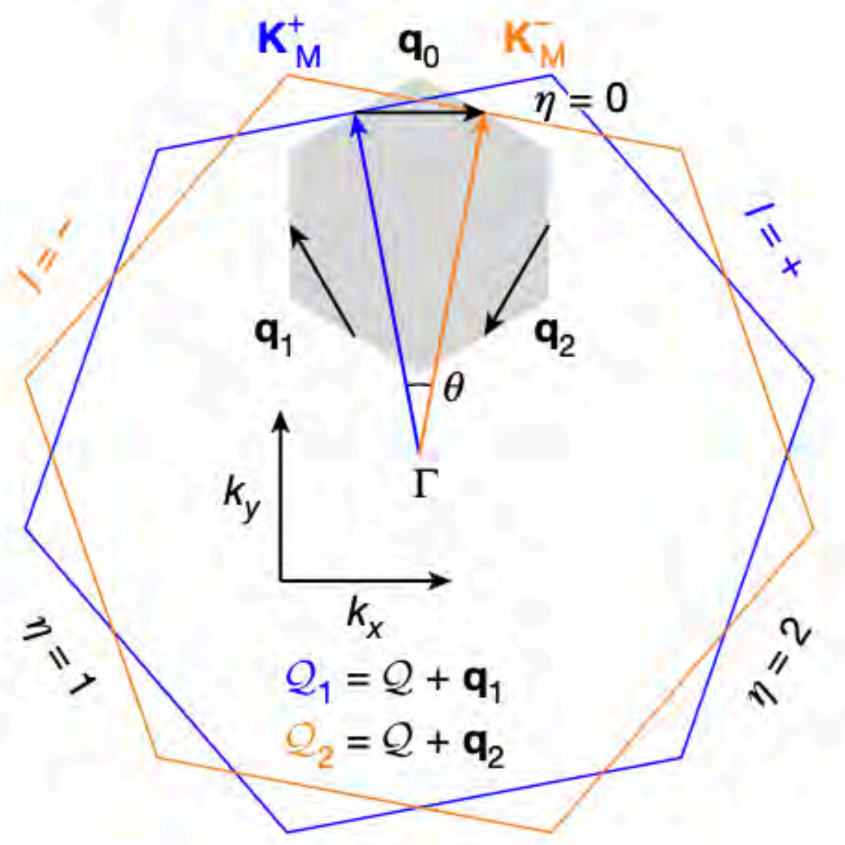

moiré reconstruction

These lectures

[Calugaru et al *Nature* **643**, 376 (2025)]

[cf T. Kariyado & A Vishwanath, Phys. Rev. Research **1**, 033076 (2019)]

Division of Topics

Lecture 1: Basic Principles of Moiré Reconstruction applied to M-point Materials

[mostly adapted from Calugaru et al *Nature* **643**, 376 (2025) and its 100+ page supplementary material]

Lecture 2: Sign-Free Quantum Monte Carlo for (some) M-point Materials

[mostly adapted from M.-R. Li, …, SAP,…, H. Hu 2508.10098 + work in progress]

Moiré Reconstruction

Origin of moiré bands: modification of intra-/inter-layer dispersions b/c emergent (quasi) periodicity

$$\begin{pmatrix} h_t(\tilde{\mathbf{k}}) & 0 \\ 0 & h_b(\tilde{\mathbf{k}}) \end{pmatrix} \to \begin{pmatrix} h_t(R_t\tilde{\mathbf{k}}) & 0 \\ 0 & h_b(R_b\tilde{\mathbf{k}}) \end{pmatrix} + \sum_{\mathbf{G}\in\mathcal{L}_M} \begin{pmatrix} V_t(\mathbf{G}) & V_{tb}(\mathbf{G}) \\ V_{bt}(\mathbf{G}) & V_b(\mathbf{G}) \end{pmatrix} e^{i\mathbf{G}\cdot\mathbf{r}}$$

untwisted — twist each layer — moiré potential — ($\tilde{\mathbf{k}}$ in full BZ)

Formally, moiré BZ only exists if twist angle/lattice mismatch is **commensurate**

Practically, for small angle/mismatch, can ignore intralayer periodicity:

— mBZ exists even if incommensurate

— can do reconstruction for separate *k*-space patches (“valleys”) for single layer

Generically: a “band folding” problem (cf. “nearly free electrons” in introductory solid-state)

Moiré Reconstruction: General Structure & Gauge Choices

Band-folding problem has form of $\mathbf{k}$-space hopping!

$$\mathcal{H} = \sum_{\mathbf{k},\mathbf{Q},\mathbf{Q}',i,j} [h_{\mathbf{Q},\mathbf{Q}'}(\mathbf{k})]_{ij} \hat{c}^\dagger_{\mathbf{k},\mathbf{Q},i} \hat{c}_{\mathbf{k},\mathbf{Q}',j}$$

$\mathbf{k} \in$ moiré BZ, i, j contain all "internal" indices

$\mathbf{Q} \in$ "momentum space lattice" (not necessarily $\mathscr{L}_M$)

There is a "gauge choice" of where to put the "zero" of $\mathbf{k} - \mathbf{Q}$ in each layer

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Moiré Reconstruction: Full Procedure

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Hierarchical Procedure:

less specific

Step 1: fix the moiré reciprocal lattice (monolayer lattice vectors)

Step 2: fix the $\mathbf{Q}$-lattice (minima of monolayer)

Step 3: identify exact/approximate symmetries (broad details eg. stacking arr.)

Step 4: actually obtain $[h_{\mathbf{Q},\mathbf{Q}'}(\mathbf{k})]_{ij}$ & diagonalize (fine details: continuum model/*ab initio*)

modeling detail

more specific

Step #1: Fixing the mBZ

Consider two identical lattices 1, 2 related by a twist θ

Reciprocal lattice 1 generated by primitive vectors $\mathbf{b}_i$

Reciprocal lattice 2 generated by primitive vectors $R(\theta)\mathbf{b}_i$

} moiré reciprocal lattice generated by

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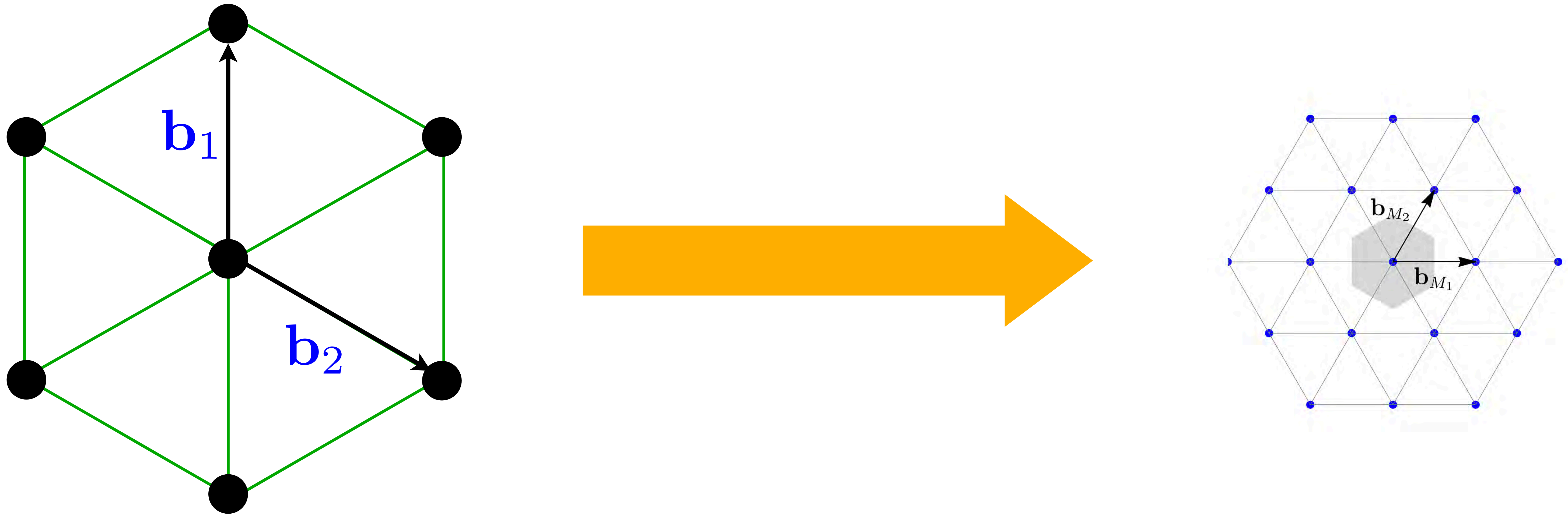
$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \approx \begin{pmatrix} 1 & -\theta \\ \theta & 1 \end{pmatrix} = \mathbf{1} + \theta\hat{z}\times$$

for small twists θ

$\mathbf{b}_{Mi} \approx \theta\hat{z}\times\mathbf{b}_i$: moiré RL = monolayer RL rotated by $\pi/2$ and scaled by θ



Step #2: Fixing the $\mathbf{Q}$-Lattice: Intuitive Picture

$$\mathcal{H} = \sum_{\mathbf{k},\mathbf{Q},\mathbf{Q}',i,j} [h_{\mathbf{Q},\mathbf{Q}'}(\mathbf{k})]_{ij} \hat{c}^{\dagger}_{\mathbf{k},\mathbf{Q},i} \hat{c}_{\mathbf{k},\mathbf{Q}',j}$$

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$$\hat{c}_{\mathbf{k},\mathbf{Q},\eta,j} = \hat{a}_{\mathbf{P}^l_\eta + \mathbf{k} - \mathbf{Q},l,j}$$

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When tunneling from $\hat{c}_{\mathbf{k},\mathbf{Q}_1,l_1}$ to $\hat{c}_{\mathbf{k},\mathbf{Q}_2,l_2}$ electron changes momentum from $\mathbf{P}^{l_1}_{\eta} + \mathbf{k} - \mathbf{Q}_1$ to $\mathbf{P}^{l_2}_{\eta} + \mathbf{k} - \mathbf{Q}_1$

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moiré translation symmetry ⇒ this difference needs to be a moiré reciprocal lattice vector $\mathbf{G}$:

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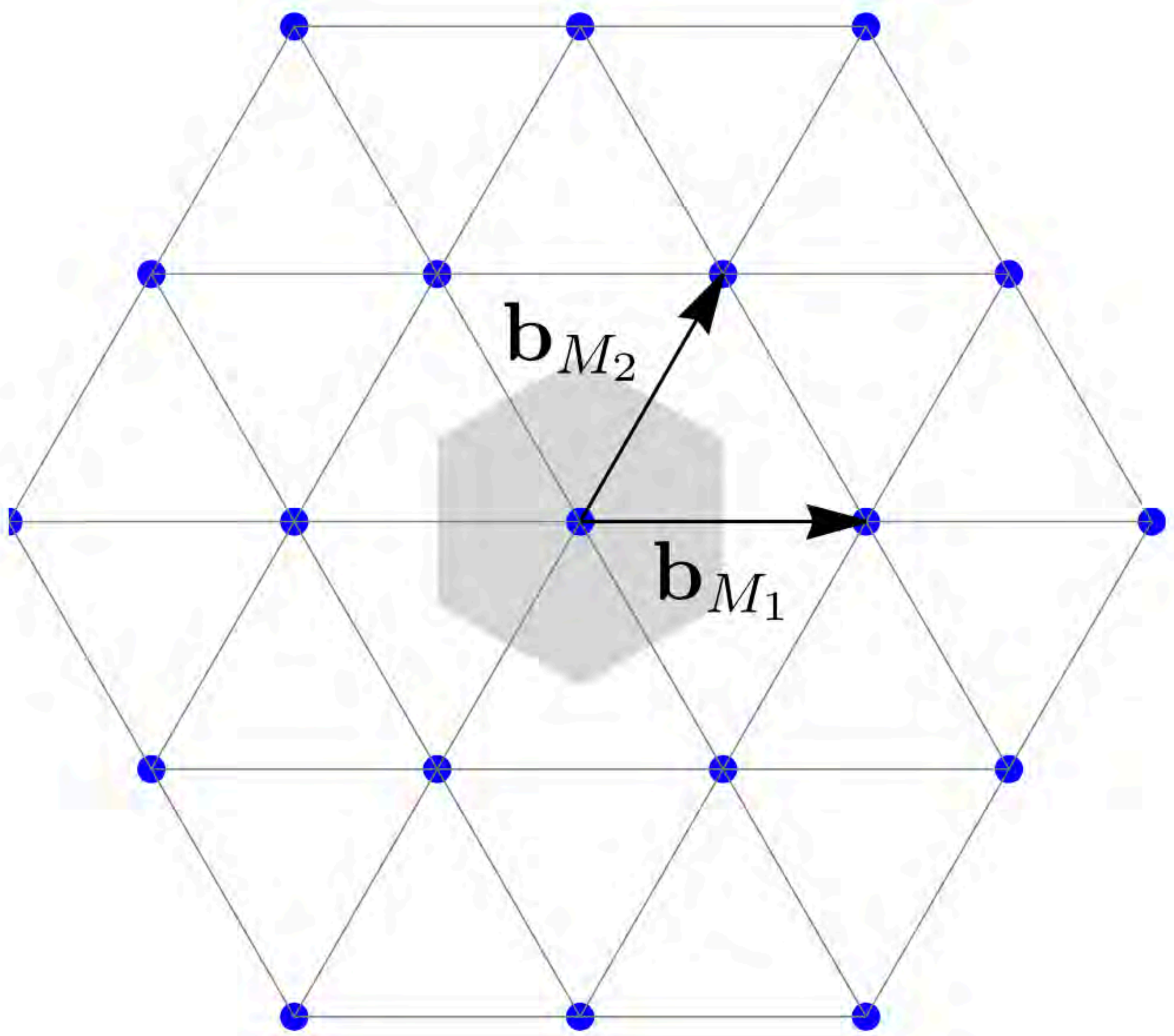
For $\mathbf{P}^l_\eta \neq 0, \mathbf{P}^1_\eta - \mathbf{P}^2_\eta$ cannot be moiré RLV $\Rightarrow$ $\mathbf{Q}$-lattice has sublattice structure beyond moire translation!

Step #2: Fixing the $\mathbf{Q}$-Lattice: Γ-point Twisting

For Γ-point materials both gauge choices coincide!

$$\hat{c}_{\mathbf{k},\mathbf{Q},\eta,j} = \hat{a}_{\mathbf{k}-\mathbf{Q},l,j}$$

$\mathbf{Q}$-lattice = **triangular** (=moiré reciprocal lattice)



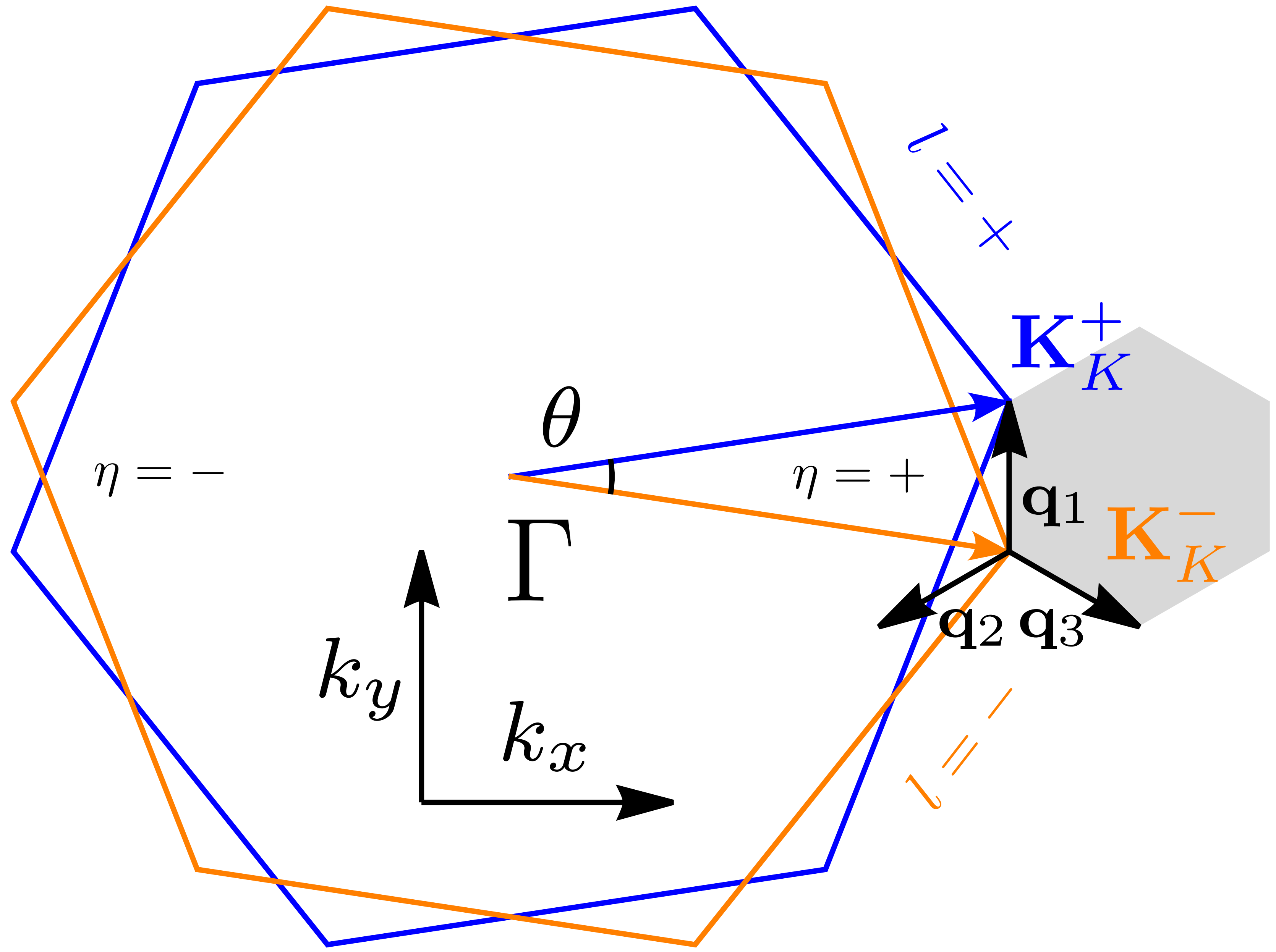
Example: valence bands of TMDs

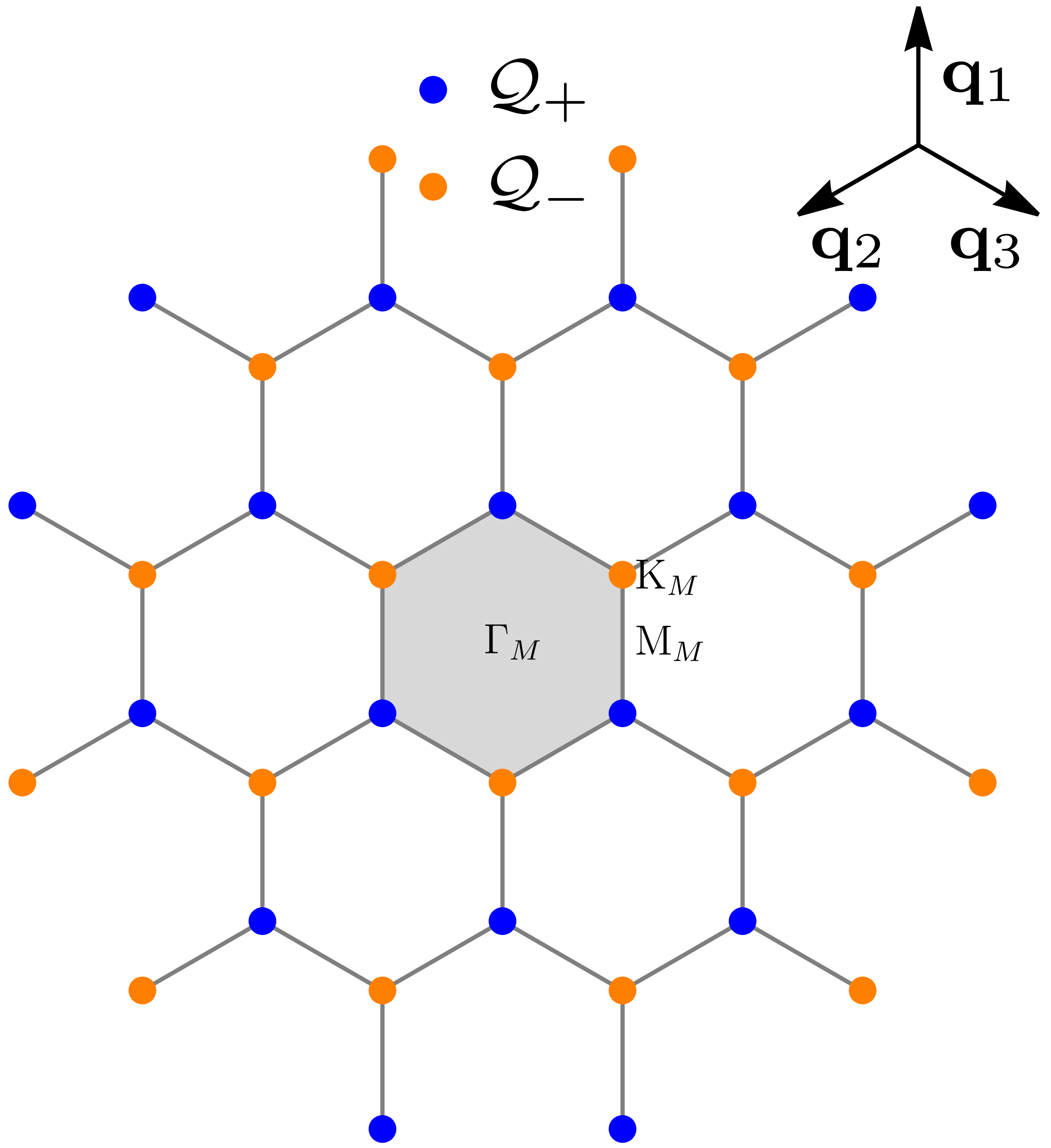
Step #2: Fixing the $\mathbf{Q}$-Lattice: K-point Twisting

For $\mathbf{K}$-point materials: pick $\mathbf{P}^l_\eta$ to be the rotated $\mathbf{K}$-pt in valley $\eta = \pm$:

$$\hat{c}_{\mathbf{k},\mathbf{Q},\eta,j} = \hat{a}_{\eta K^l_{\mathrm{K}}+\mathbf{k}-\mathbf{Q},l,j}$$

$\mathbf{Q}$-lattice = honeycomb



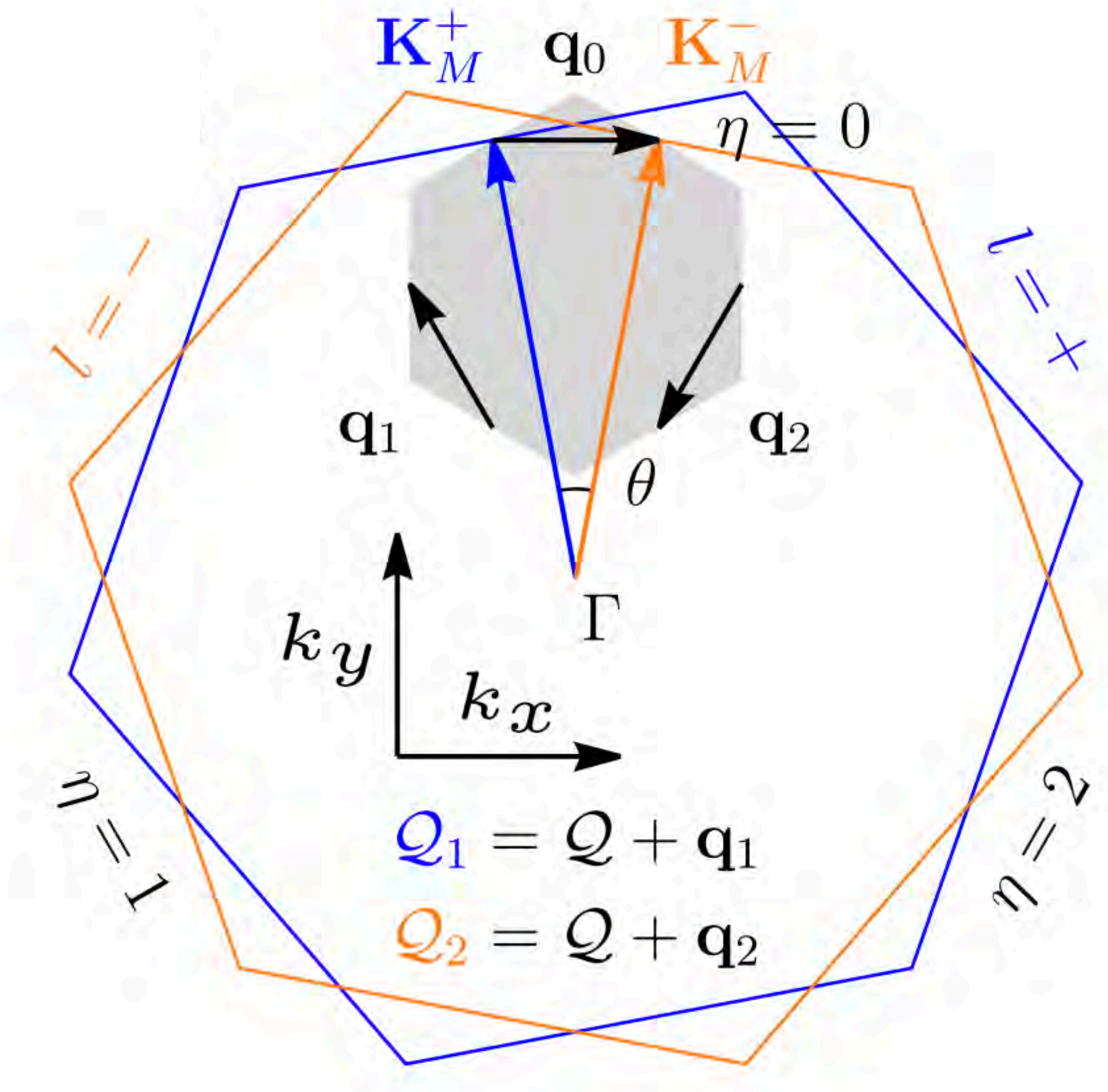


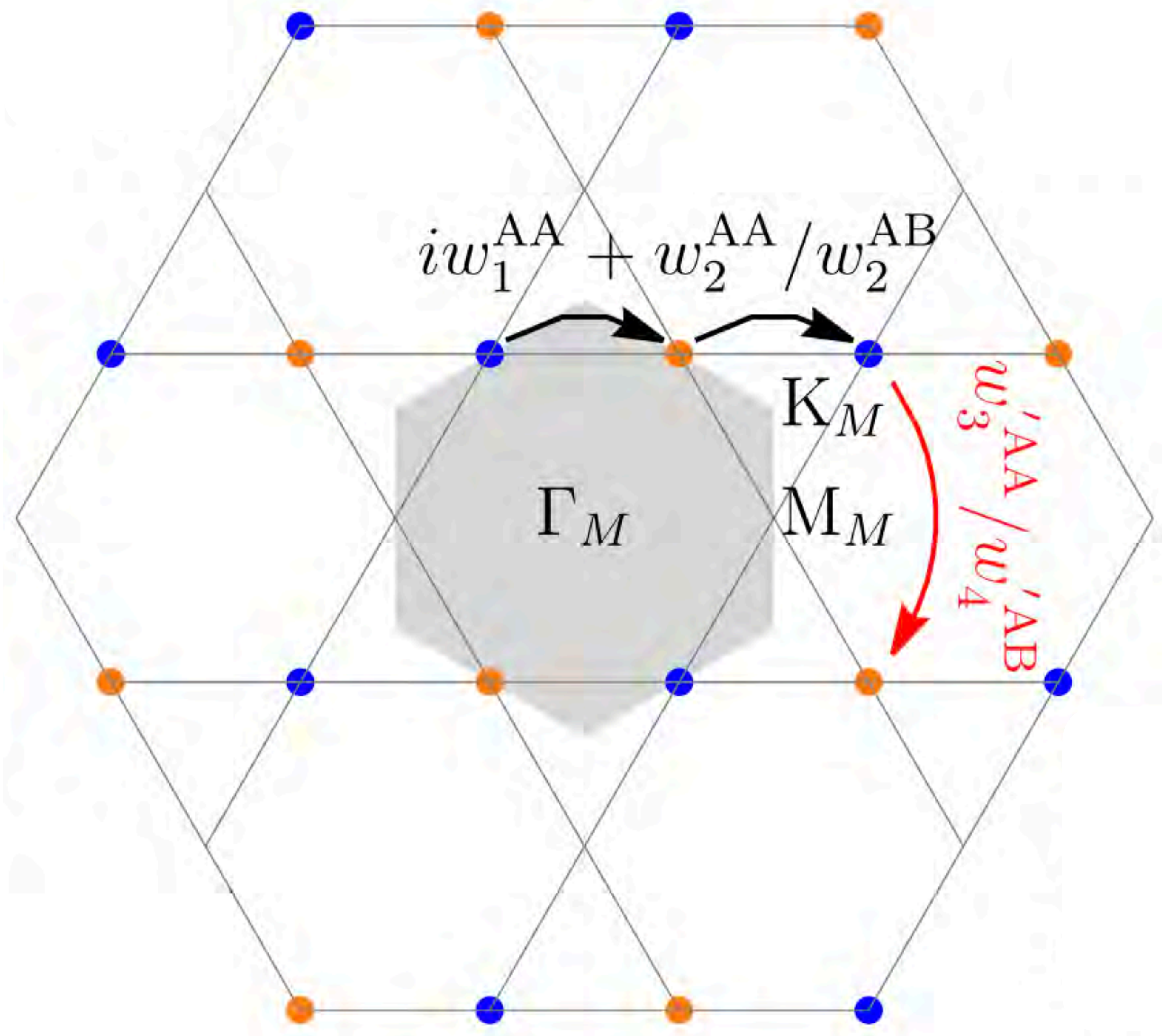
Example: moiré graphene, conduction bands of TMDs

Step #2: Fixing the $\mathbf{Q}$-Lattice: M-point Twisting

For $\mathbf{M}$-point materials: pick $\mathbf{P}^l_\eta$ to be the rotated $\mathbf{M}$-pt in valley $\eta = 0,1,2$: $\quad \hat{c}_{\mathbf{k},\mathbf{Q},\eta,l} = \hat{a}_{C_{3z}^\eta K_{\mathrm{M}}^l + \mathbf{k} - \mathbf{Q},l}$

$\mathbf{Q}$-lattice = kagomé





Valley-η moiré reconstruction only involves $\mathbf{Q}$-sublattices $[(\eta \pm 1) \mod 3]$: call this set $\mathcal{Q}_\eta$

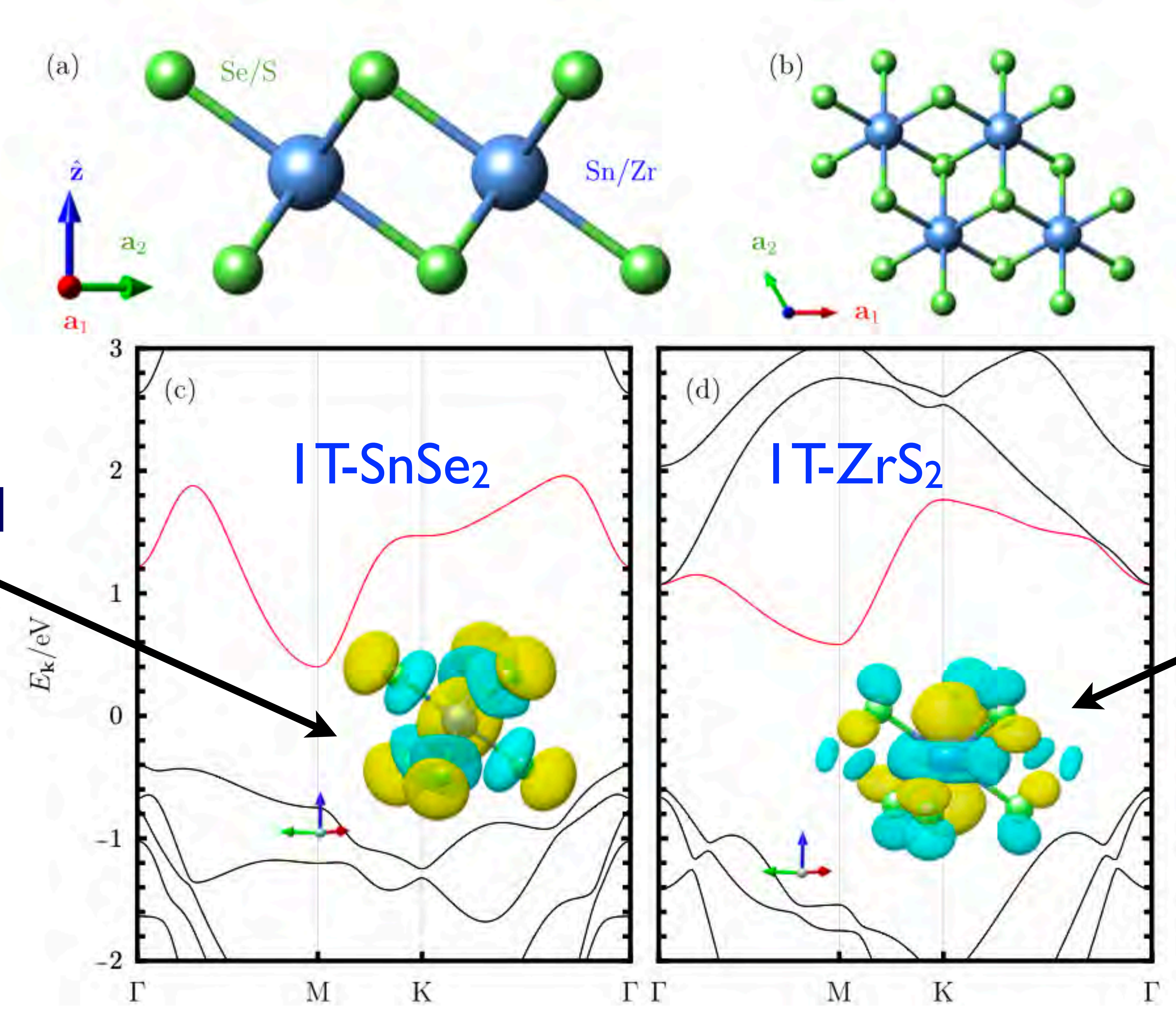
Interlude: M-point Monolayers

Exfoliable 2D materials with monolayer dispersion near **M**-points: (cf. 2D Materials Database)

1T-$SnSe_2$, 1T-ZrS_2 + similar: 1T-$ZrSe_2$, 1T-SnS_2, 1T-$HfSe_2$, 1T-HfS_2, …; also GaTe (diff. structure)

2411.09741

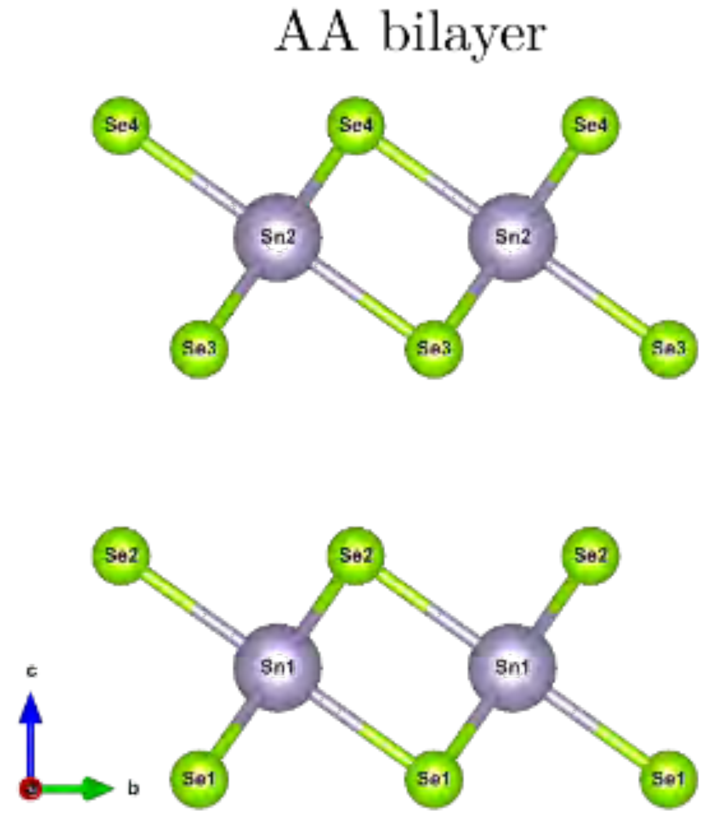
s-like molecular orbital centered at Sn

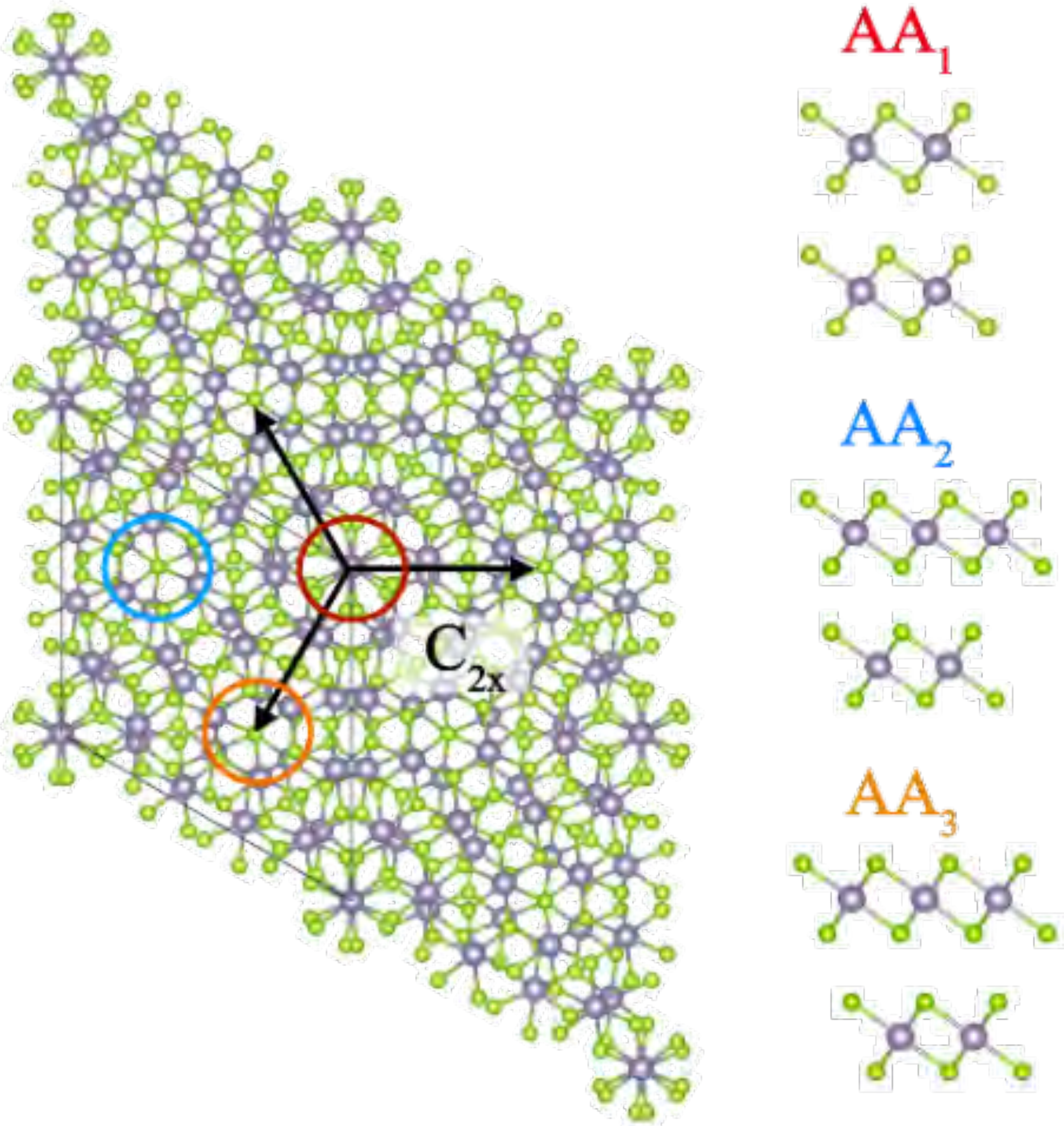


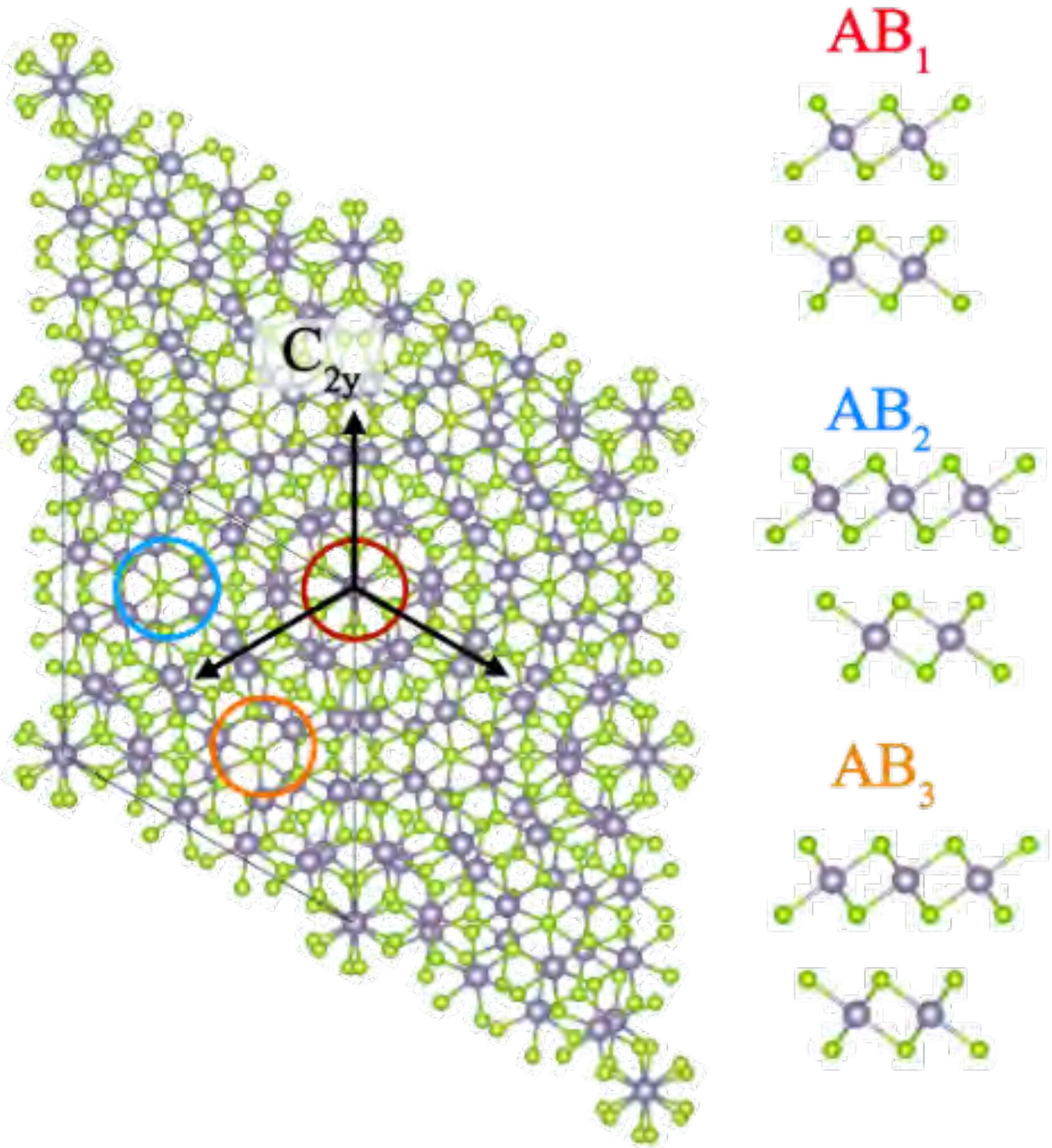
mainly d_z-like molecular orbital of Zr

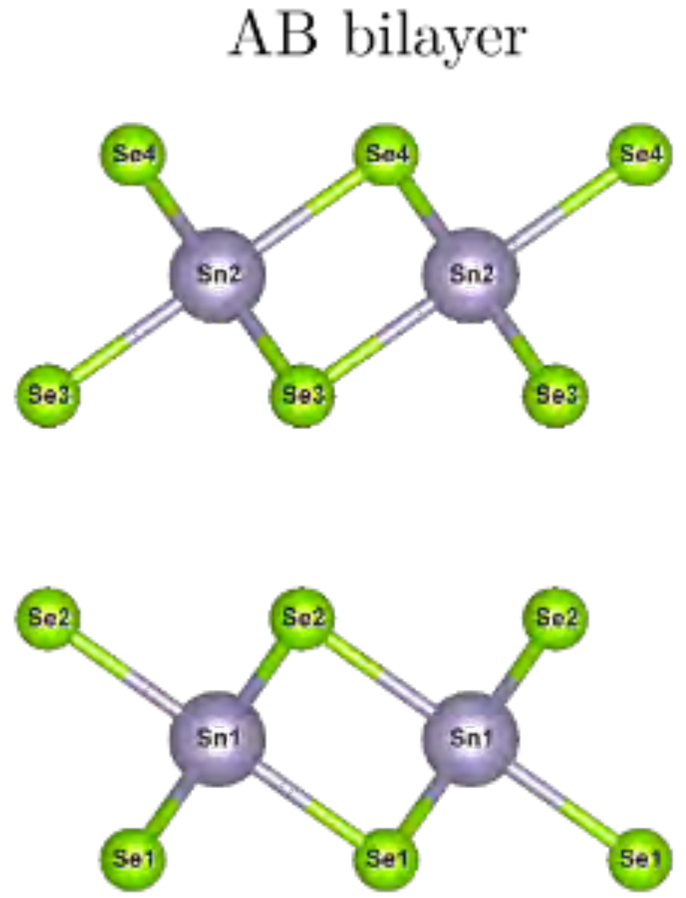
Interlude: Stacking Configurations

Since these materials have inequivalent A and B sites, two inequivalent ways to stack!









AA Stacking

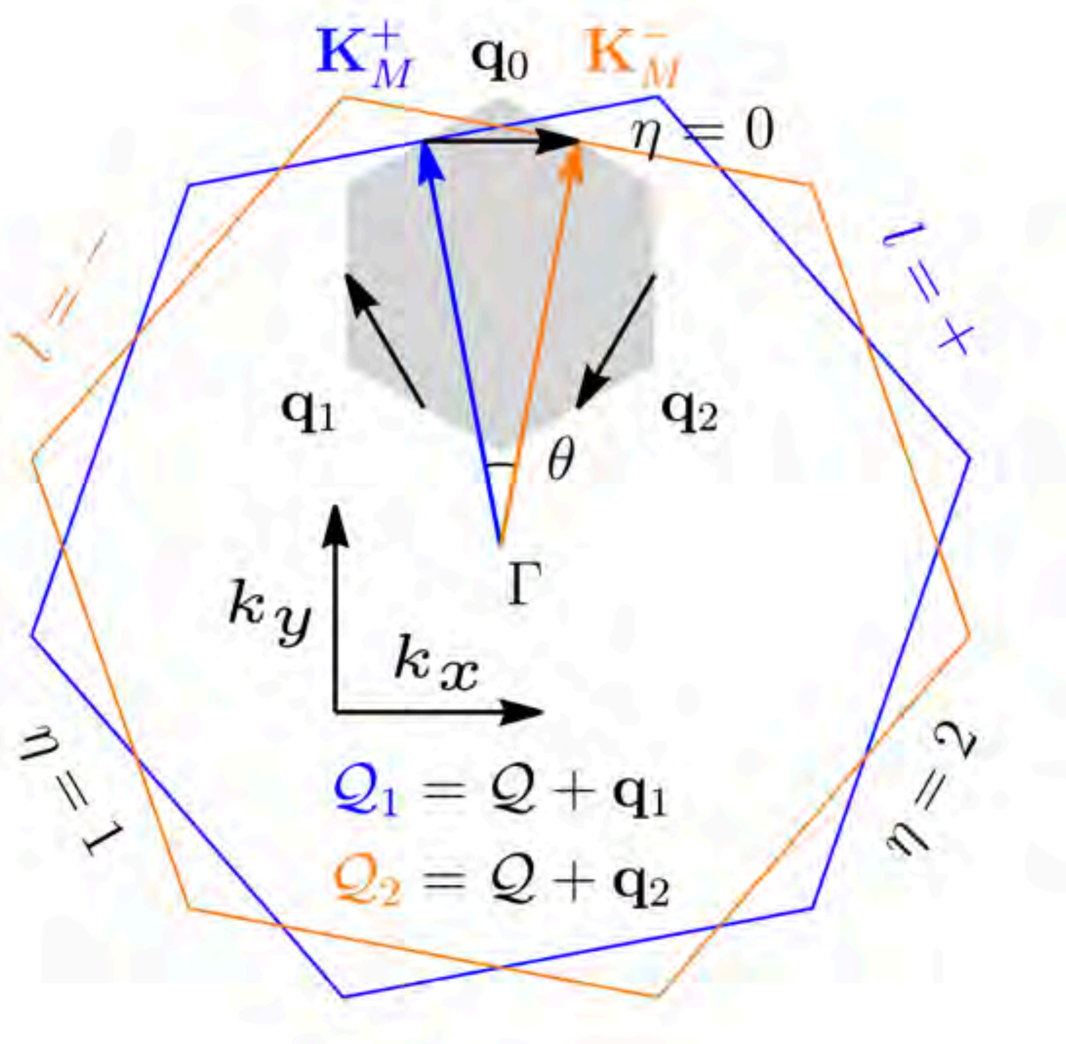
AB Stacking

The two stacking configurations give different symmetry properties for the moiré problem

Interlude: Approximate Continuum Model

Preliminary *ab initio* modelling* suggests a simplified toy model (shown for $\eta = 0$):

$$[h_{\mathbf{Q},\mathbf{Q}'}(\mathbf{k})]_{ls,l's'} = \delta_{\mathbf{Q},\mathbf{Q}'}\delta_{ss'}\delta_{ll'}\left[\frac{(k_x - Q_x)^2}{2m_x} + \frac{(k_y - Q_y)^2}{2m_y}\right] + [T_{\mathbf{Q},\mathbf{Q}'}]_{l;l's'}$$



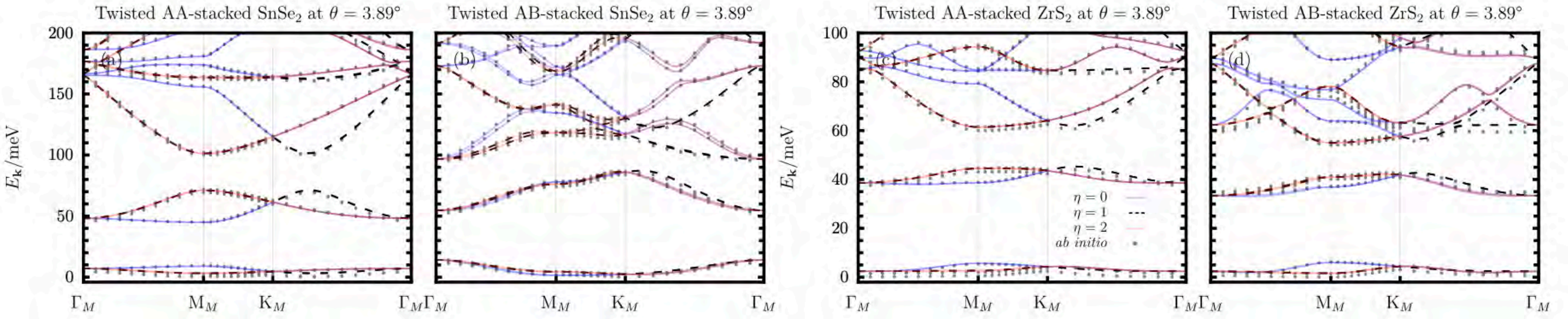
AA case: $$[T^{AA}_{\mathbf{Q},\mathbf{Q}'}]_{ls;(-l)s} = (\pm i w_1^{AA} + w_2^{AA})\delta_{\mathbf{Q}\pm\mathbf{q}_0,\mathbf{Q}'} + w_3'^{AA}\delta_{\mathbf{Q}\pm\mathbf{q}_1-\mathbf{q}_2,\mathbf{Q}'}$$

AB case: $$[T^{AB}_{\mathbf{Q},\mathbf{Q}'}]_{ls;(-l)s} = w_2^{AB}\delta_{\mathbf{Q}\pm\mathbf{q}_0,\mathbf{Q}'} + w_4'^{AB}\delta_{\mathbf{Q}\pm\mathbf{q}_1-\mathbf{q}_2,\mathbf{Q}'}$$

Parameters fit to *ab initio*

Monolayer	m_x	m_y	w_1^{AA}	w_2^{AA}	$w_3'^{AA}$	w_2^{AB}	w_4^{AB}
$SnSe_2$	0.21	0.73	66.38	88.80	−18.94	−77.80	27.04
ZrS_2	0.29	1.86	−12.35	50.50	−19.83	−35.88	−16.88

Caveat:
3-parameter models don't fit *ab initio* too well, but **4-5 param. models do ▶**



* via "local stacking approx"

Interlude: Non-Symmorphic Symmetries

For M-point twisting, new kind of emergent symmetry is helpful in organizing moiré reconstruction

Usually, non-symmorphic symmetries in 2d real space: involve reflection + partial lattice translation

Non-symmorphic symmetries in $\mathbf{k}$-space are unusual (usually only relevant for huge $\boldsymbol{B}$-field!)

$\mathbf{M}$- point moiré materials end up having such a symmetry! (Detailed origin is stacking-dependent):

$$\tilde{M}_z \hat{c}^\dagger_{\mathbf{k},\mathbf{Q},s,l} \tilde{M}_z^{-1} = \hat{c}^\dagger_{\mathbf{k}+\mathbf{q}_\eta,\mathbf{Q}+\mathbf{q}_\eta,s,l}, \quad \text{for } \mathbf{Q} \in \mathcal{Q}_{\eta+l}$$

$$\tilde{M}_z \hat{\psi}^\dagger_{\eta,s,l}(\mathbf{r}) \tilde{M}_z^{-1} = \hat{\psi}^\dagger_{\eta,s,-l}(\mathbf{r})$$

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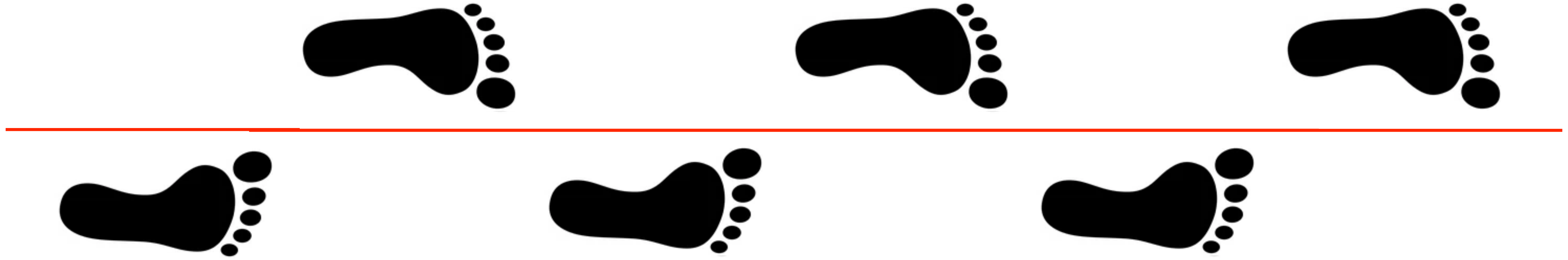

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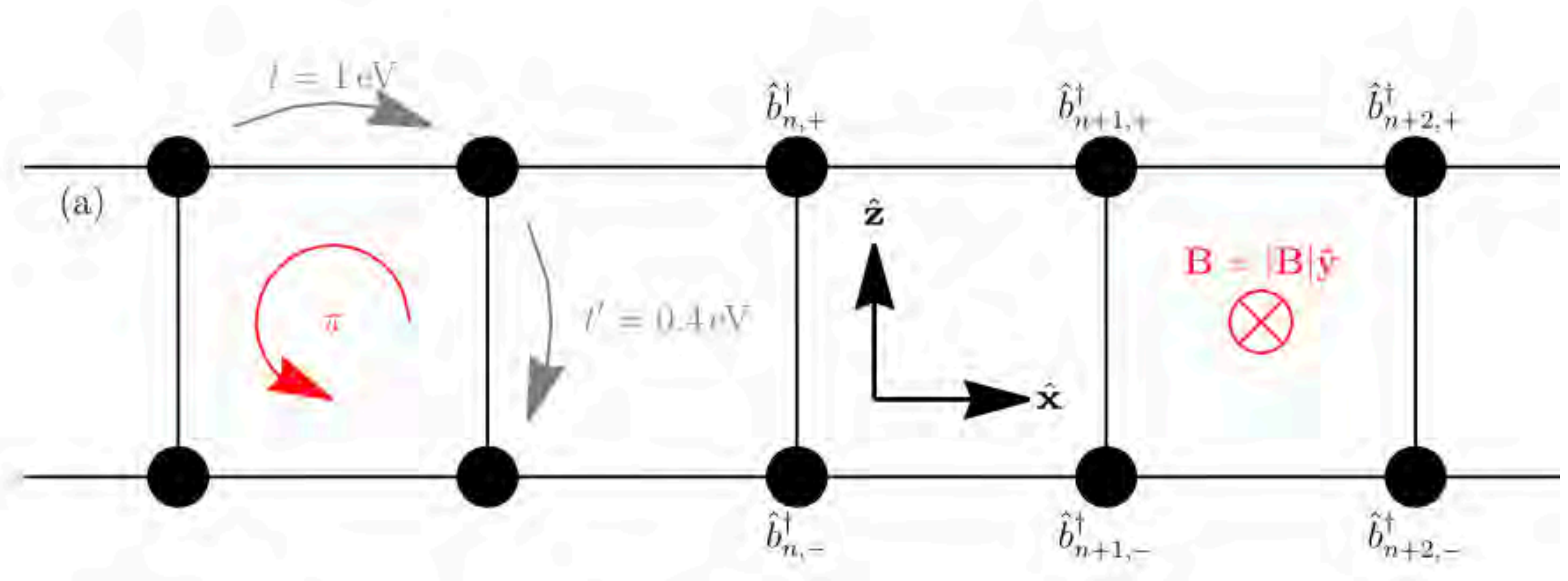
Role of Non-Symmorphic Symmetries

1d toy Model: π-flux ladder



$$T\hat{b}^\dagger_{n,l}T^{-1} = \hat{b}^\dagger_{n+1,l}$$

$$\tilde{M}_z\hat{b}^\dagger_{n,l}\tilde{M}_z^{-1} = \hat{b}^\dagger_{n,-l}(-1)^n$$

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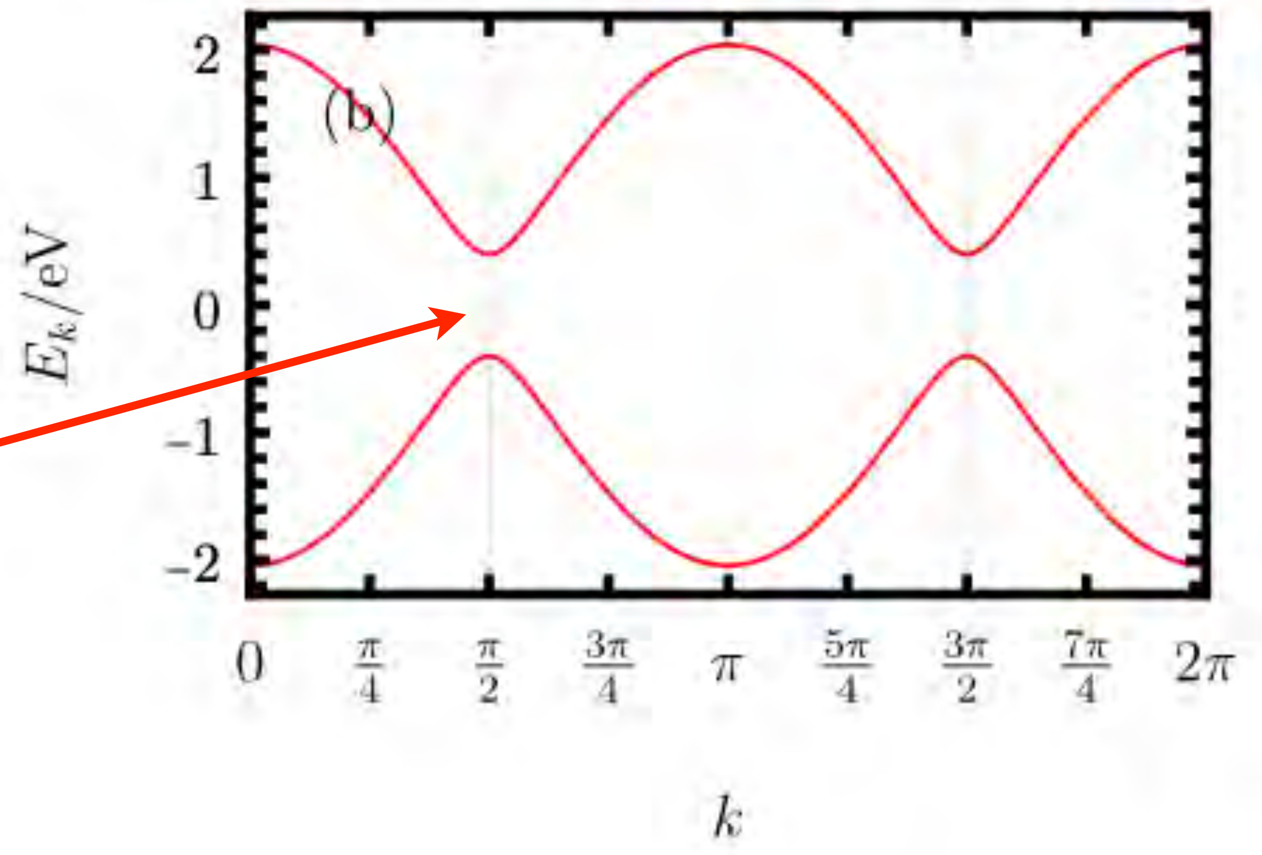

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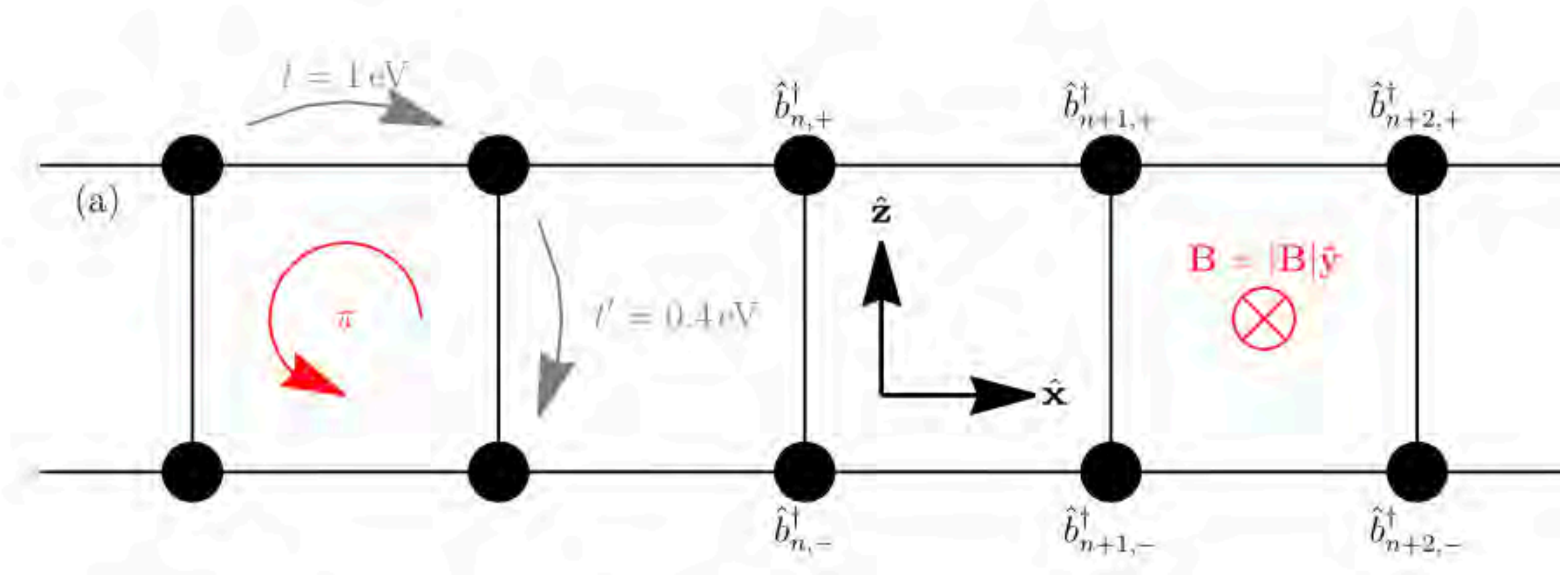

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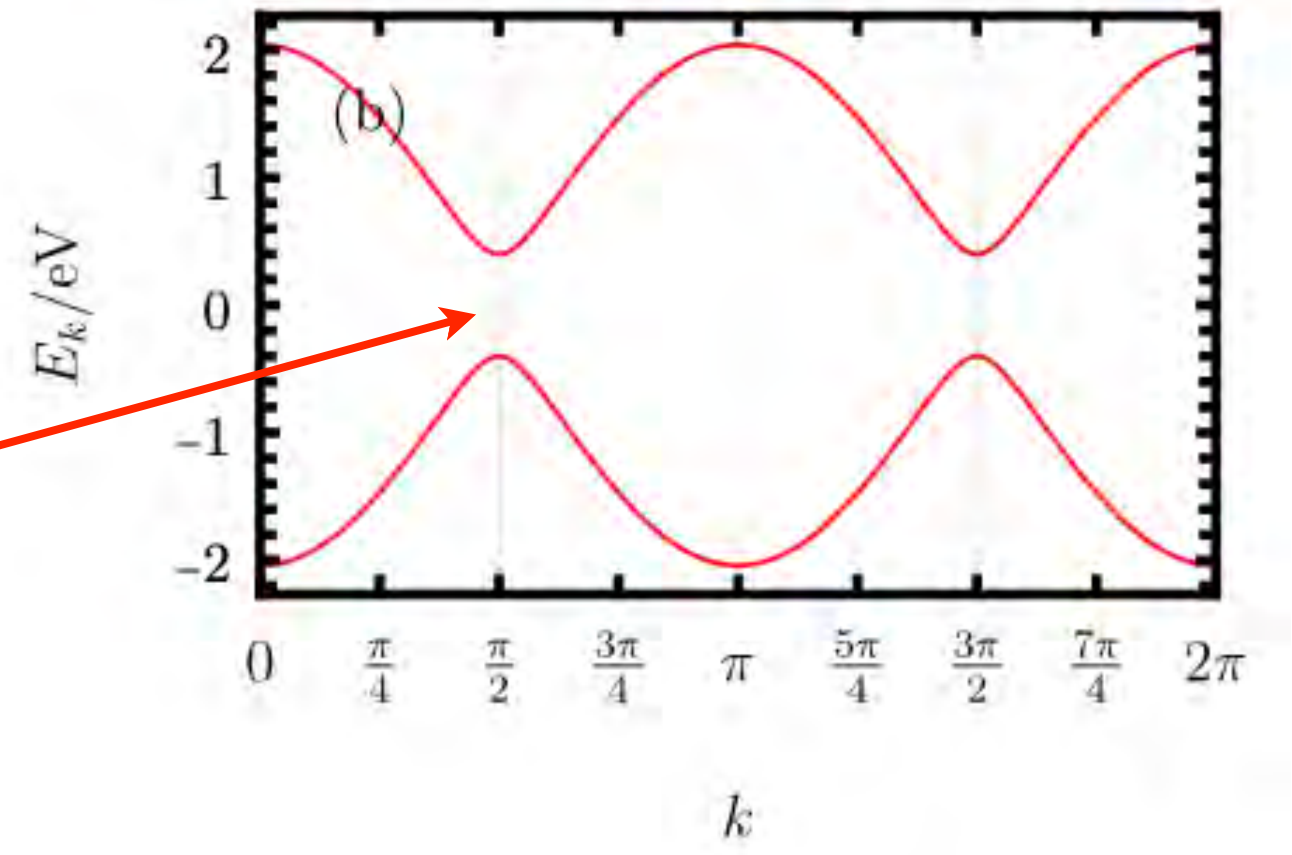
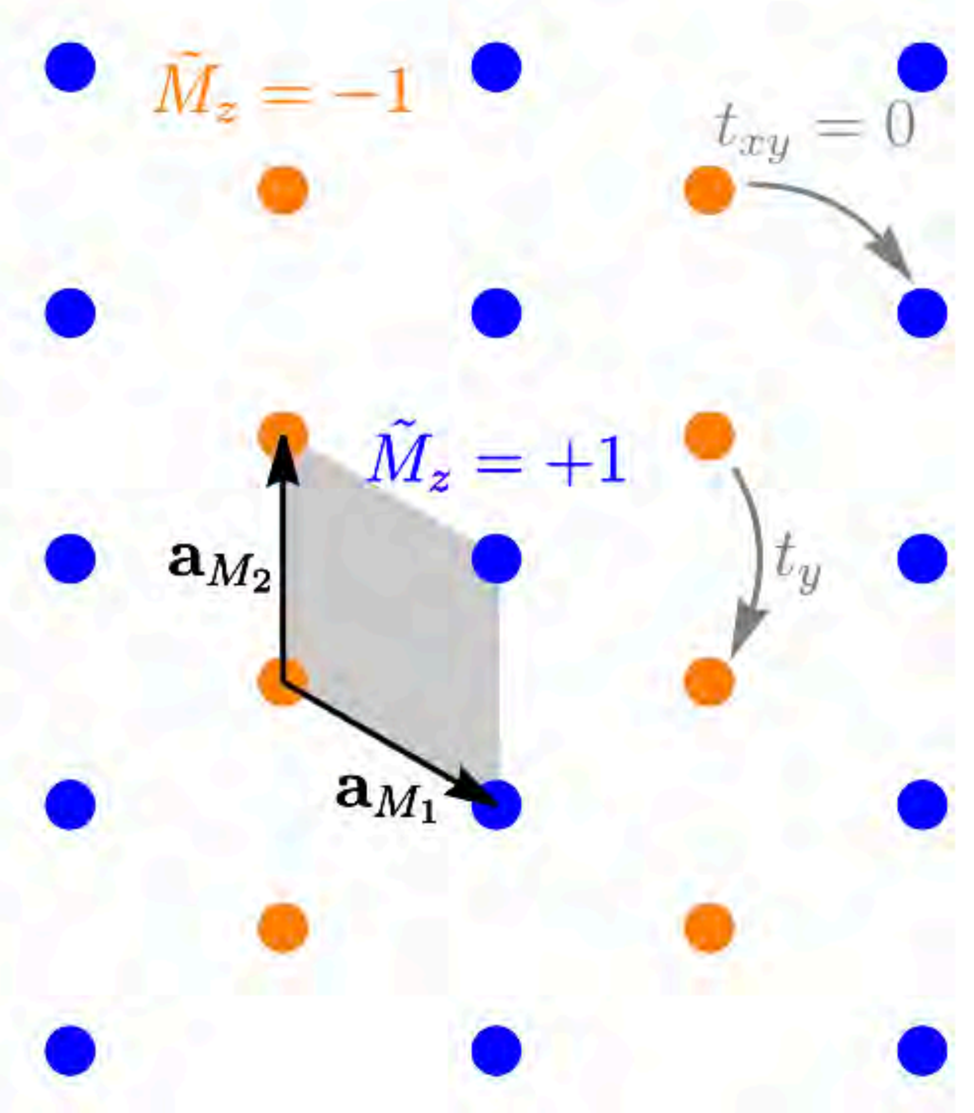


In 2D $\mathbf{M}$-point moirés: $\tilde{M}_z$ forbids certain hoppings!

e.g. consider $\eta = 0$ valley in real space for AA stacking

$\tilde{M}_z$ axis is $\parallel \hat{y}$ + can show $[T_{\mathbf{a}_{M_1}}, \tilde{M}_z] = \{T_{\mathbf{a}_{M_2}}, \tilde{M}_z\} = 0$

$\Rightarrow$ no hopping between sites w/ different $\tilde{M}_z$-eigenvalue (± 1)



Step #3: Exact & Approximate Symmetries of M-point Twisting

Approx. continuum model results can be generalized by examining symmetries of moiré potential

At small twist angles, "zero twist" symmetries are useful guide (cf. ≈PHS in TBG)

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Most important symmetries are non-symmorphic:

AA stacking: monolayer inversion $I \Rightarrow$ **moiré non-symmorphic mirror** $\tilde{M}_z$

AB stacking: monolayer mirror $M_z \Rightarrow$ **moiré non-symmorphic inversion** $\tilde{I}$

(sends $\mathbf{k}, l \rightarrow -\mathbf{k} + \mathbf{q}_\eta, -l$)

$\tilde{I}$ combines with *approx*. moire C_{2z} to give nonsymmorphic mirror: $\tilde{M}_z = \tilde{C}_{2z}\tilde{I}$

(less ideal than in AA)

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Spoiled by relaxation — which is *worse* at smaller twists (!) — but still good starting point

Step #4: Moiré Bandstructure Calculations & Caveats

Continuum model (∼BM): two-center approximation ($t_{inter}(\mathbf{r}, \mathbf{r}') = t_{inter}(\mathbf{r} - \mathbf{r}')$) + first harmonic

"accidental symmetry" : continuous translation symmetry along one direction!

More general moiré potentials (symmetry-constrained) give better results

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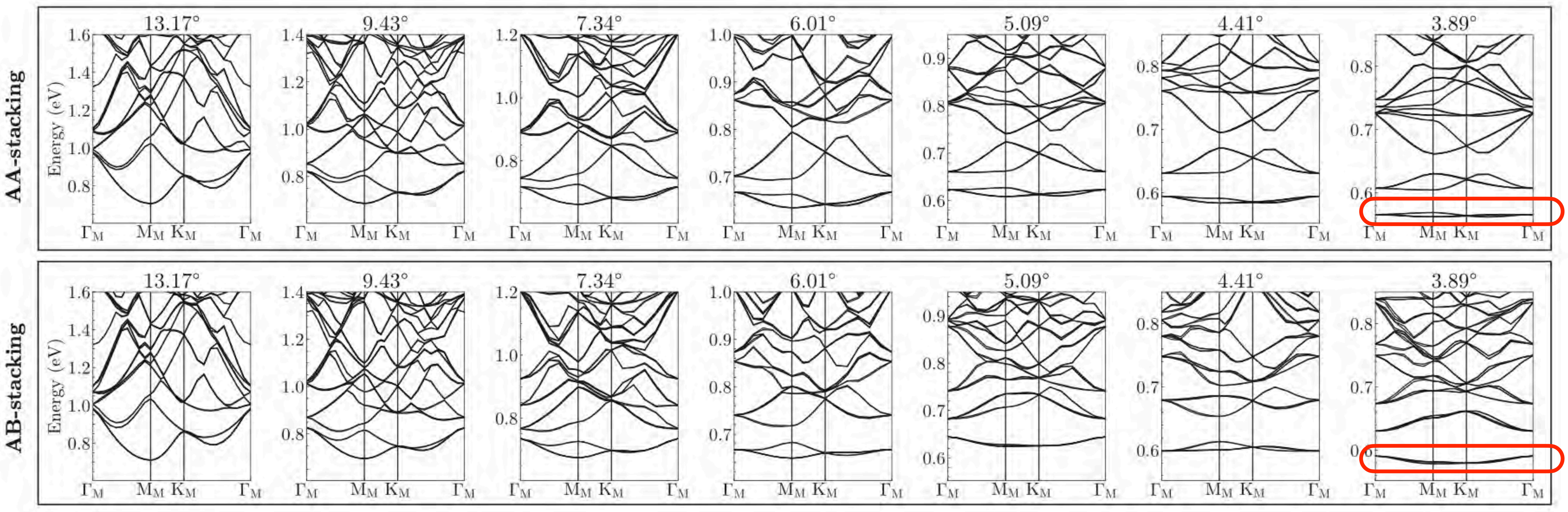
Relaxation plays important role in modifying some of the symmetries from exact → approximate

Ab initio Results: $tSnSe_2$

Flat bands appear at small twist angles ($\theta \sim 3.89°$) for both stacking



6 = (2 spin)×(3 valley) flat bands, topological trivial, can Wannierize to get effective tight-binding model

Real-Space Picture from Tight-Binding

Real-space placement of orbitals depends on stacking

Interplay of orbital placement with nonsymmorphic symmetries influences hopping

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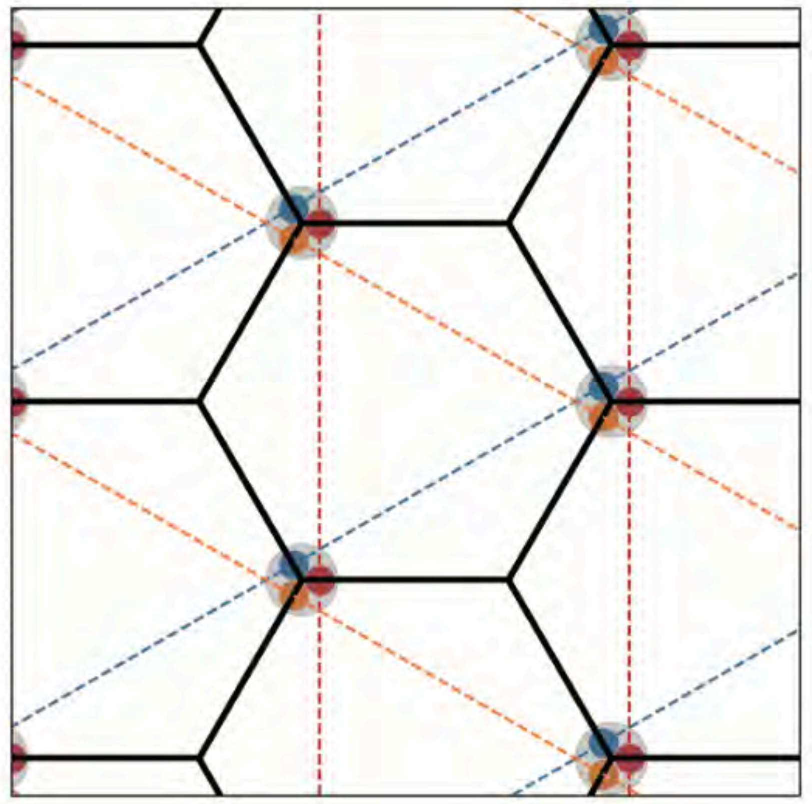
AA-stacked $tSnSe_2$



orbital from 3 valleys nearly coincide:
triangular lattice

valley-selective, quasi-1D hopping
enables sign-free QMC

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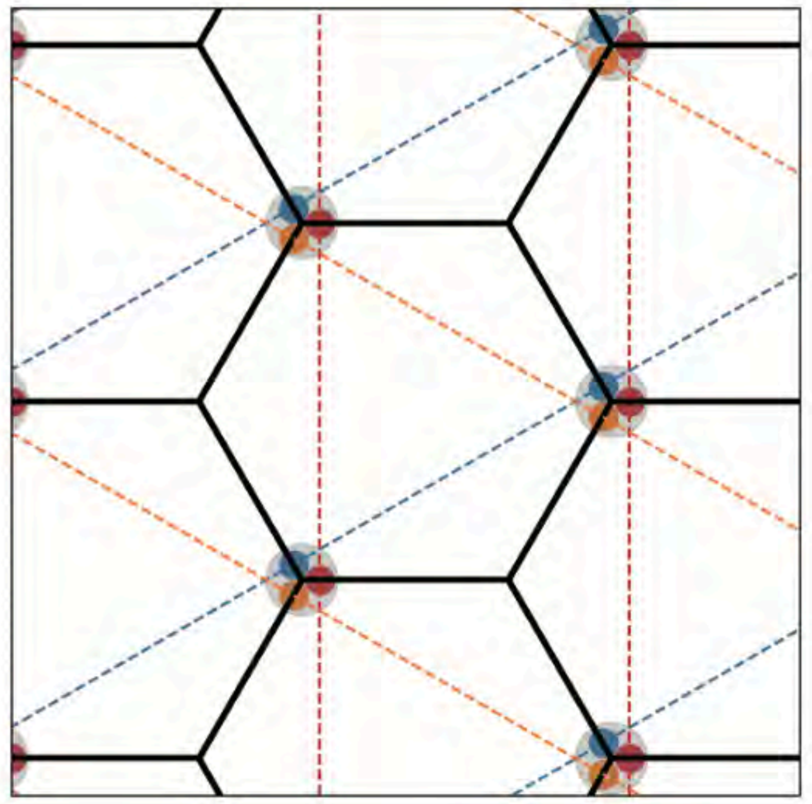

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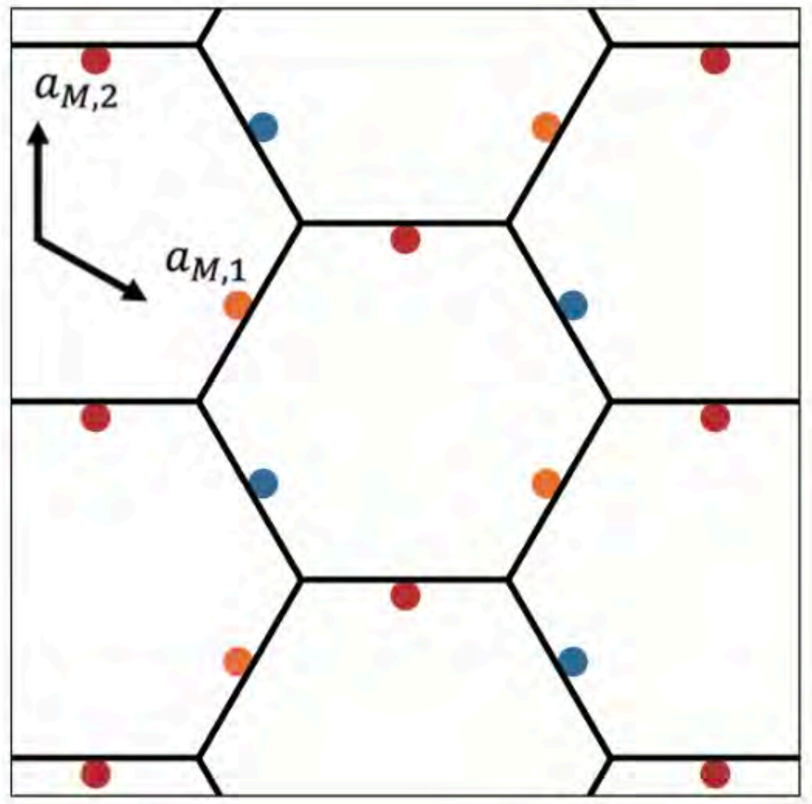
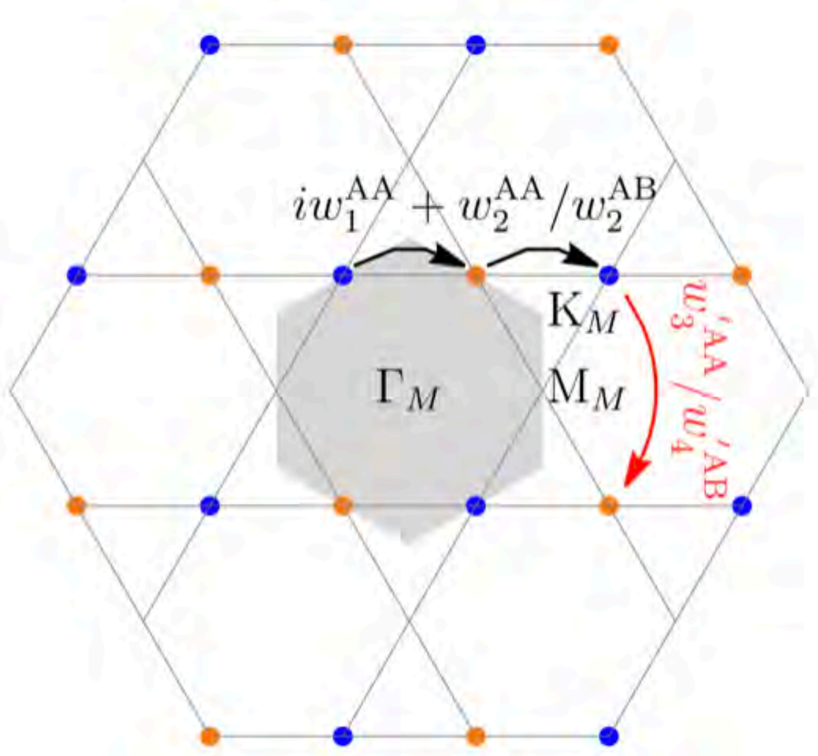


orbitals from 3 valleys displaced: kagomé lattice

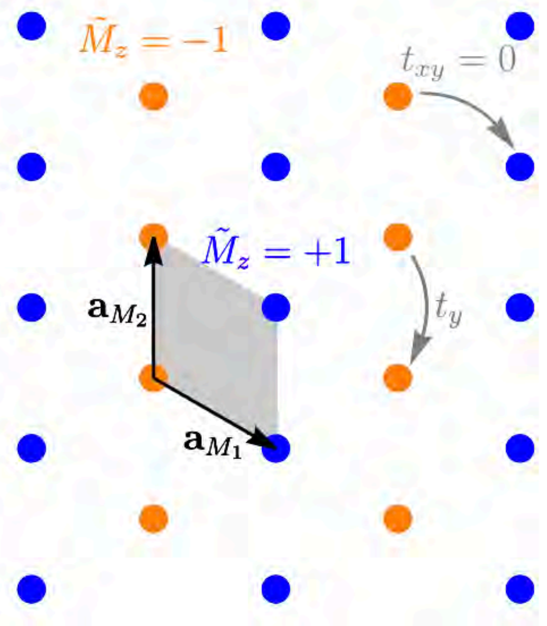
2D but no n.n. inter-valley hopping — different from usual kagomé

Summary of Lecture 1

Twisting $\mathbf{M}$-point monolayers unlocks a new array of moiré materials



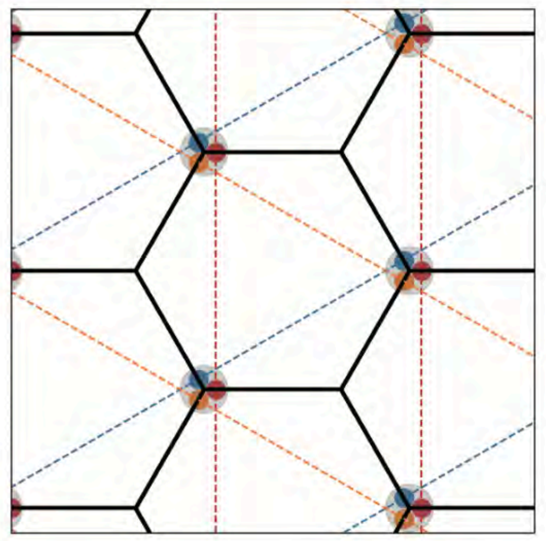
Easiest understanding of single-particle moiré problem is via studying momentum-space hopping problem



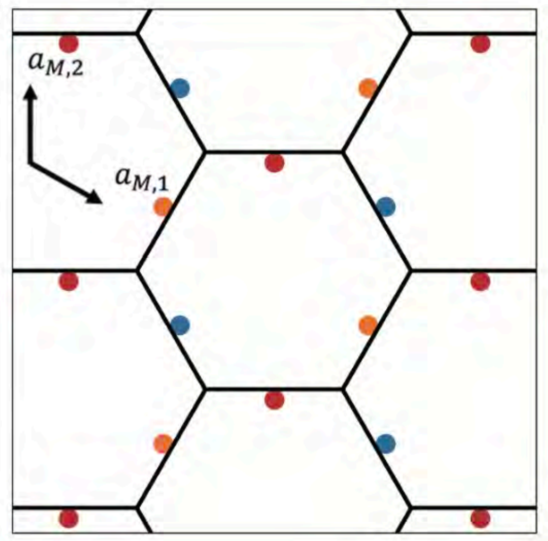
Emergent momentum-space non-symmorphic symmetries play key role!

Two examples in $tSnSe_2$:

AA stacking: triangular lattice w/ quasi-1d hopping



AB stacking: kagome lattice



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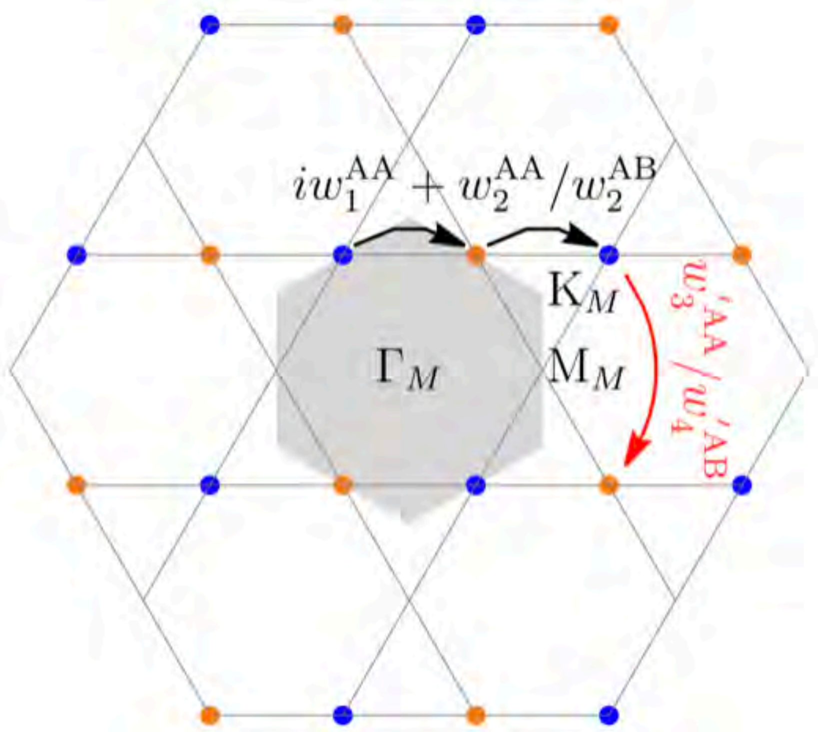

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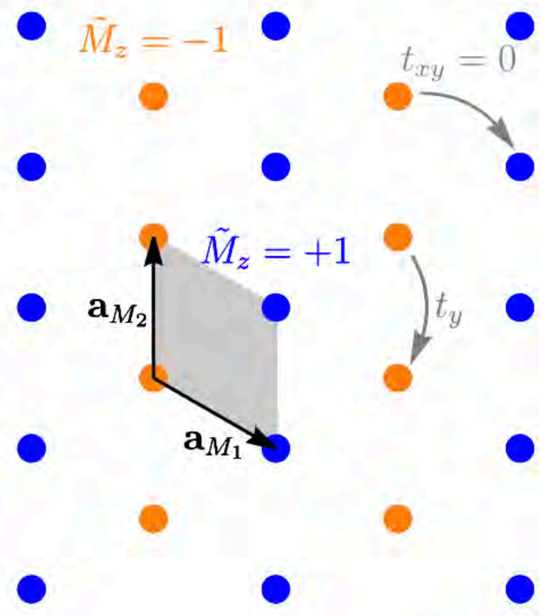

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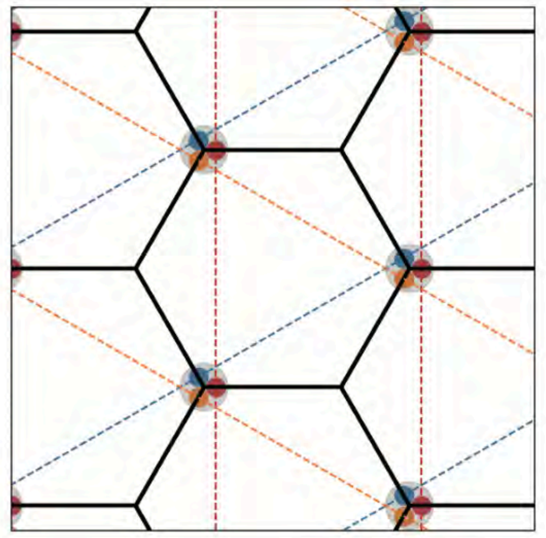
Lecture 2!

AA stacking: triangular lattice w/ quasi-1d hopping



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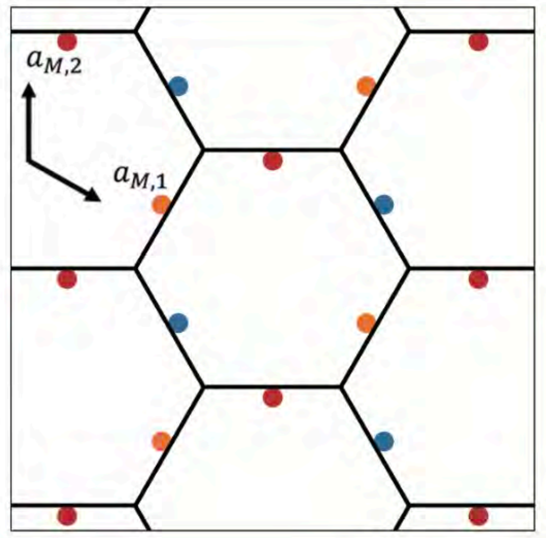

Extra Slides

Material Variability