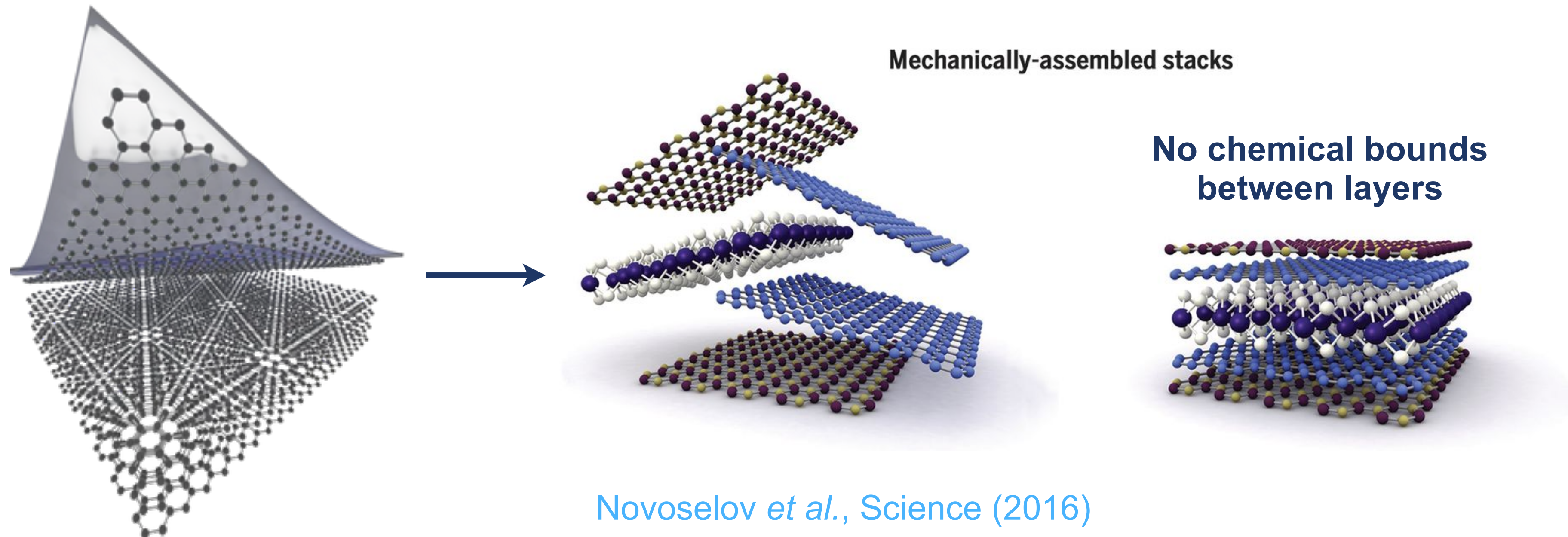


Perturbative symmetry indicators for moiré materials discovery

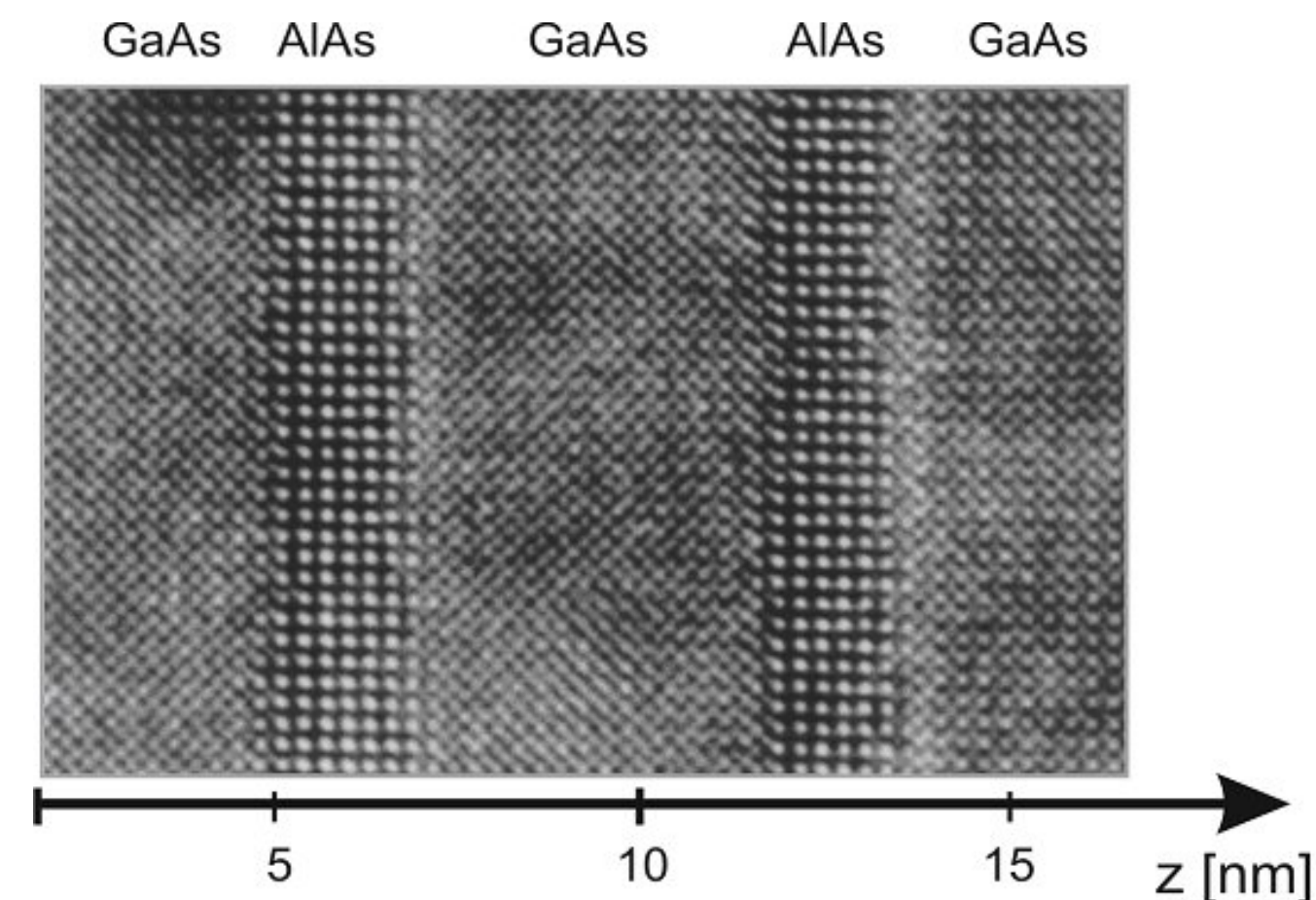
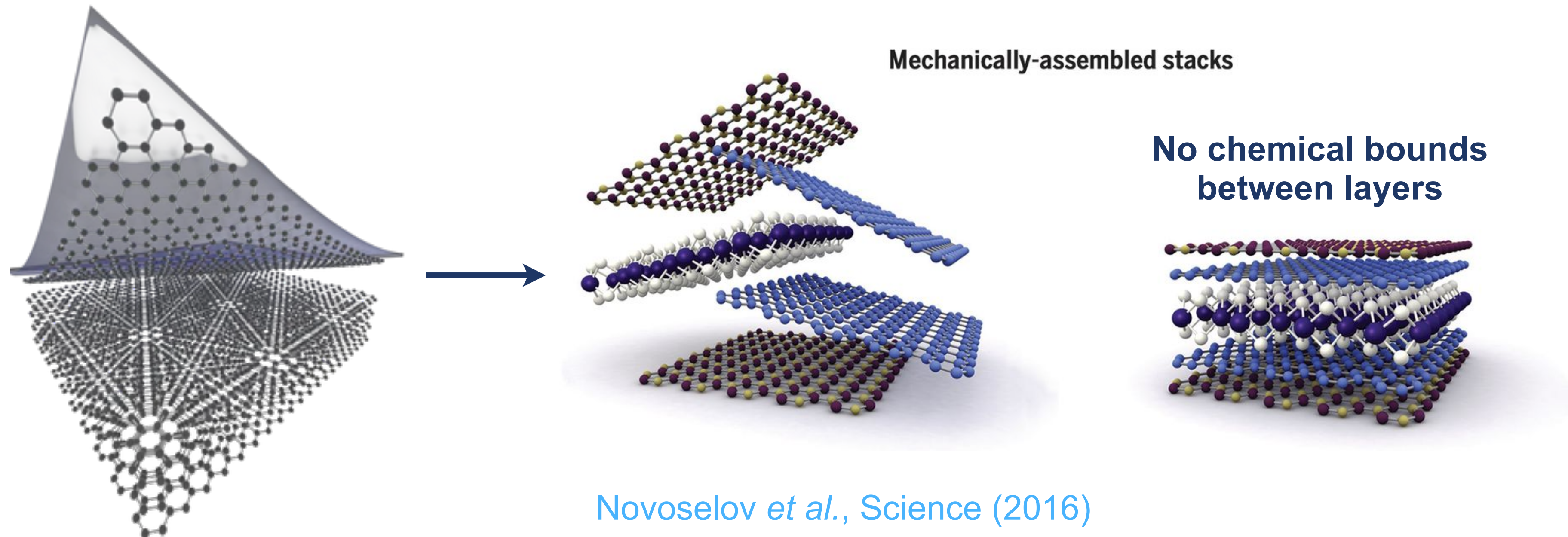
8 June 2026, IMSI

Valentin Crépel

Very brief intro: the promise of van der Waals heterostructures



Very brief intro: the promise of van der Waals heterostructures



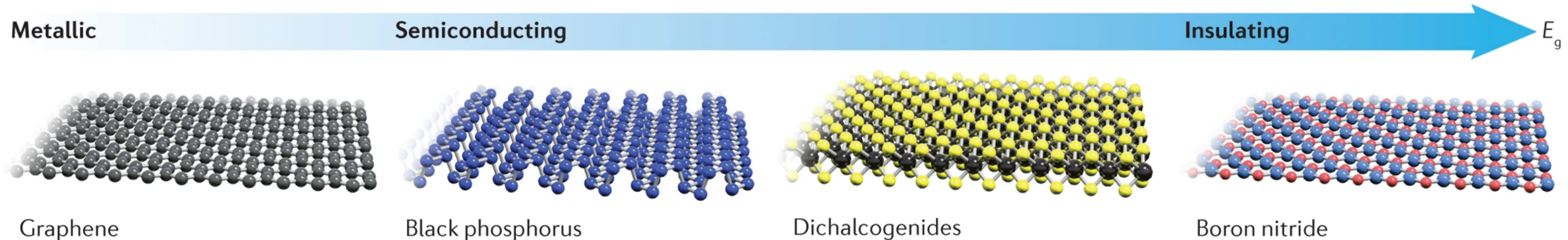
Chemical bounds: only grow materials that are *alike*, both lattice structure and properties.

Versatility of van der Waals heterostructures

- Choice within more than 2000 exfoliable materials (online databases)

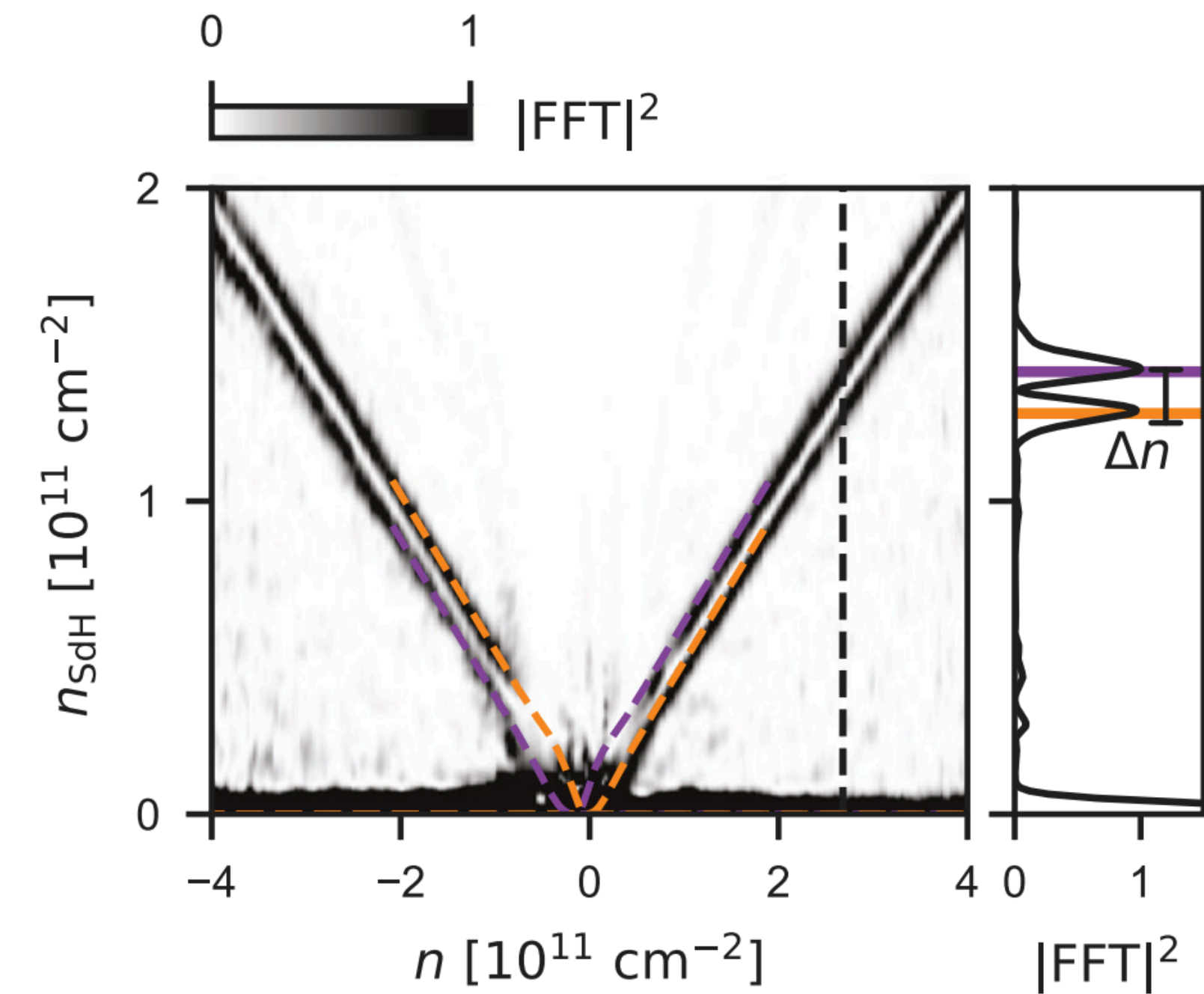
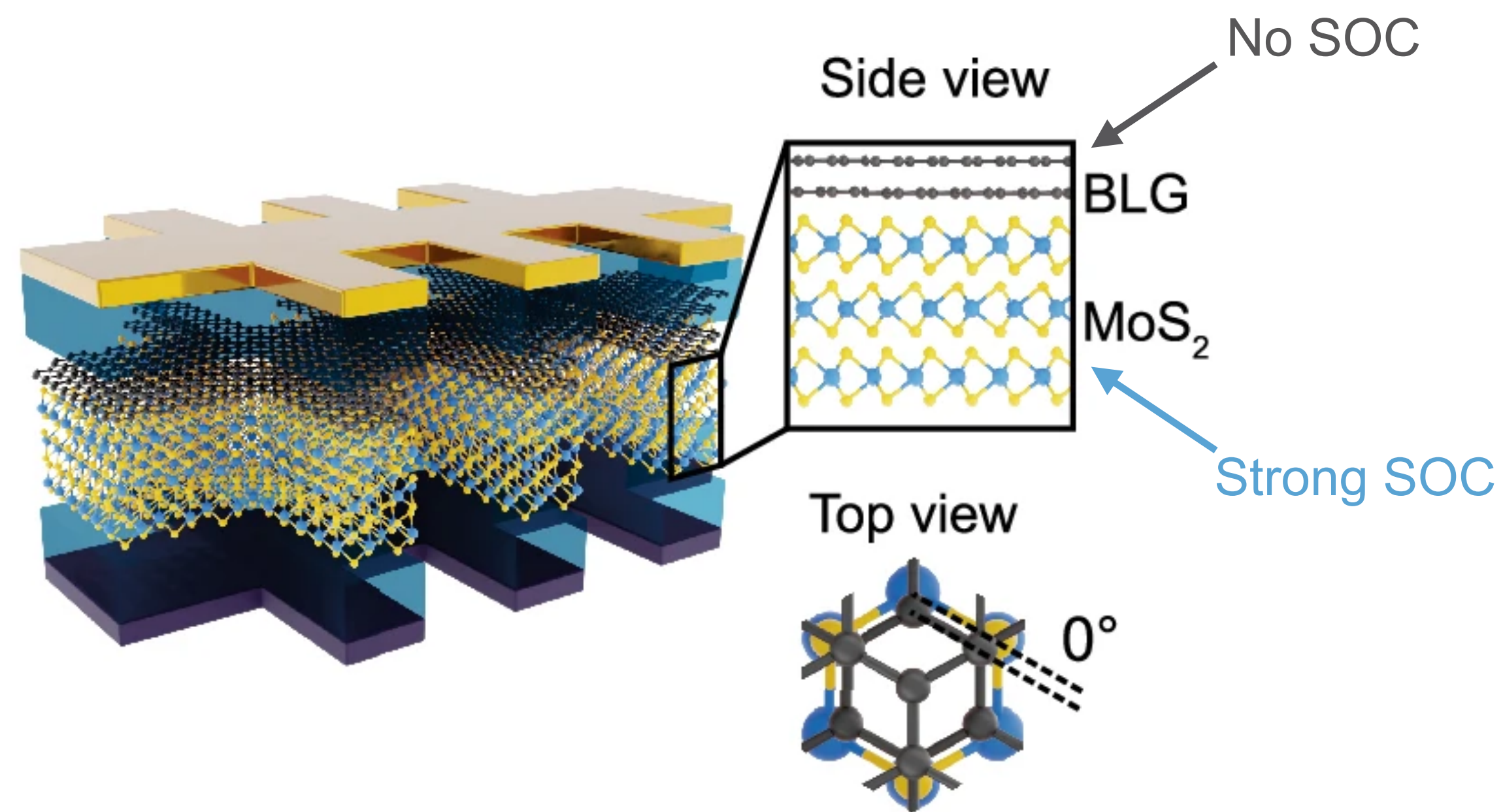
[Haastrup *et al.*, 2D Materials \(2018\)](#); [Mounet *et al.*, 2D Materials \(2021\)](#); [Jiang ... Bernevig, arXiv:2411.09741 \(2024\)](#)

- With different properties (metal, semiconductors, superconductors, ...) that can be admixed!



[Liu *et al.*, Nature Reviews Materials \(2016\)](#)

Versatility of van der Waals heterostructures

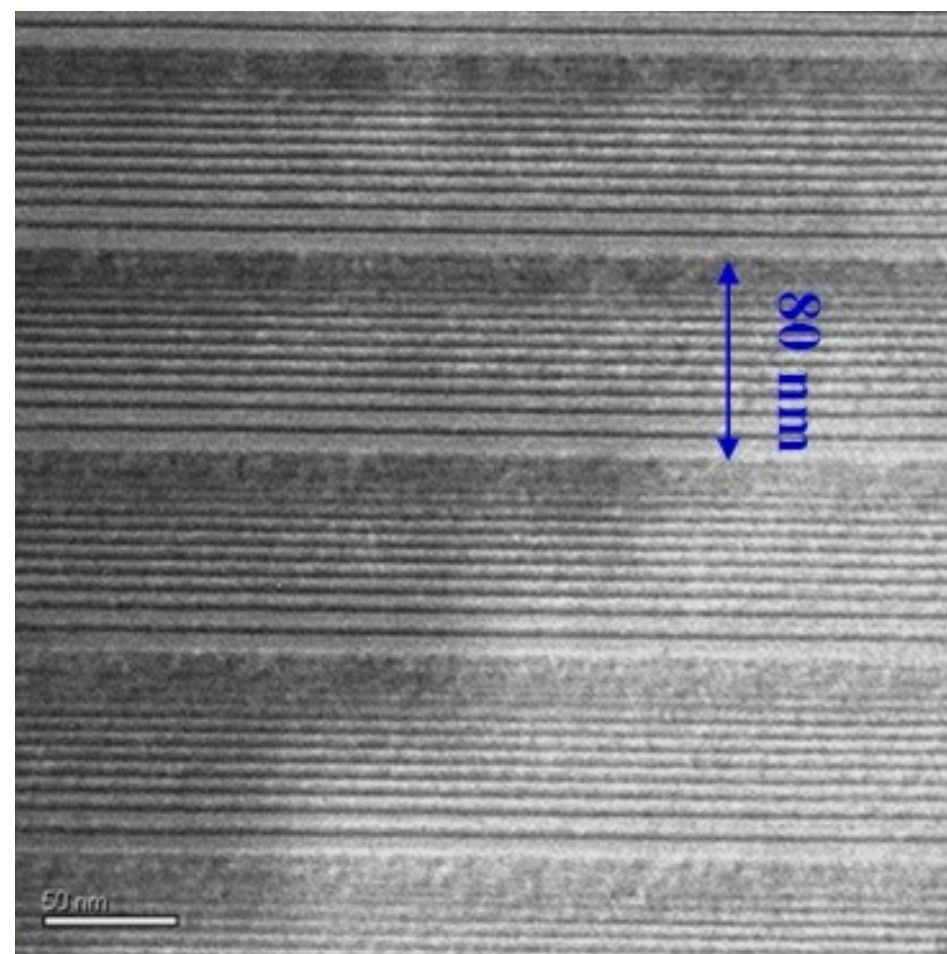


“Spin-orbit proximity in MoS₂/bilayer graphene heterostructures”, Masseroni ... Ensslin and Duprez, Nat. Commun. (2024)

Tunability of van der Waals heterostructures

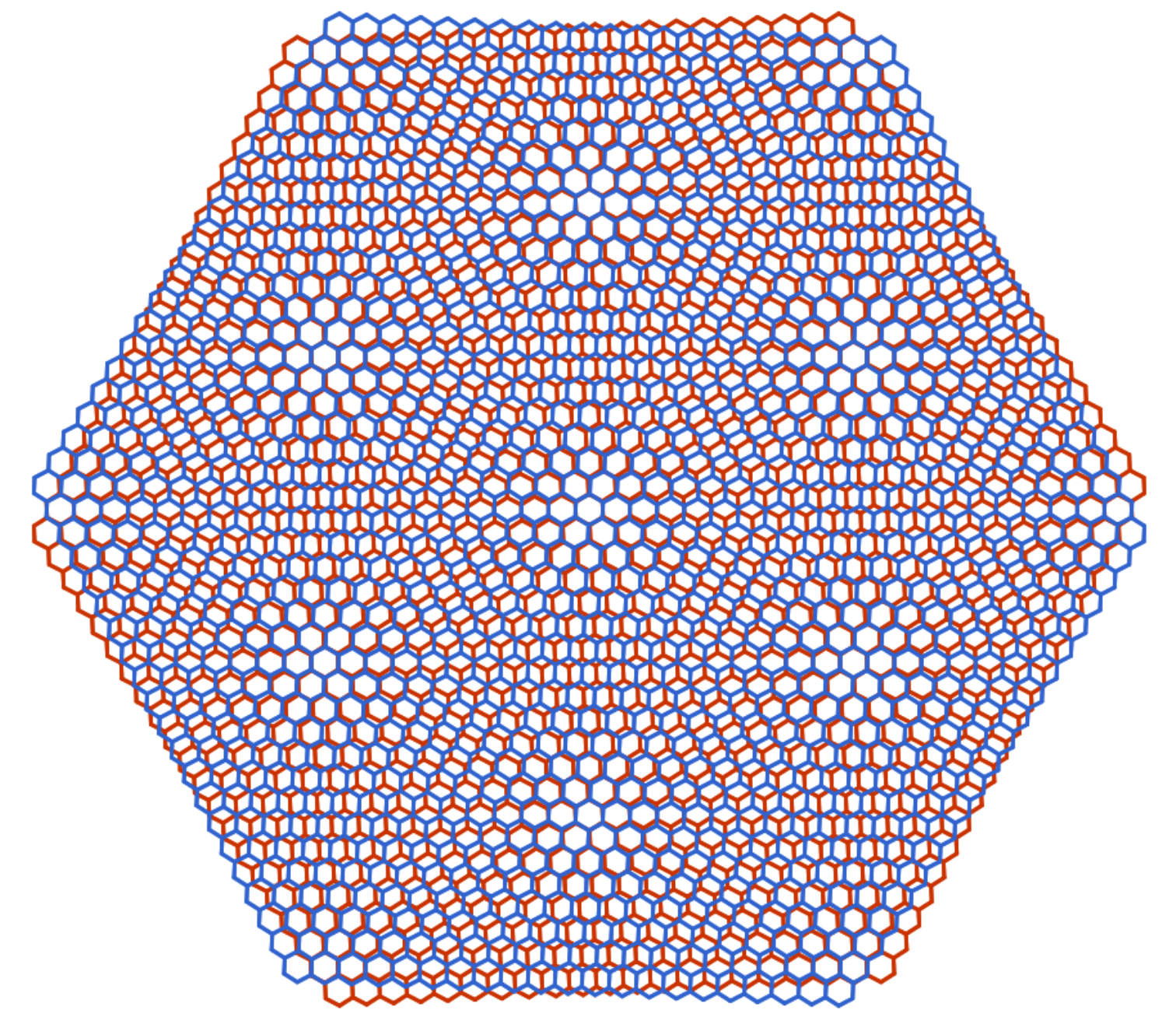
- Choice within more than 2000 exfoliable materials (online databases)
- Structural design (superlattice) to alter properties: moiré patterns

1d superlattice:
Quantum cascade laser



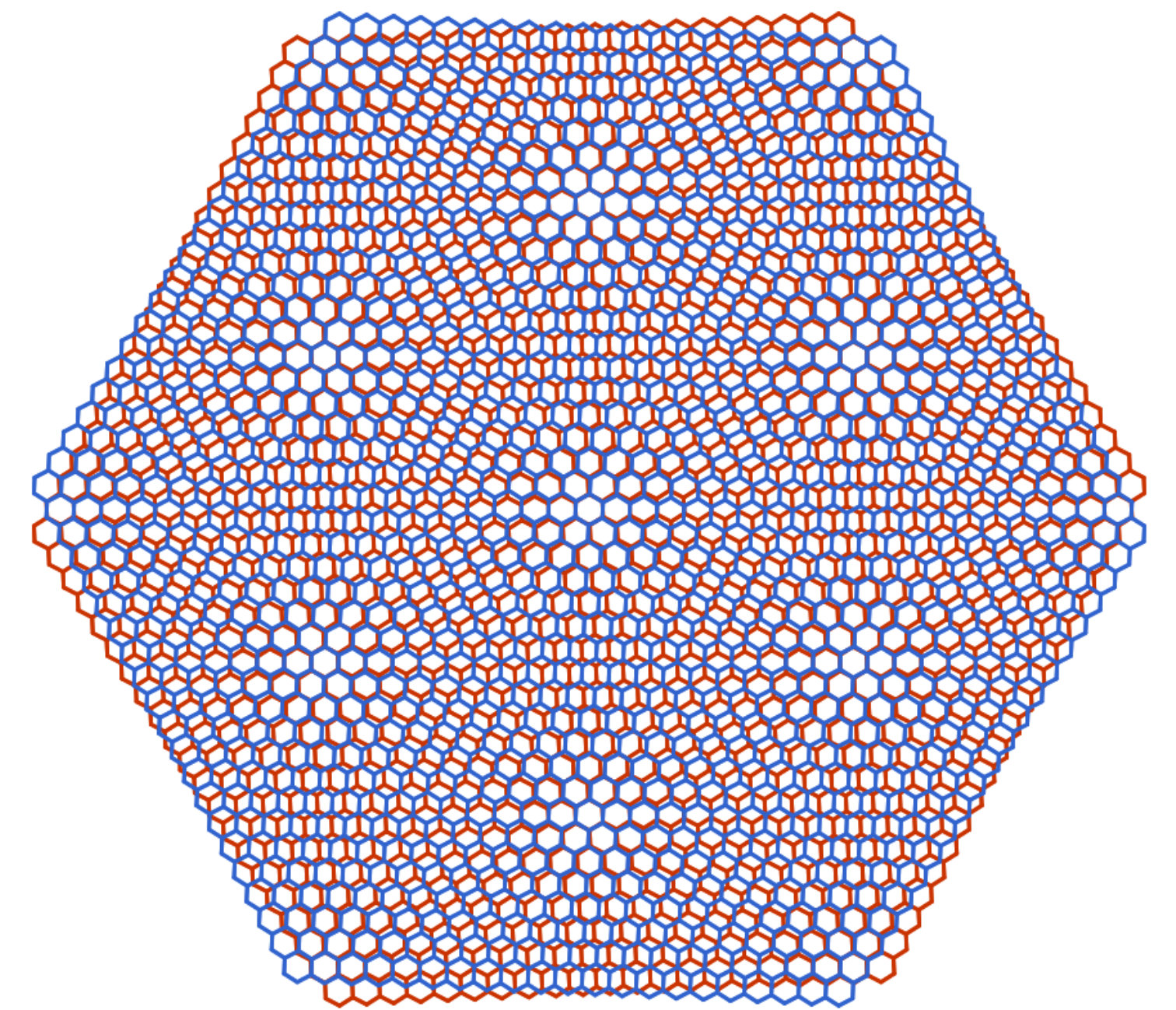
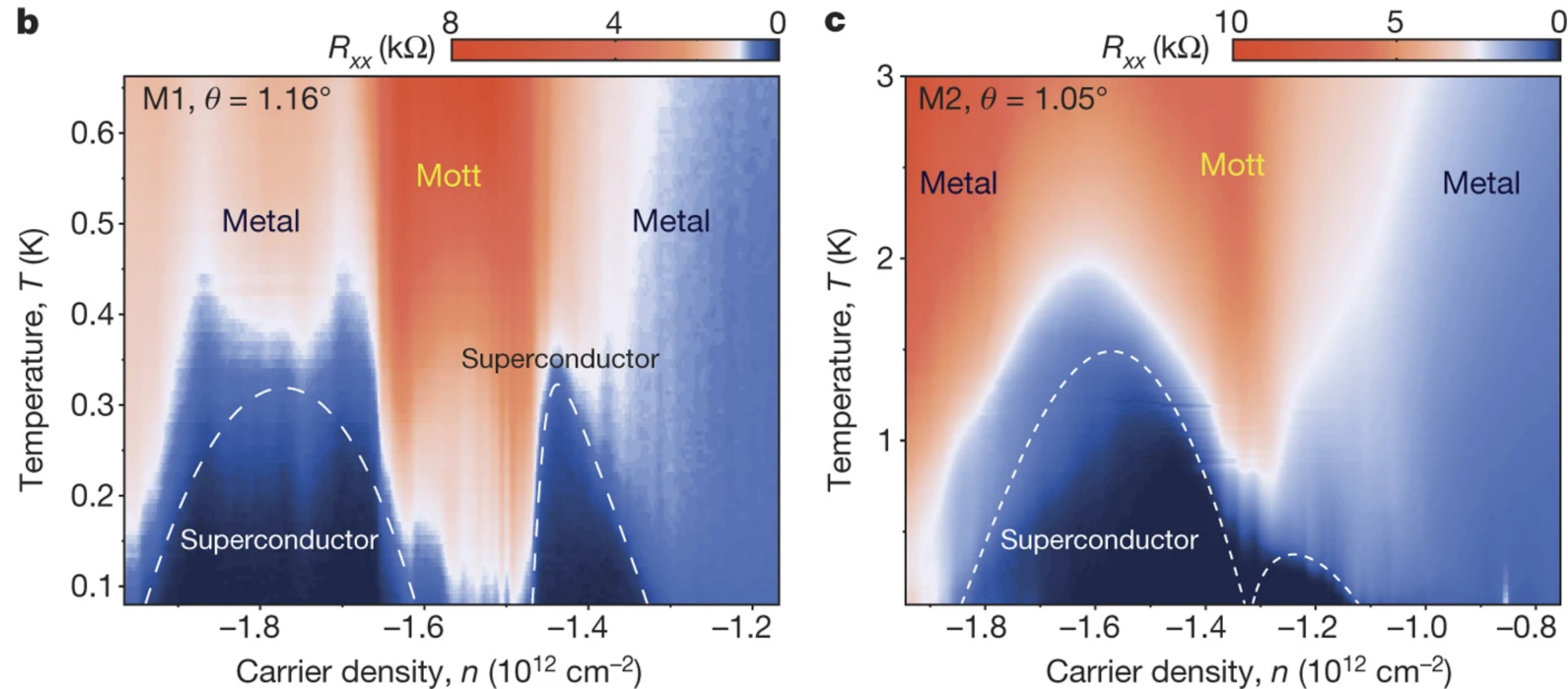
Faist *et al.*, Science (1994)

Generalization to 2d: moiré



Tunability of van der Waals heterostructures

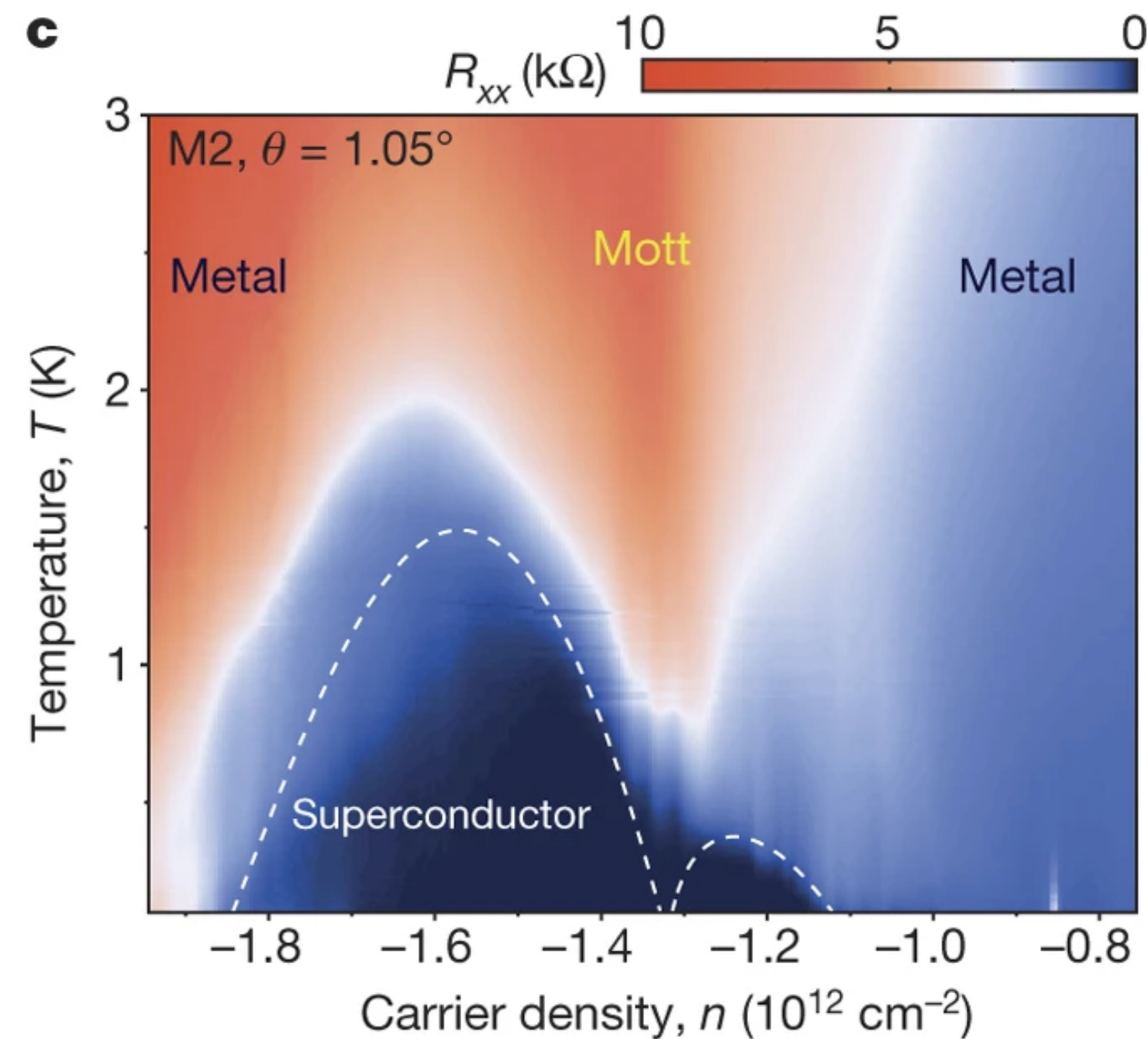
- Choice within more than 2000 exfoliable materials (online databases)
- Structural design (superlattice) to alter properties: **USEFUL** moiré patterns



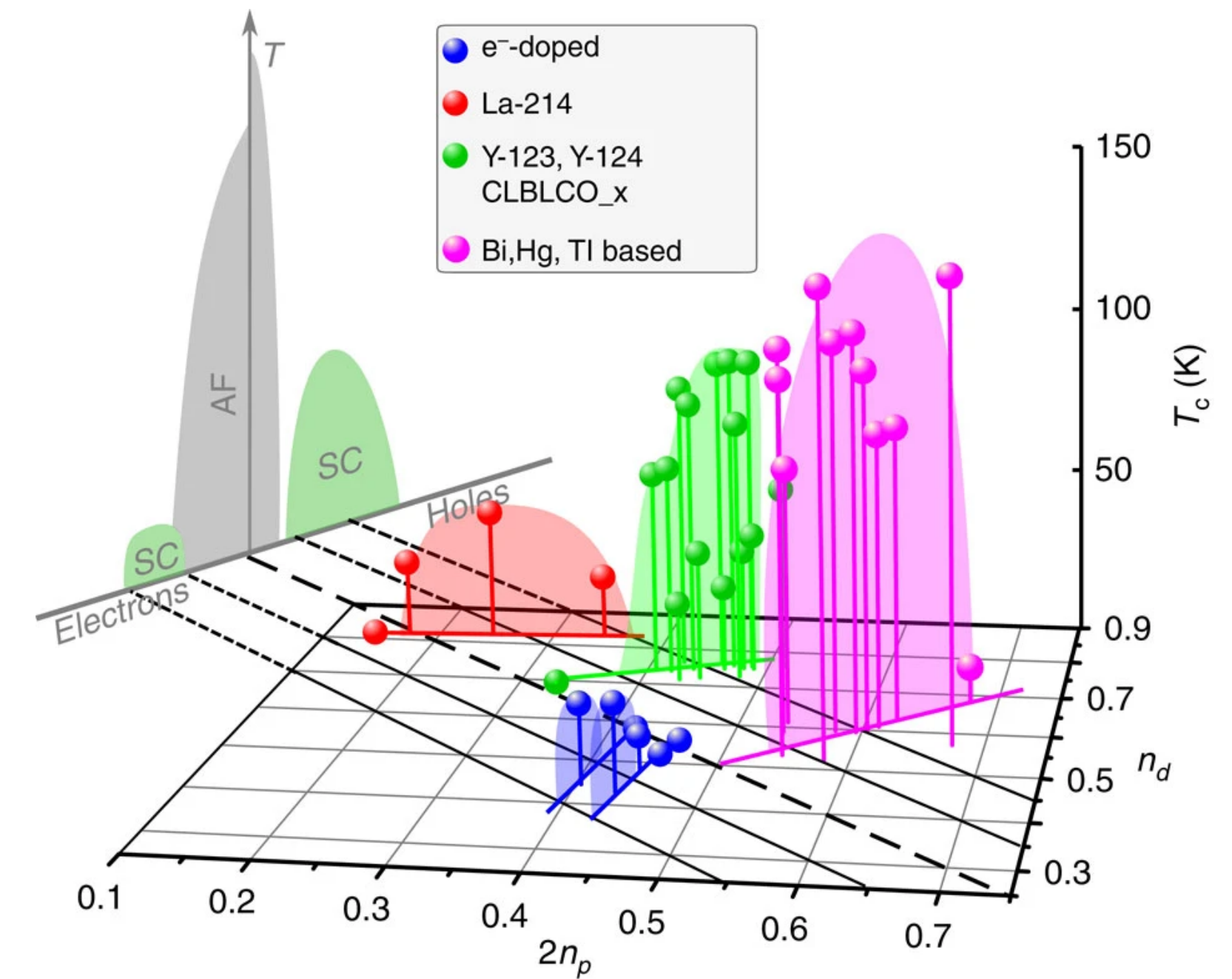
Yao ... Jarillo-Herrero, Nature (2018)

Controllability of van der Waals heterostructures

- Choice within more than 2000 exfoliable materials (online databases)
- Structural design (superlattice) to alter properties: USEFUL moiré patterns
- In-situ control by external field & continuously varying parameters



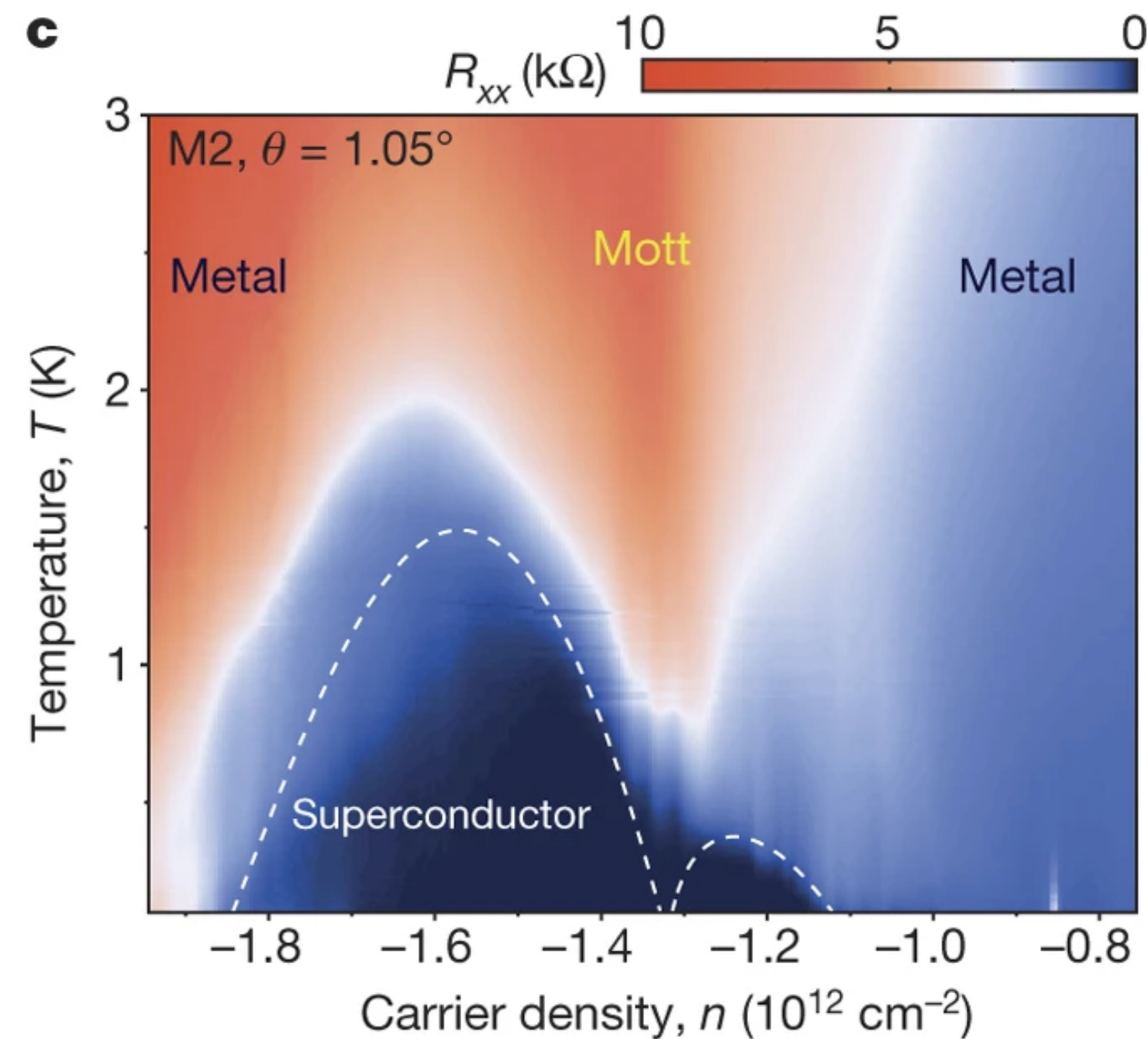
Yao ... Jarillo-Herrero, Nature (2018)



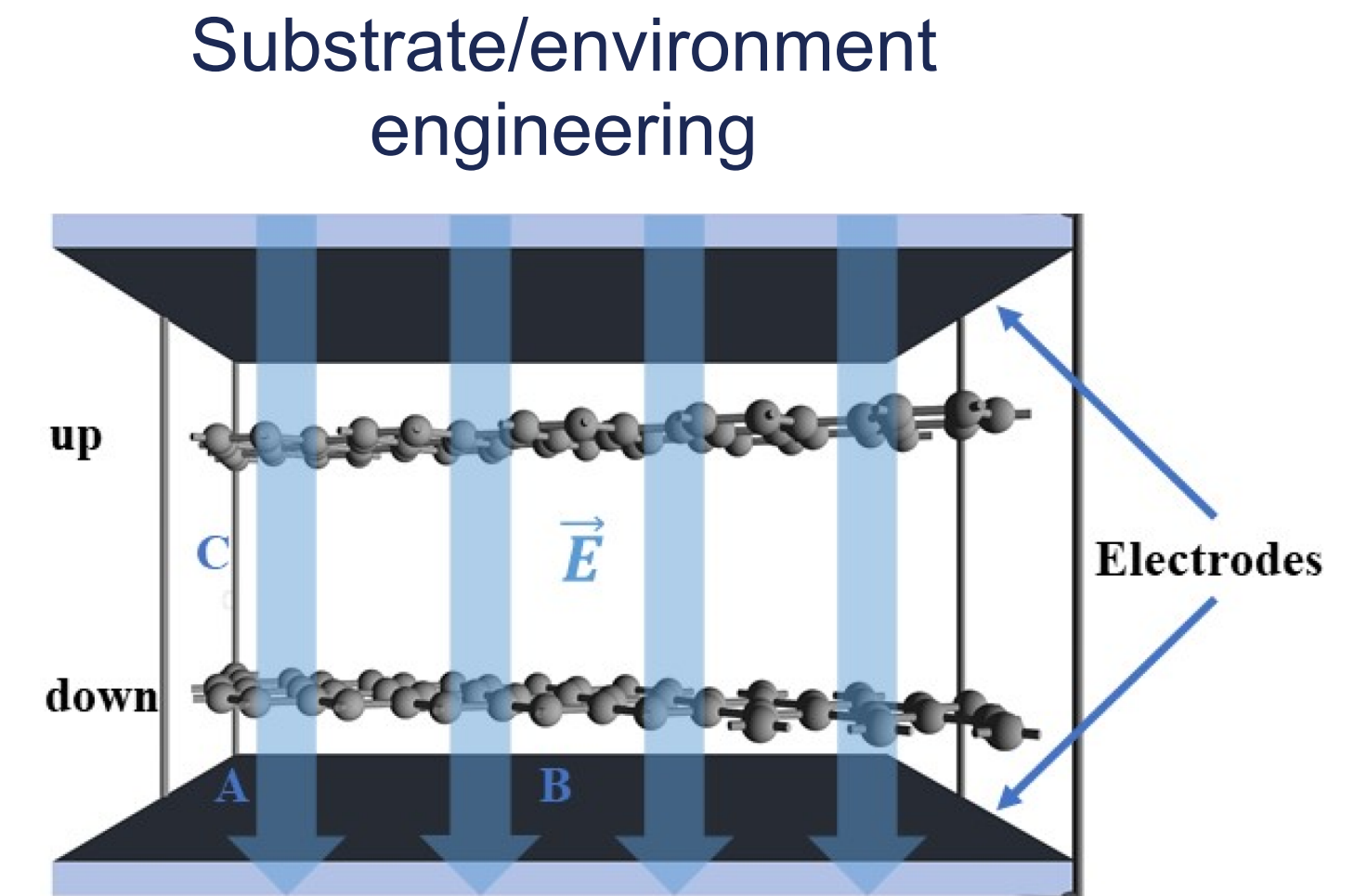
Rybicki *et al.*, Nat. Commun. (2016)

Controllability of van der Waals heterostructures

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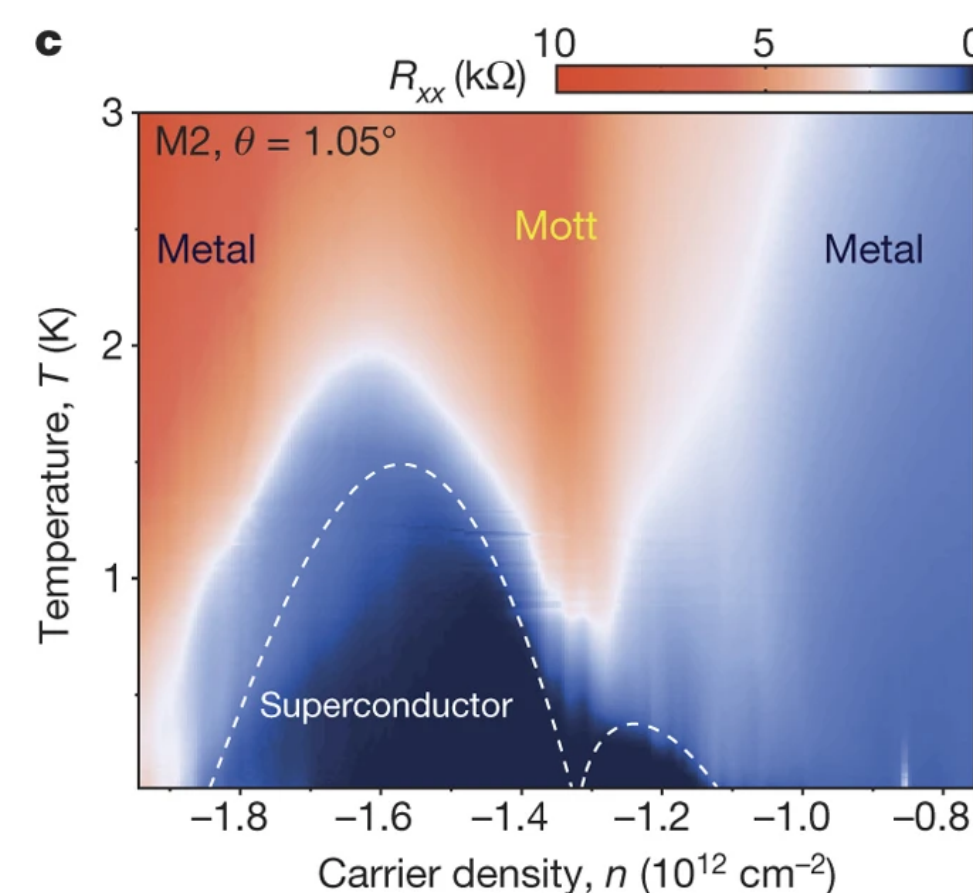
Yao ... Jarillo-Herrero, Nature (2018)



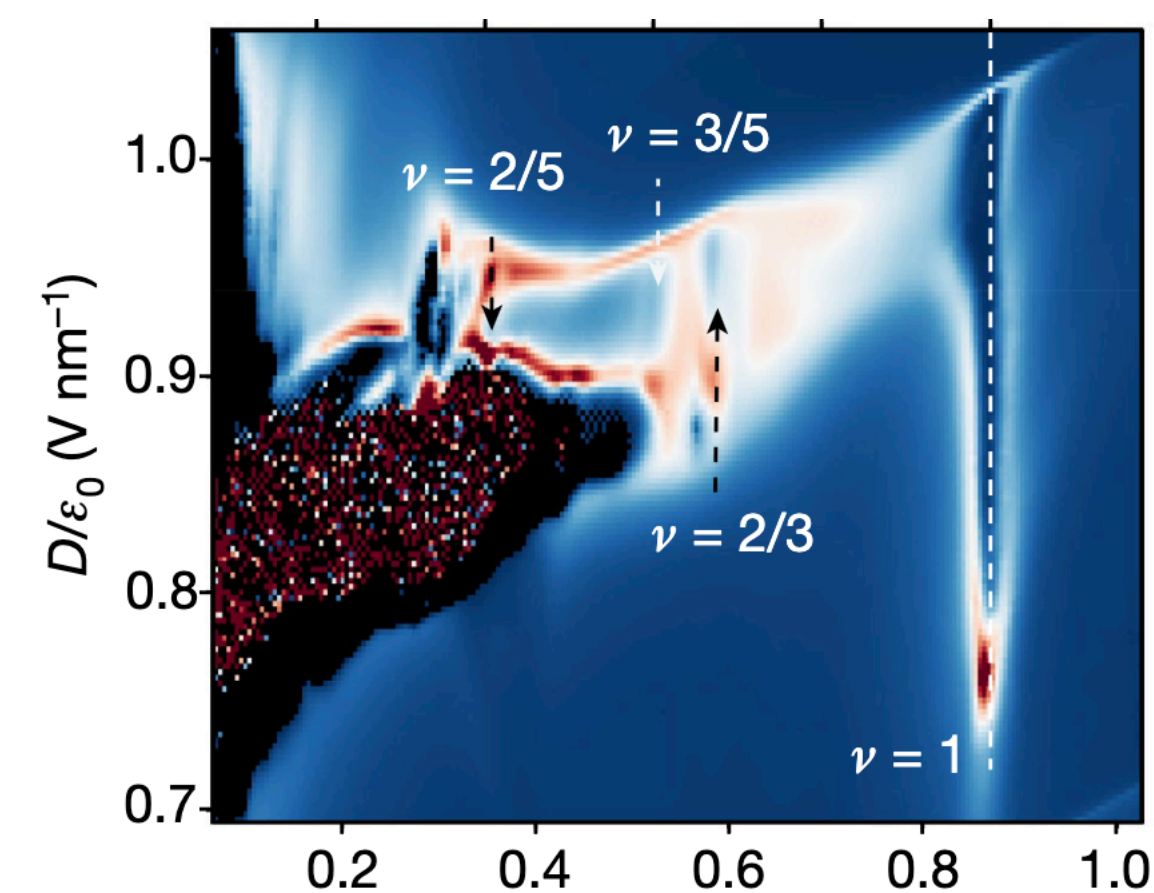
A few volts $\sim 1e/\text{moiré unit cell}$

Yankowitz ... Dean, Science (2019)

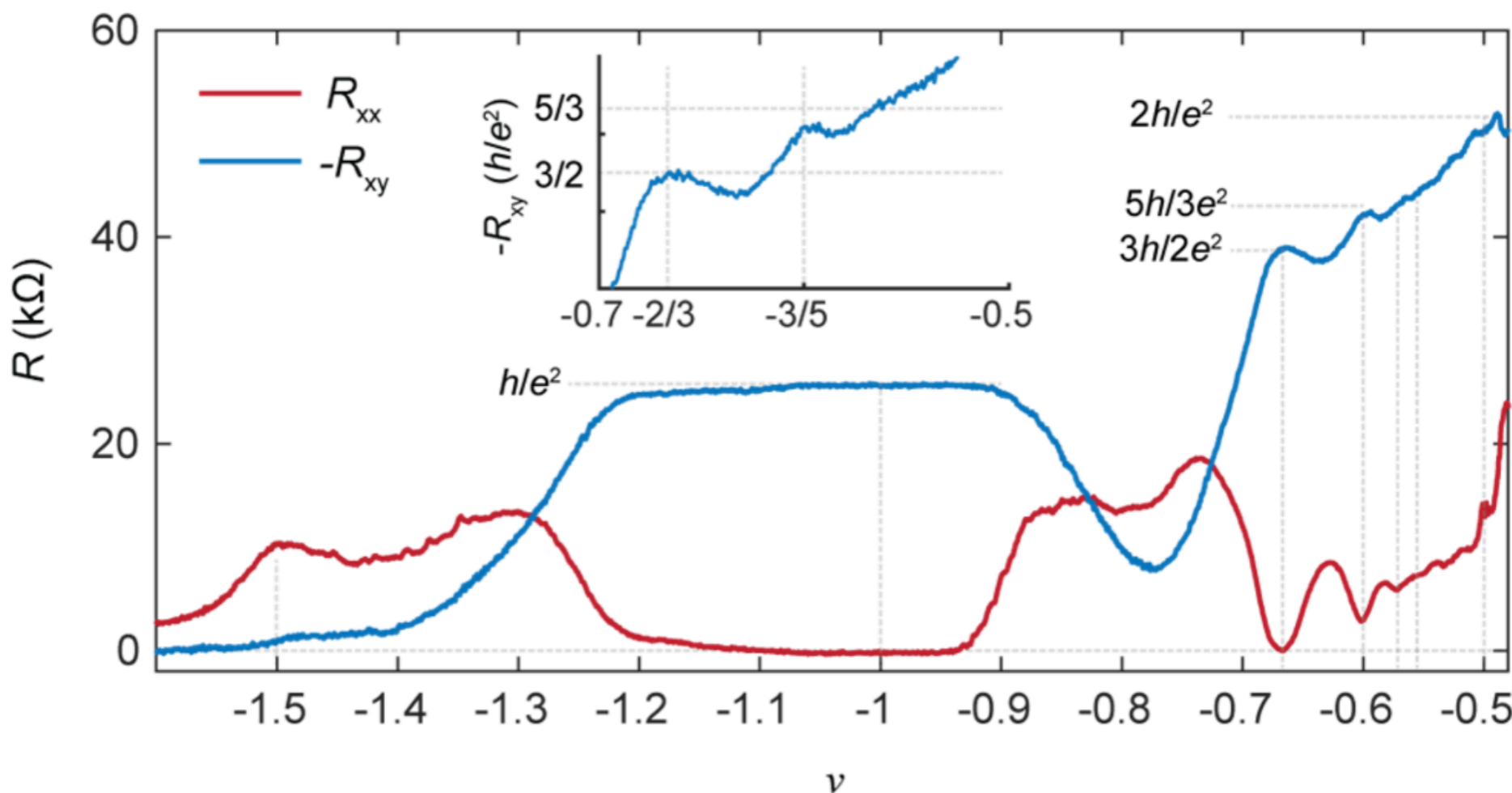
The achievements of van der Waals heterostructures



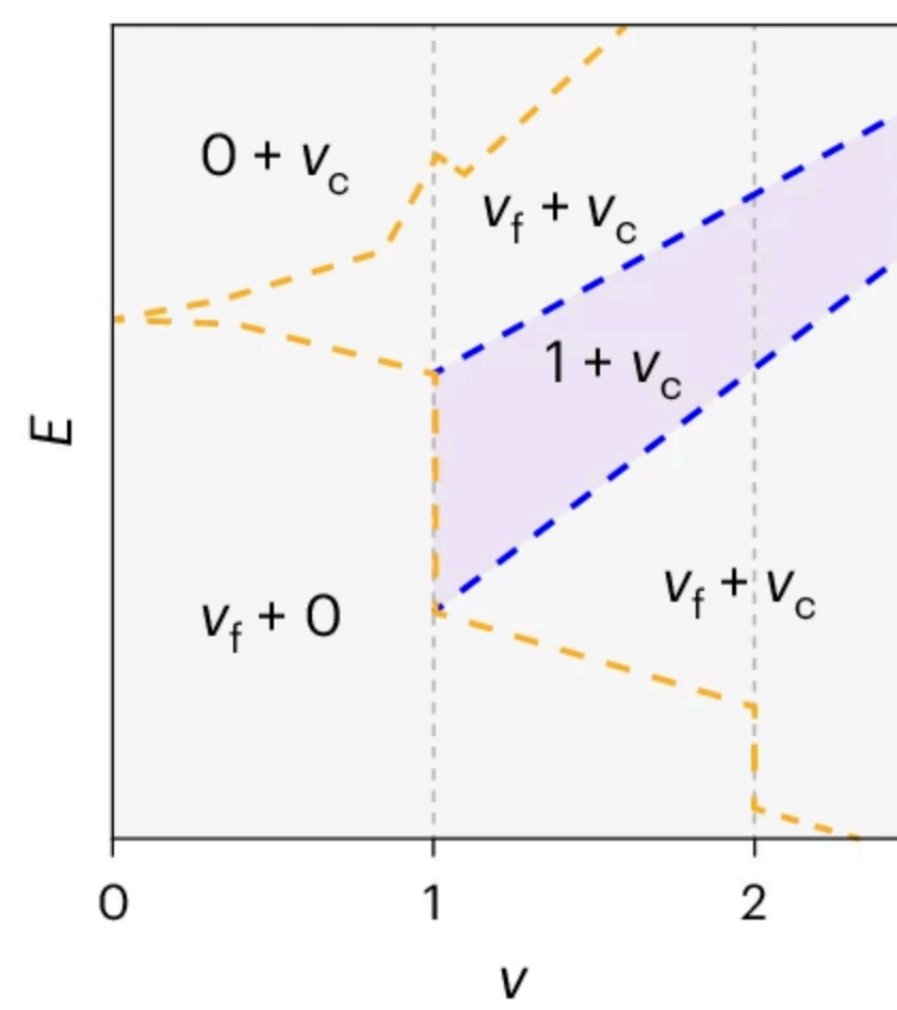
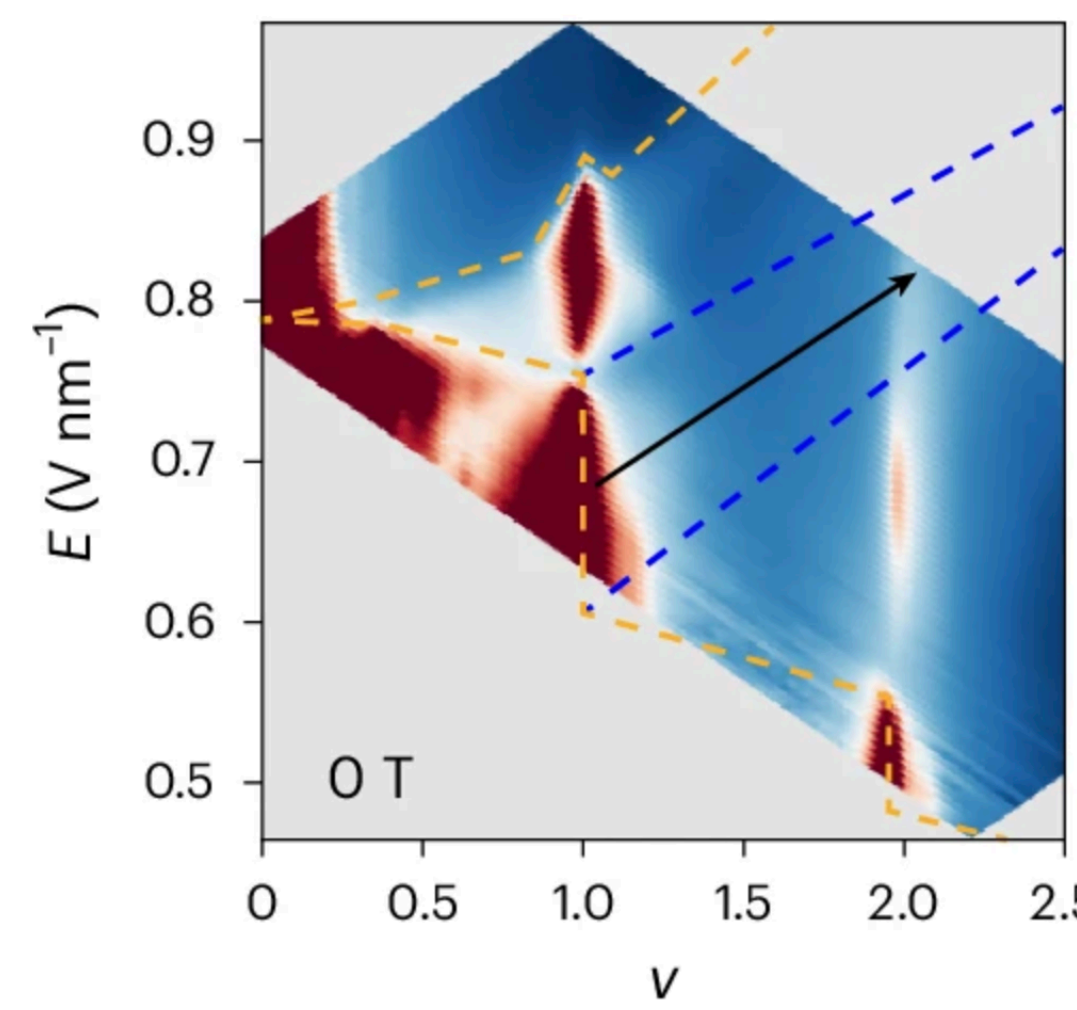
Yao ... Jarillo-Herrero, Nature (2018)



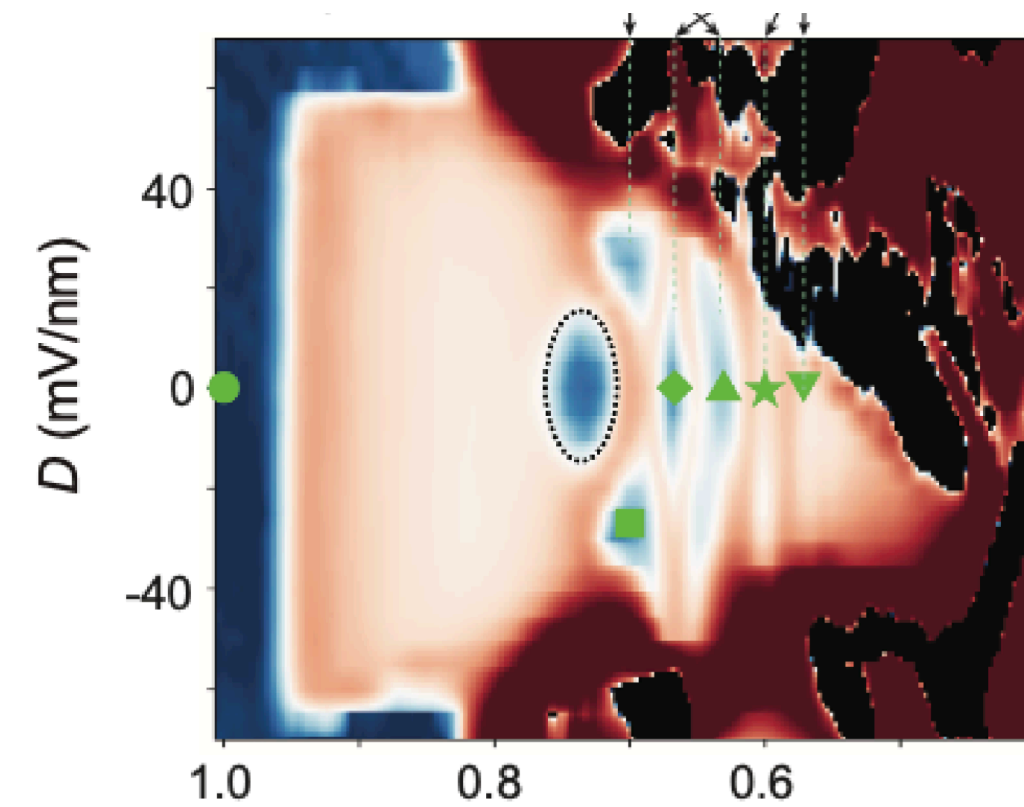
Lu ... Ju, Nature (2024)



Park ... Xu, arXiv:2503.10989



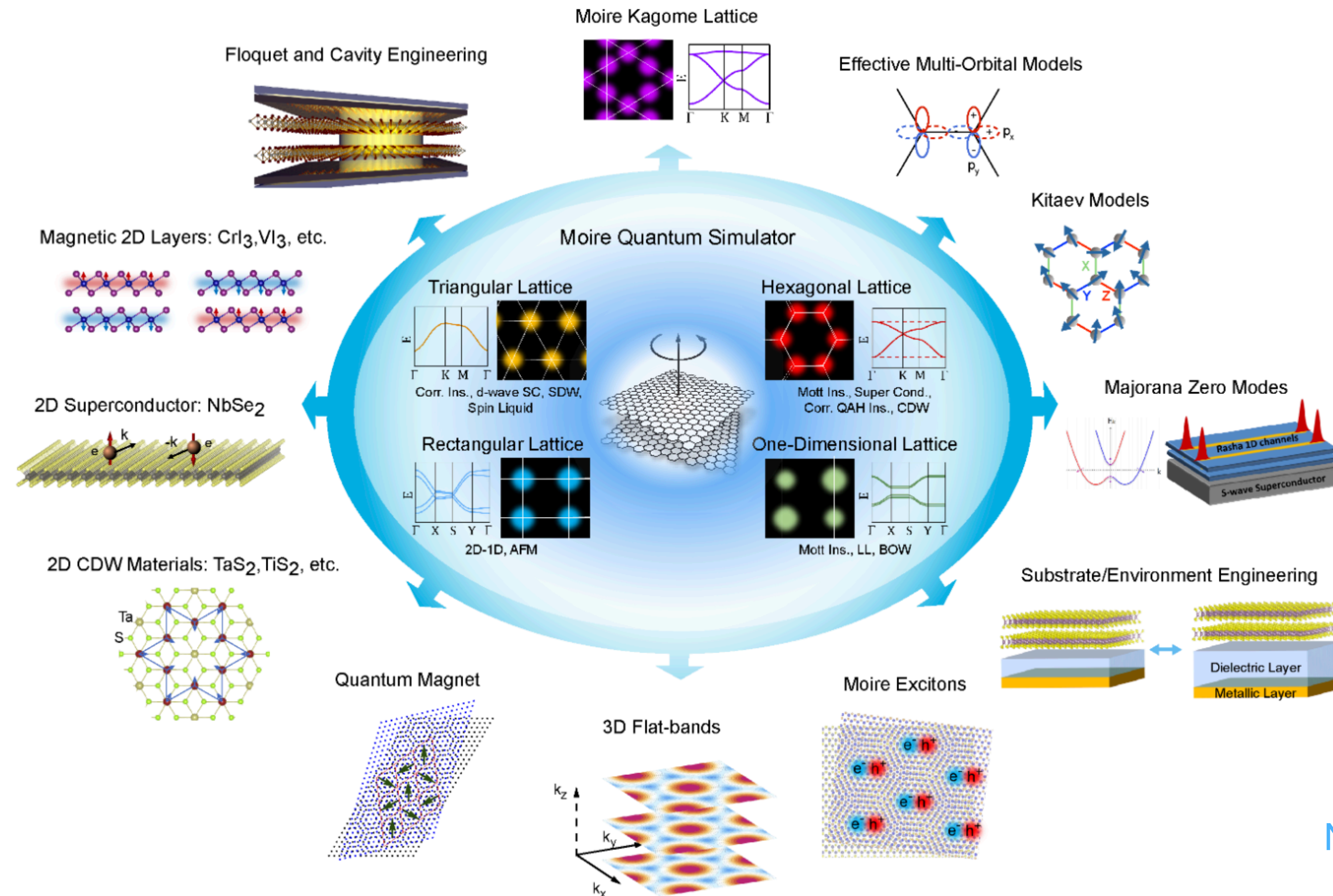
Han ... Shan&Mak, Nature (2026)



Xu ... Li, arXiv:2504.06972

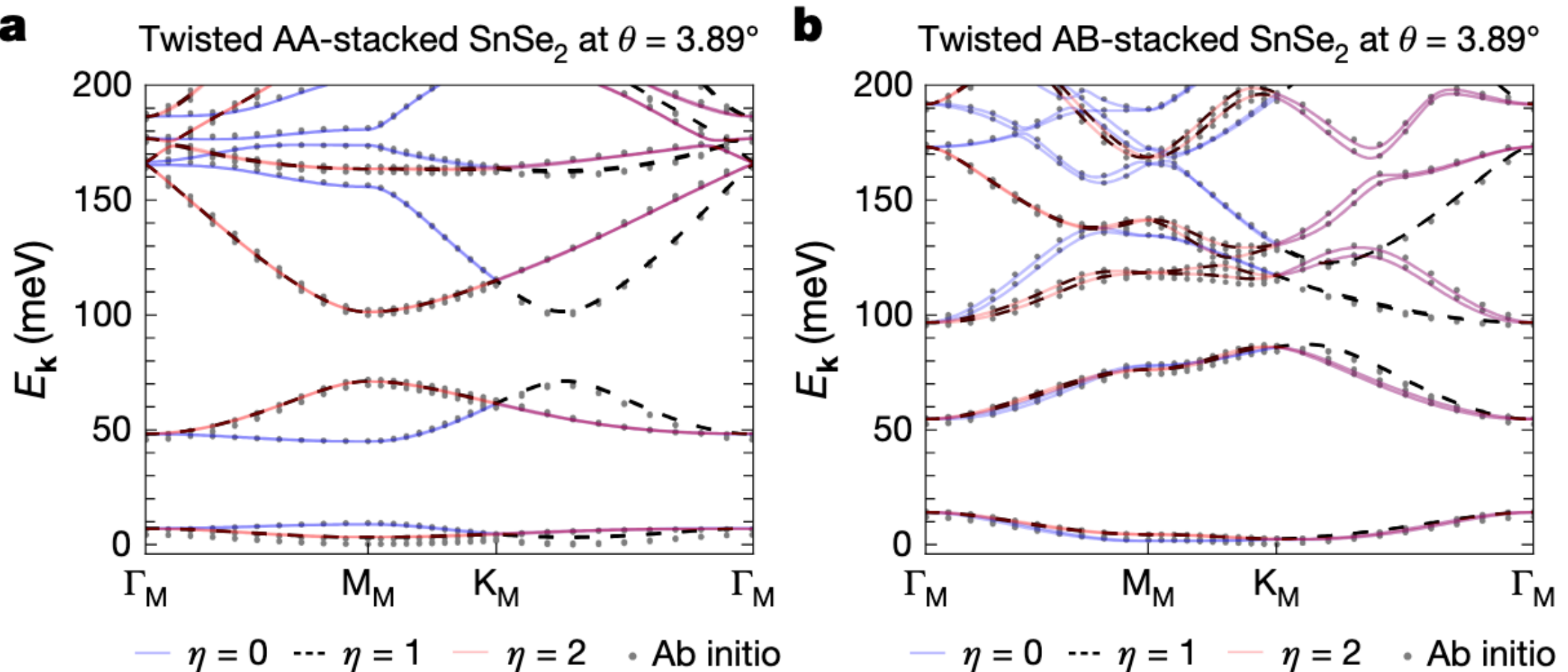
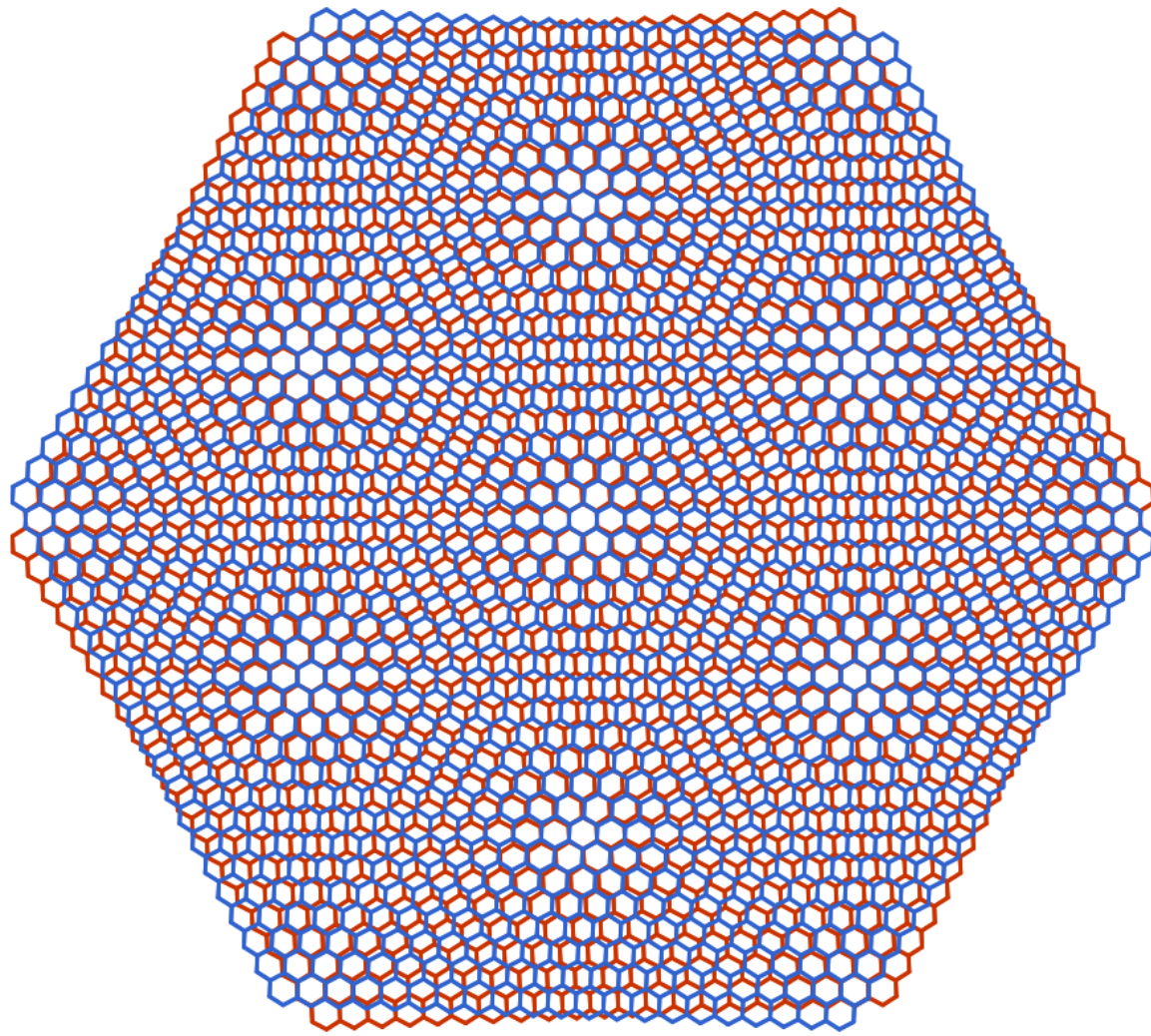
The achievements of van der Waals heterostructures

- Build from only a few: graphene (rhombo stack, or twisted) and TMDs
- Contrast with the main promise of vdW heterostructures: countless combinations!

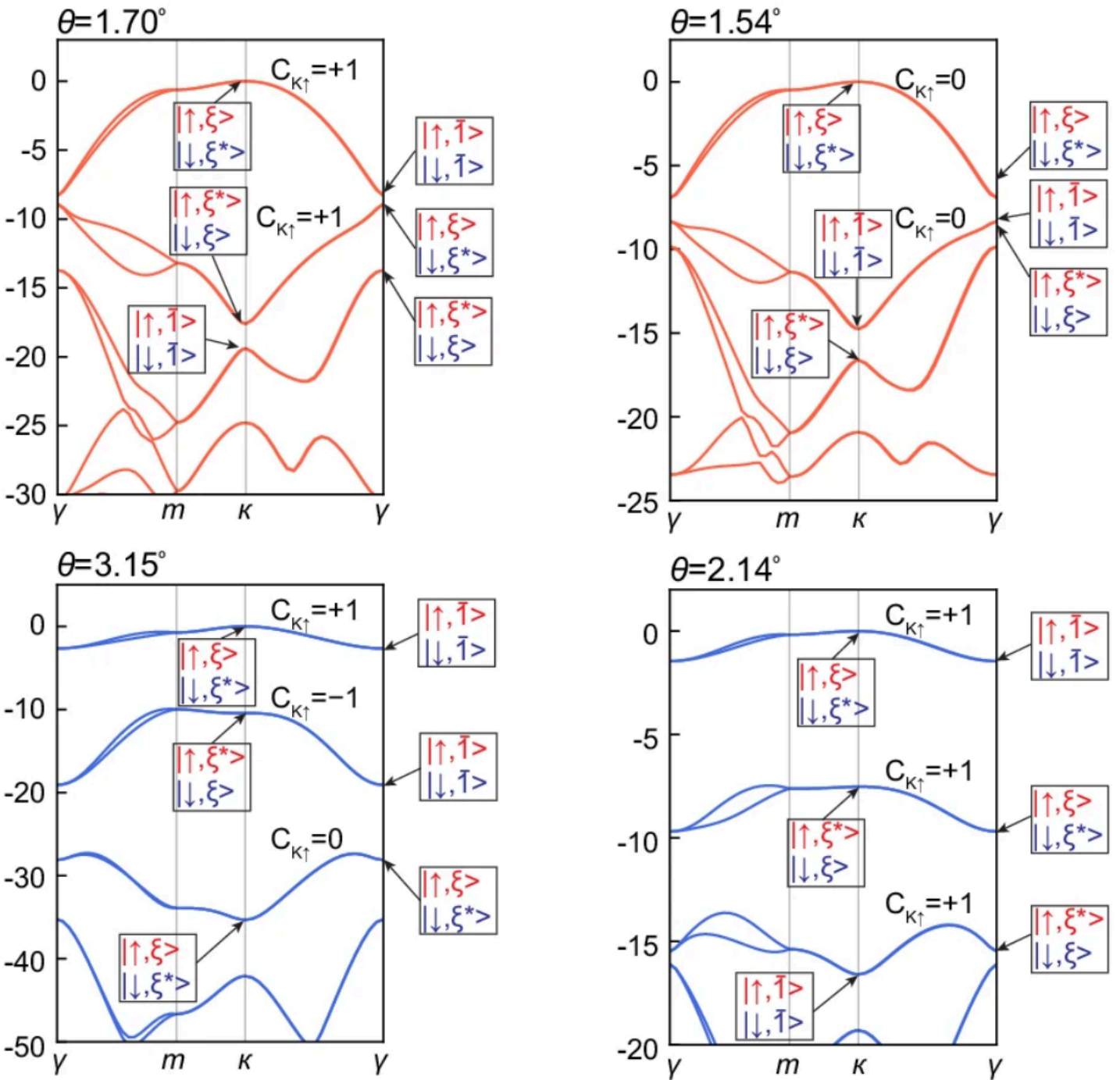


Reactive approach

- Build from only a few (graphene / TMDs): Because we exfoliate them well!
- Already rich platform, but not sure if better candidates exist!
- Hard to tell if better candidates exist (previous talk and large-scale DFT)



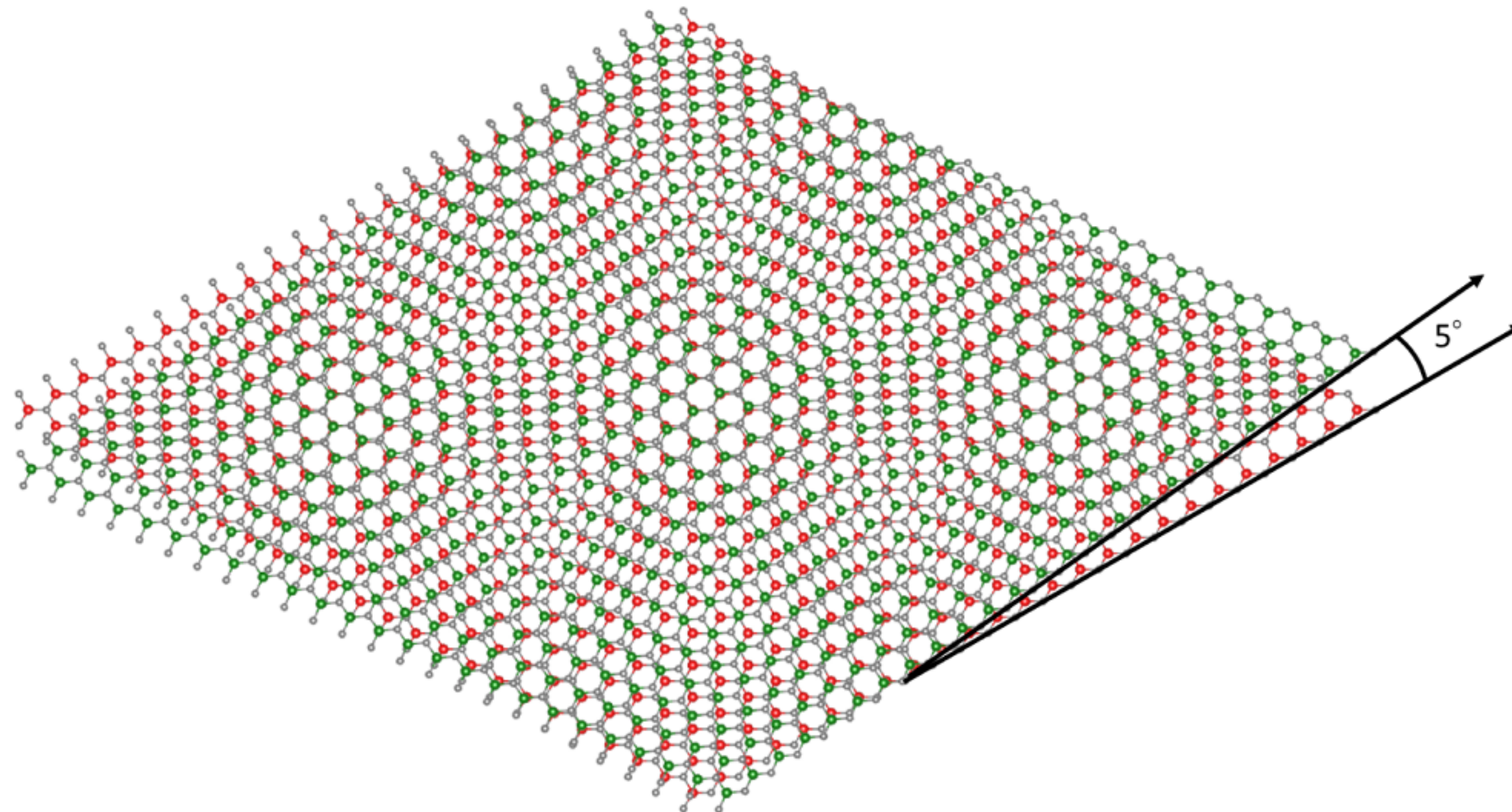
Călugăru, ..., Bernevig, Nature (2025)



Zhang, ..., Xiao, Nat Commun (2024)

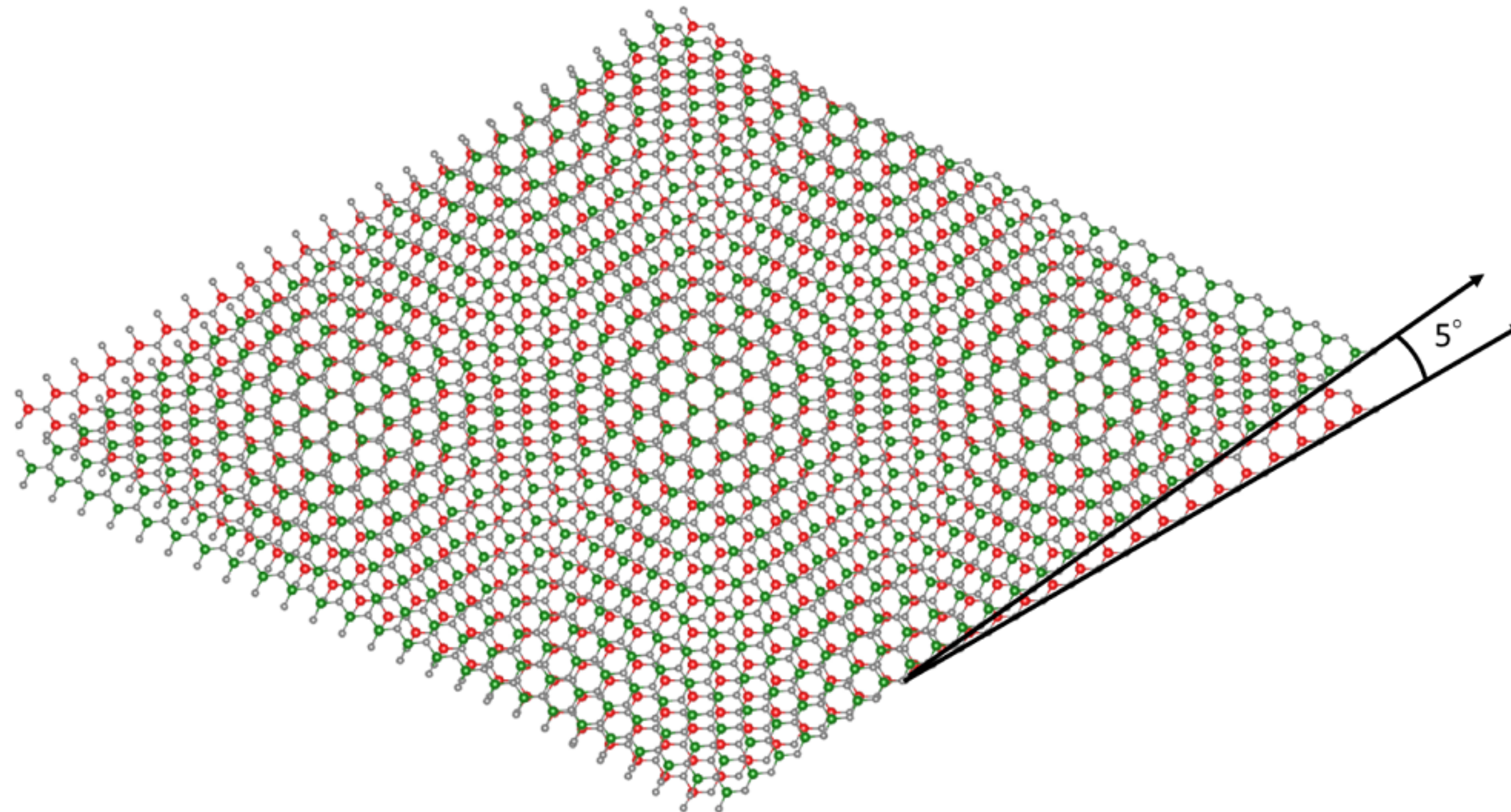
Navigating the moiré landscape

- Quantitative estimates (large-scale DFT) are difficult: value of magic angle to 0.1°
- BUT qualitative features allowing to rank all candidate materials should be simple to find
 - Moiré scale (temperature at which we resolve moire bands)
 - Topological / non-topological
- Why easy-to-compute robust qualitative features exist? Separation of scale



The perturbative limit of moiré materials

- Why easy to compute, robust qualitative features exist? Separation of scale — in the perturbative limit
- Intuitively, $a_m \gg a$ for twists $\lesssim 6^\circ$ should be enough (?) for atomic scale physics to be integrated out
- In practice, need both length scale separation AND energy scale separation

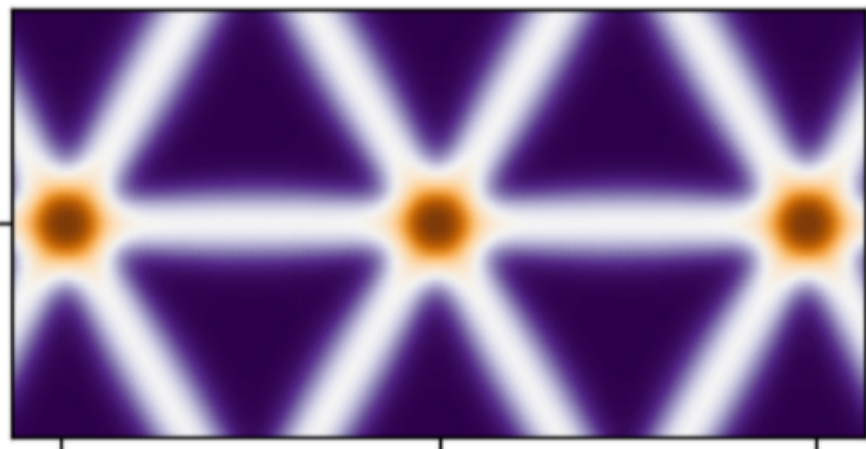


The perturbative limit of moiré materials: relaxation

Carr, ..., Luskin, Kaxiras, PRB (2018)

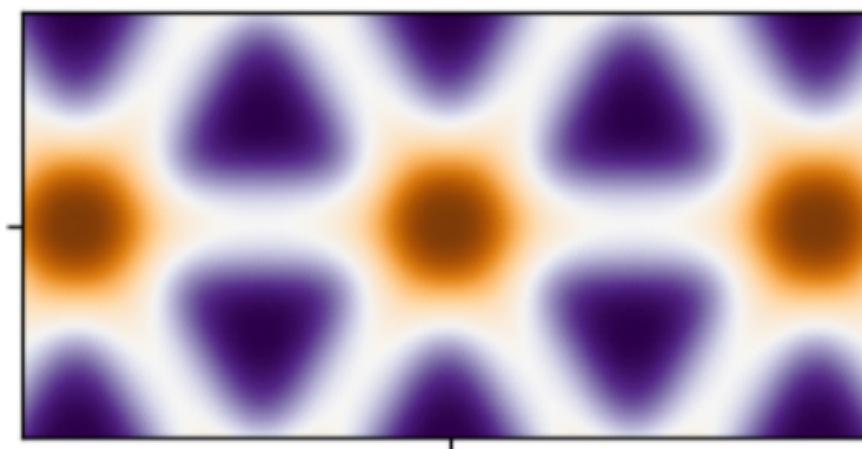
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Relaxed

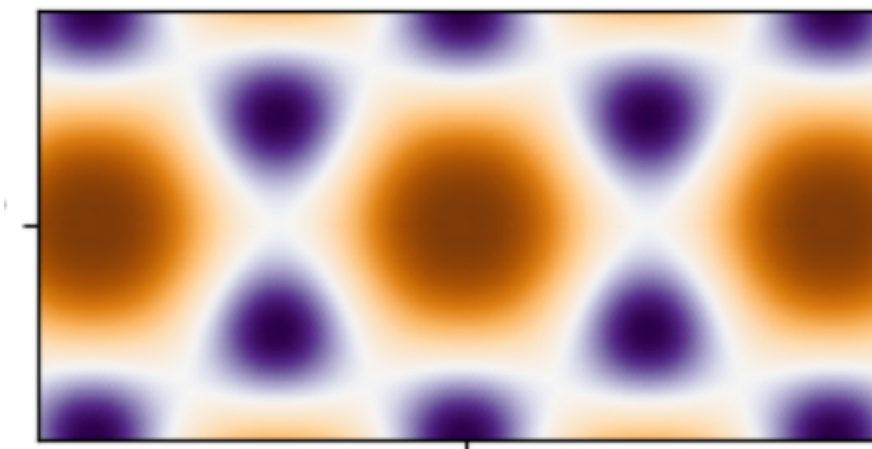


Local atomic arrangement matters
= lattice scale energetics rules
moiré physics

Crossover



Rigid



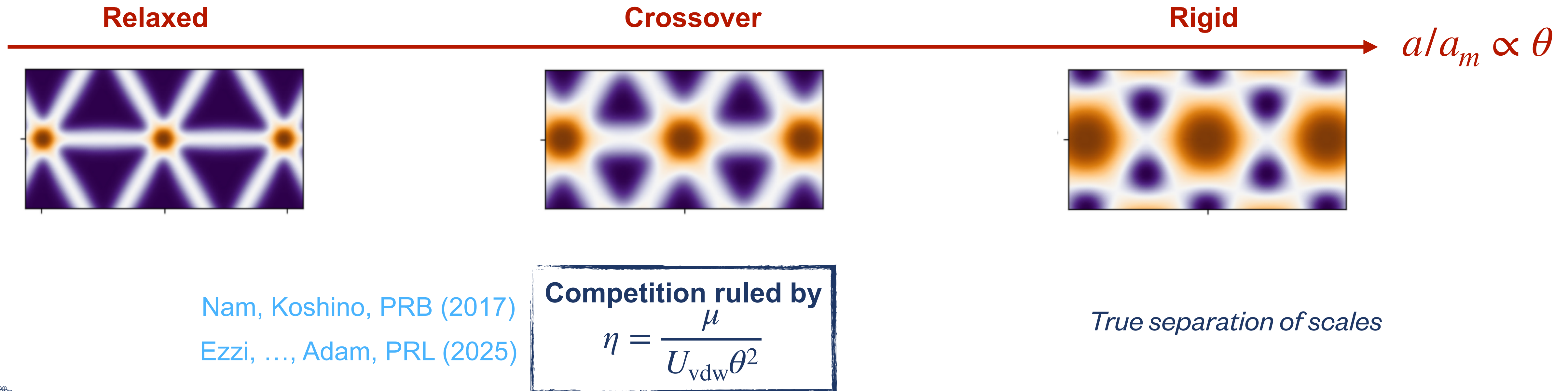
Local atomic arrangement does not matter
= low energy determined entirely by moiré
True separation of scales

$$a/a_m \propto \theta$$

The perturbative limit of moiré materials: relaxation

Carr, ..., Luskin, Kaxiras, PRB (2018)

- Why easy to compute, robust qualitative features exist? Separation of scale — in the perturbative limit
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The perturbative limit of moiré materials: kinetic

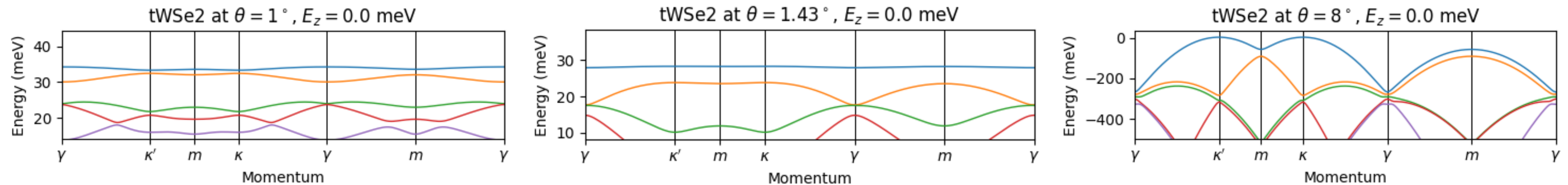
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Deep moiré

Crossover (magic)

Plane-waves

$$a/a_m \propto \theta$$



Devakul, ..., Fu, Nat. Commun. (2023)

The perturbative limit of moiré materials: kinetic

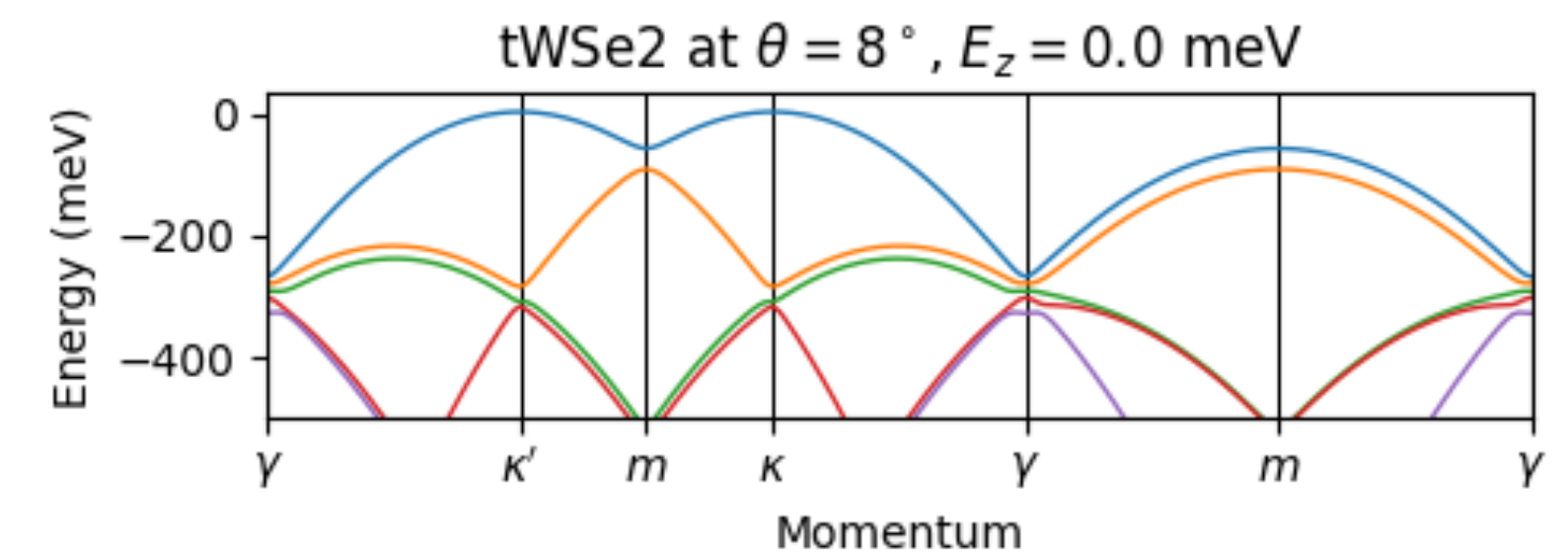
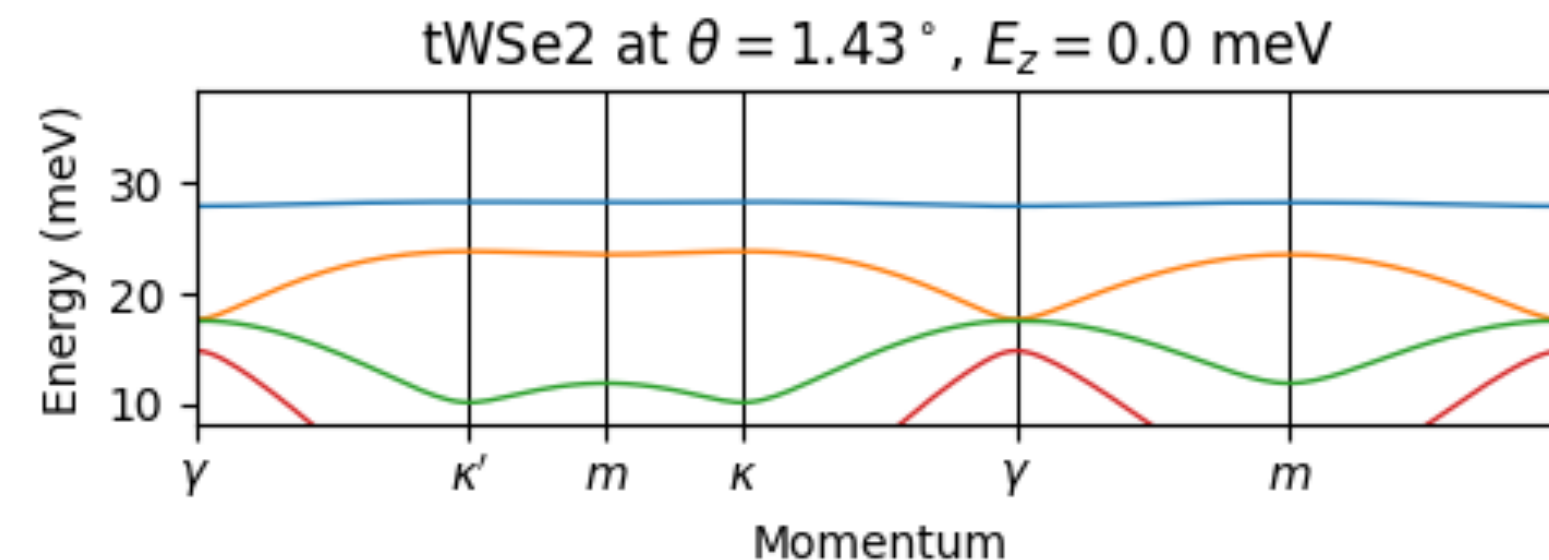
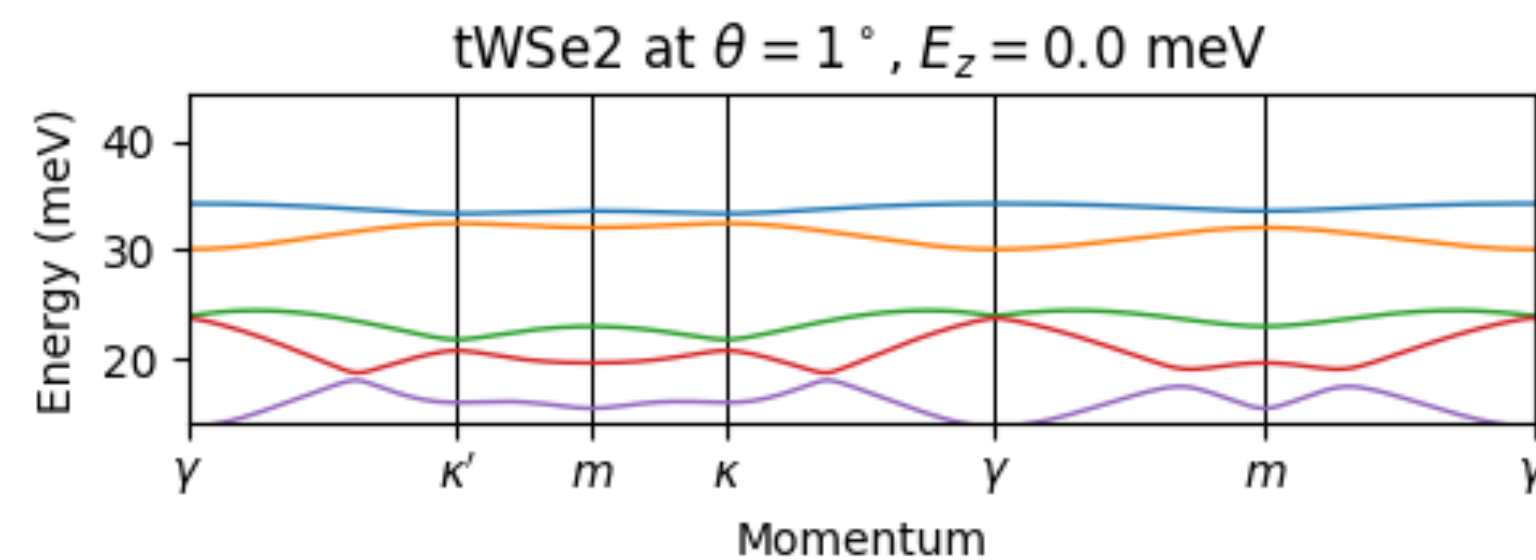
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Devakul, ..., Fu, Nat. Commun. (2023)

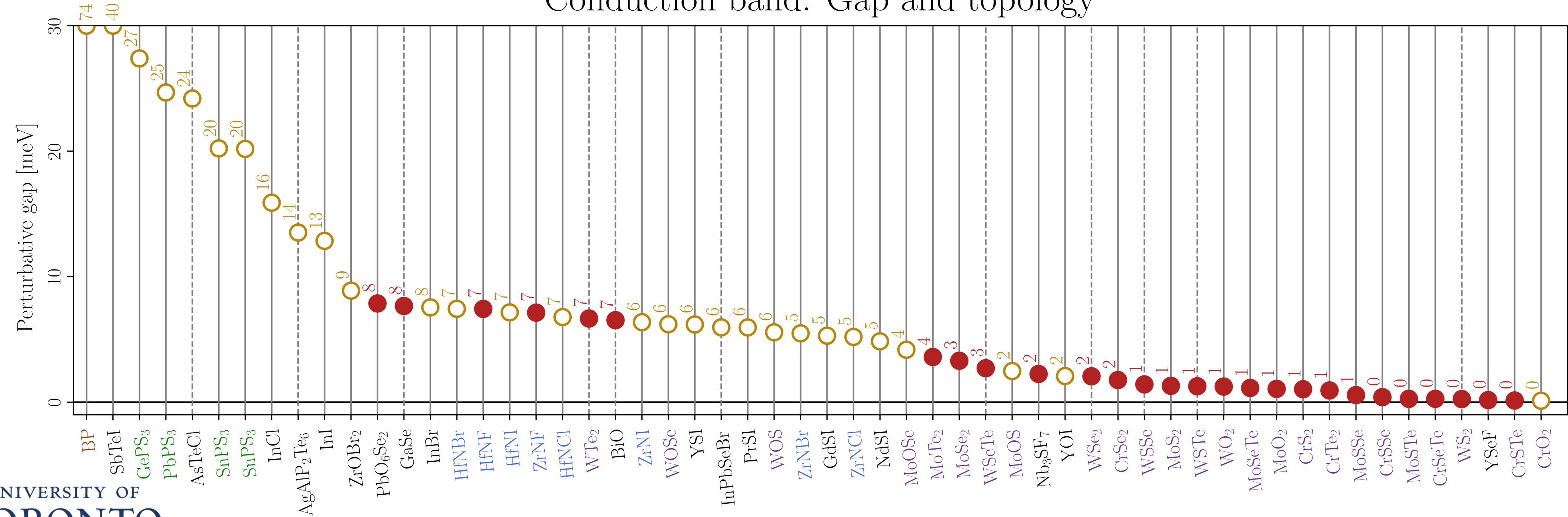
True separation of scales

Goal: Perturbative moiré limit for high-throughput discovery

- Build from only a few (graphene / TMDs): Because we exfoliate them well!
- Already rich platform, but not sure if better candidates exist!
- Hard to tell if better candidates exist (previous talk and large-scale DFT)

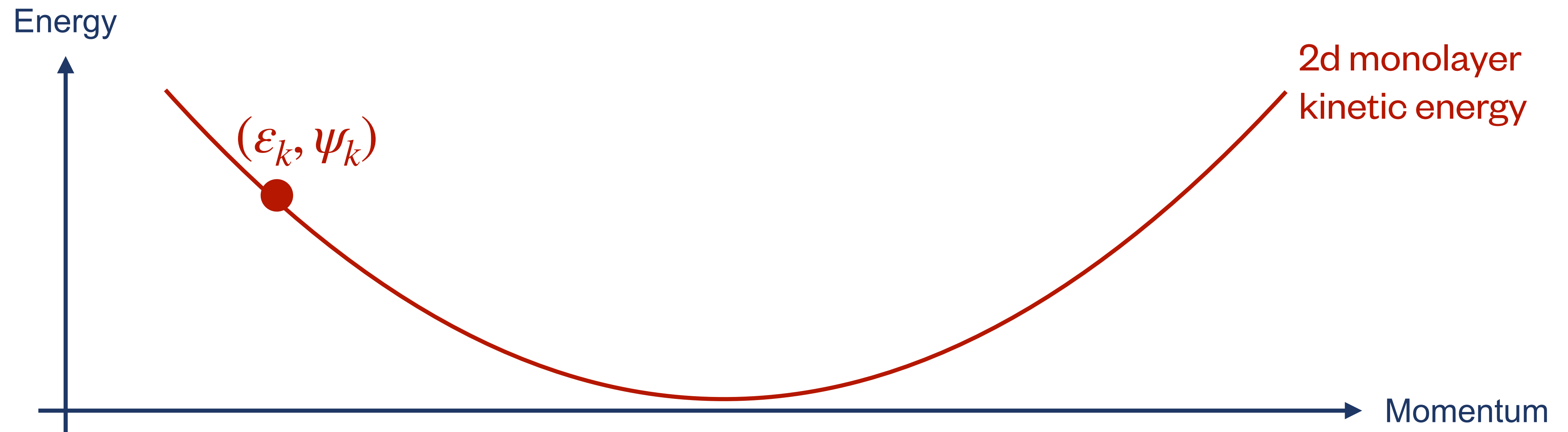
Alternative solution:
moiré perturbation theory
for qualitative but robust
features/ranking

Conduction band: Gap and topology



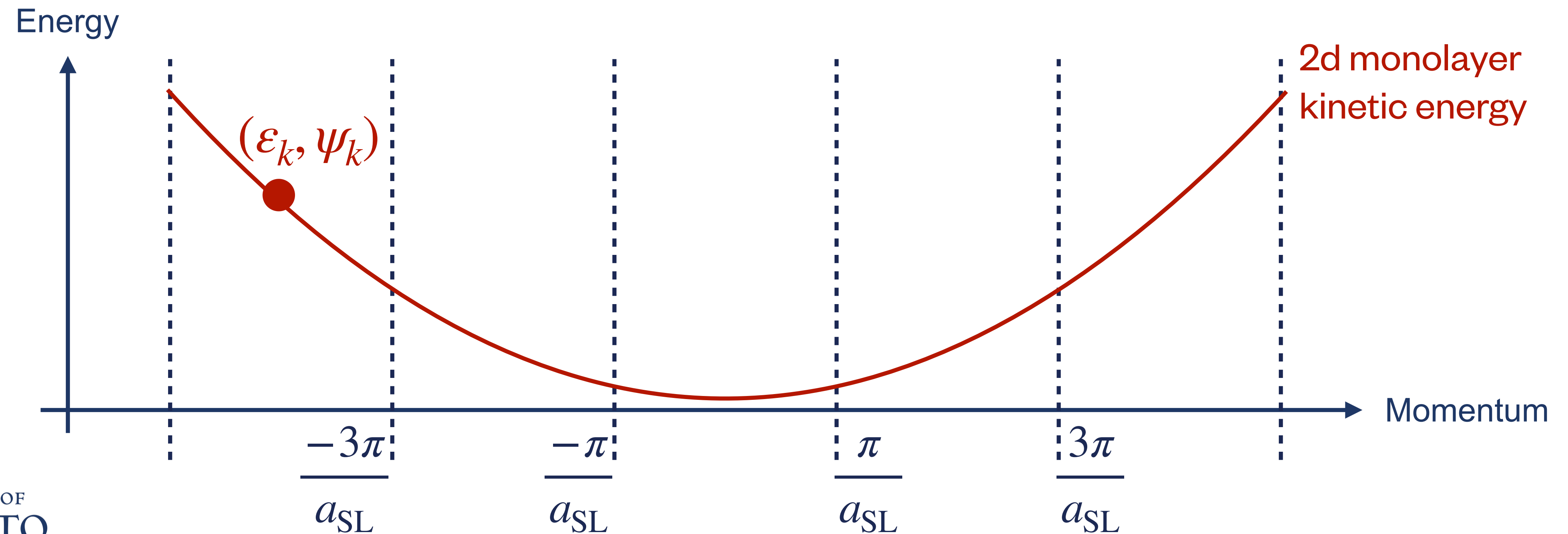
Method: Perturbative band theory

- Goal: Discard material details to extract topological invariant (universal physics)



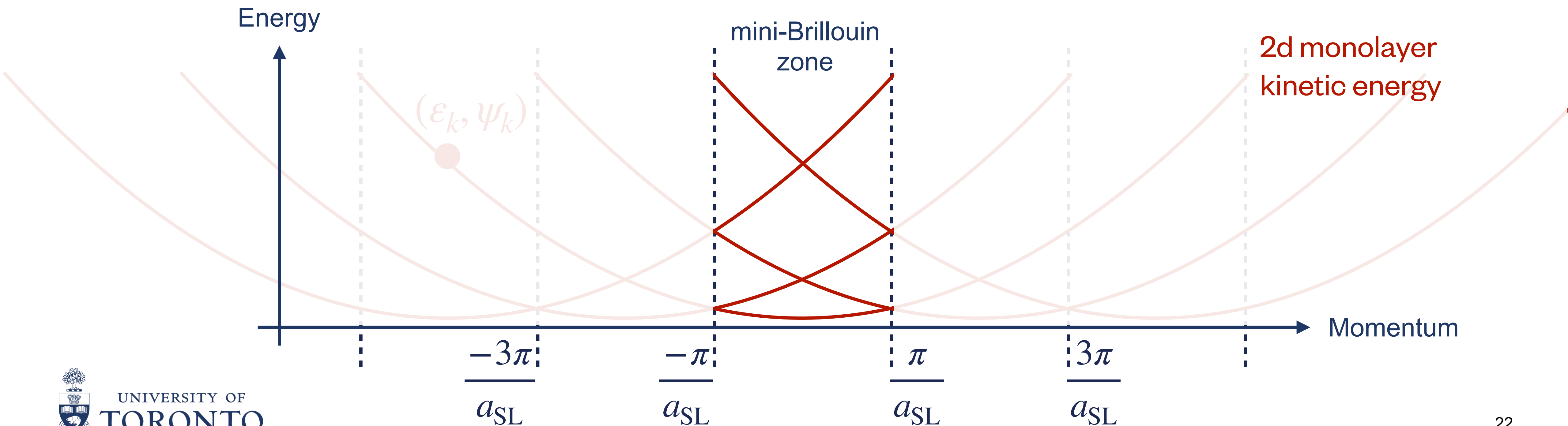
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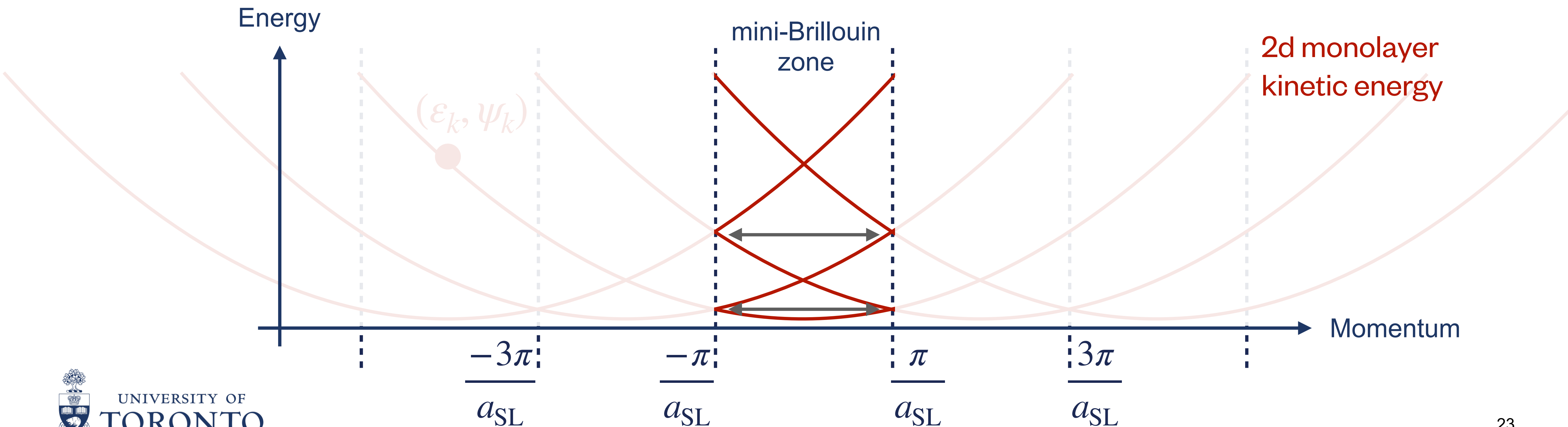
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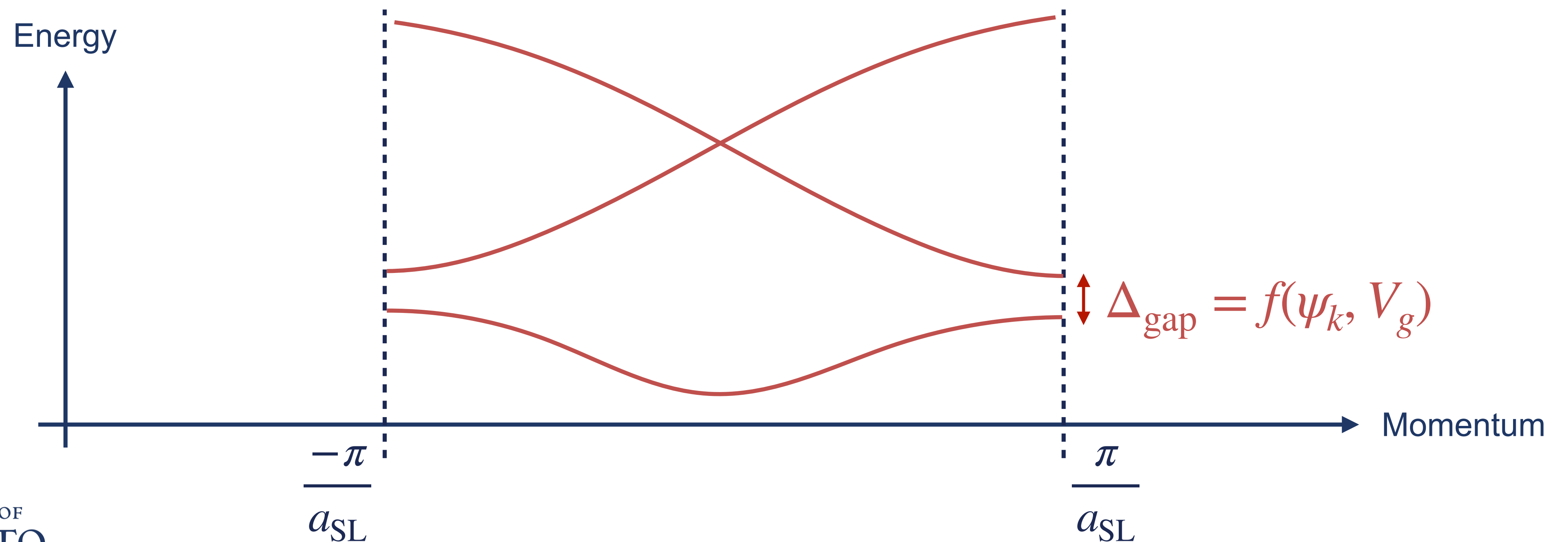
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- Step 1: Include moiré field / potential perturbatively, $V_g e^{ig \cdot r}$



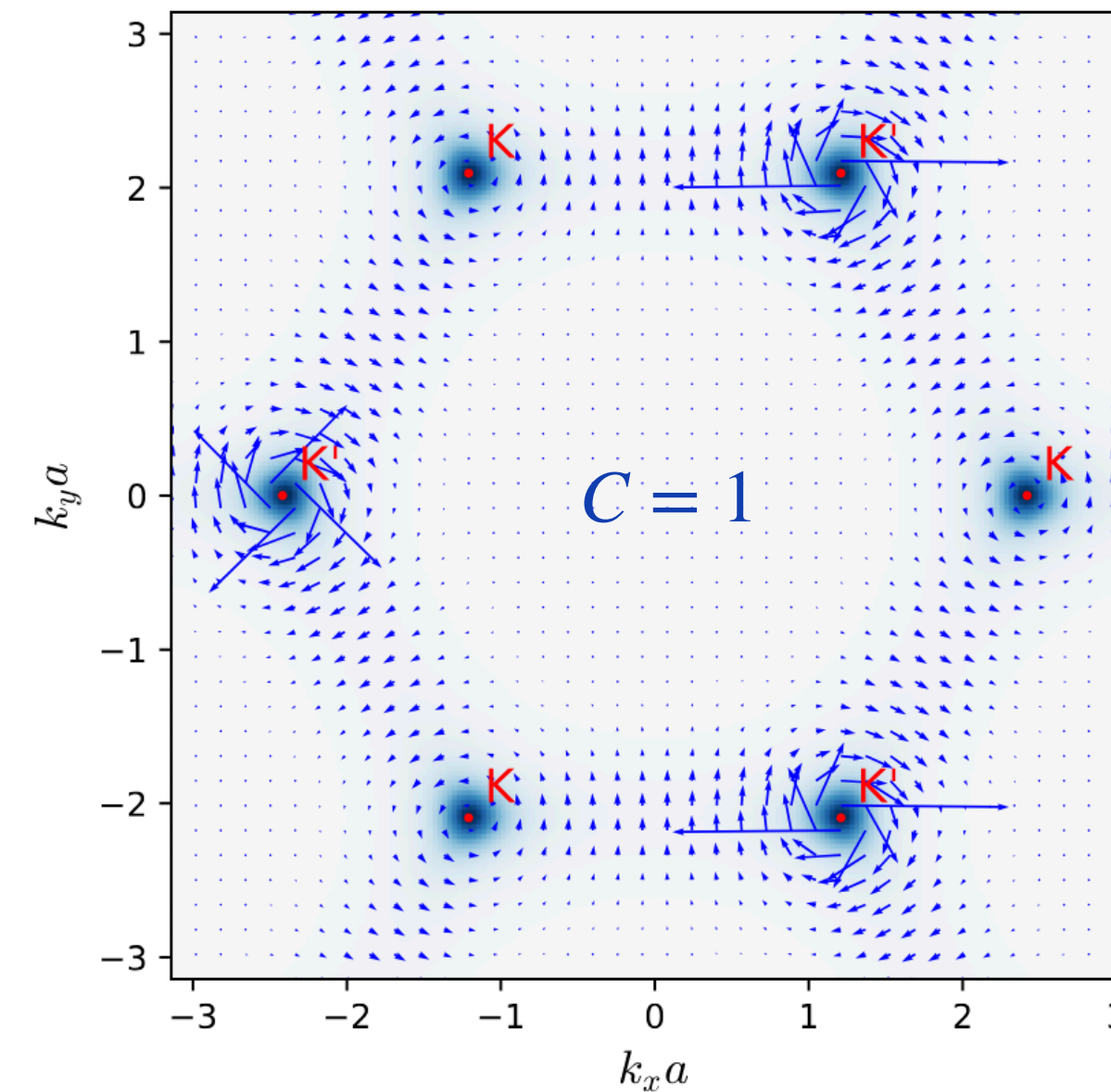
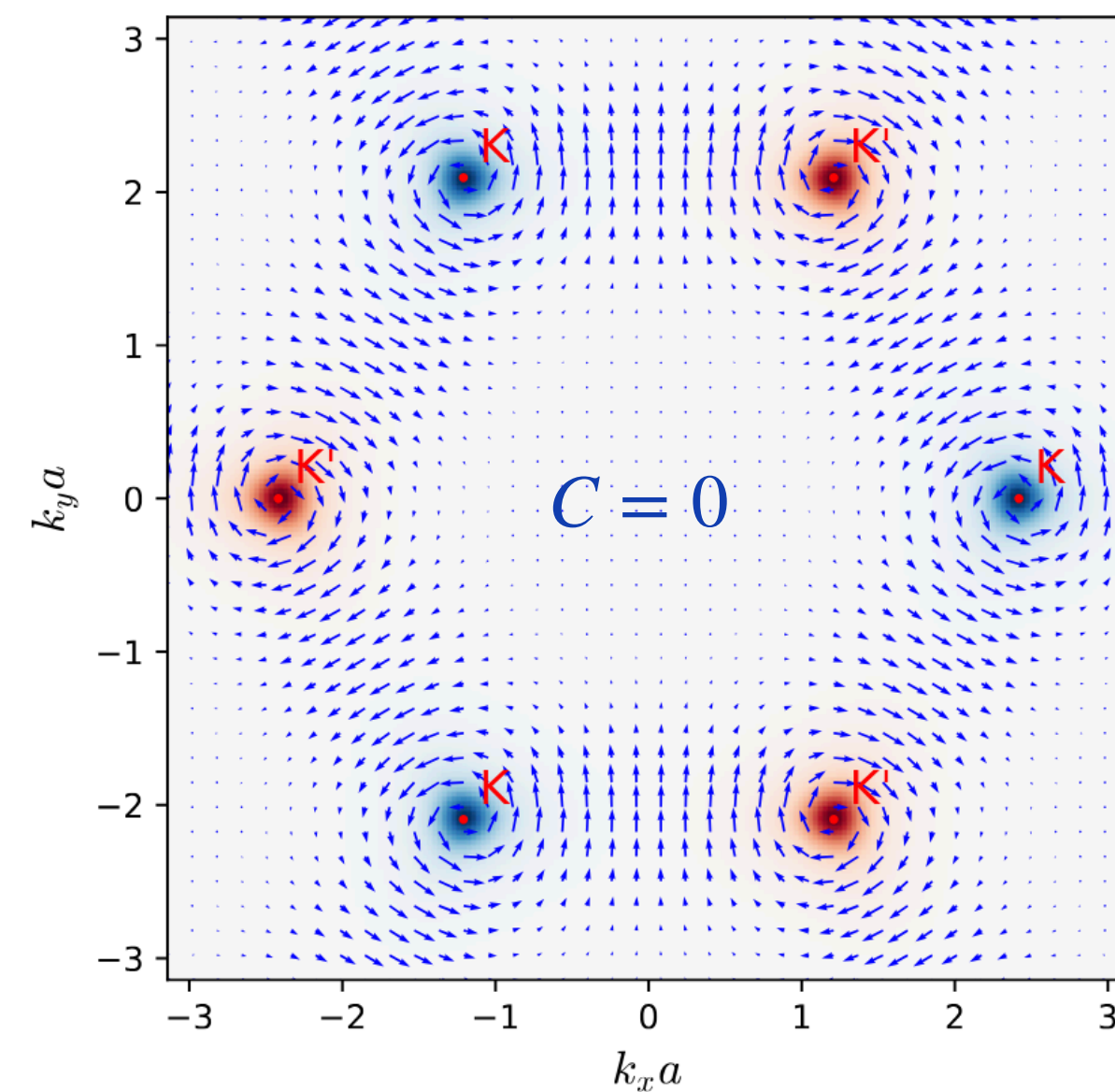
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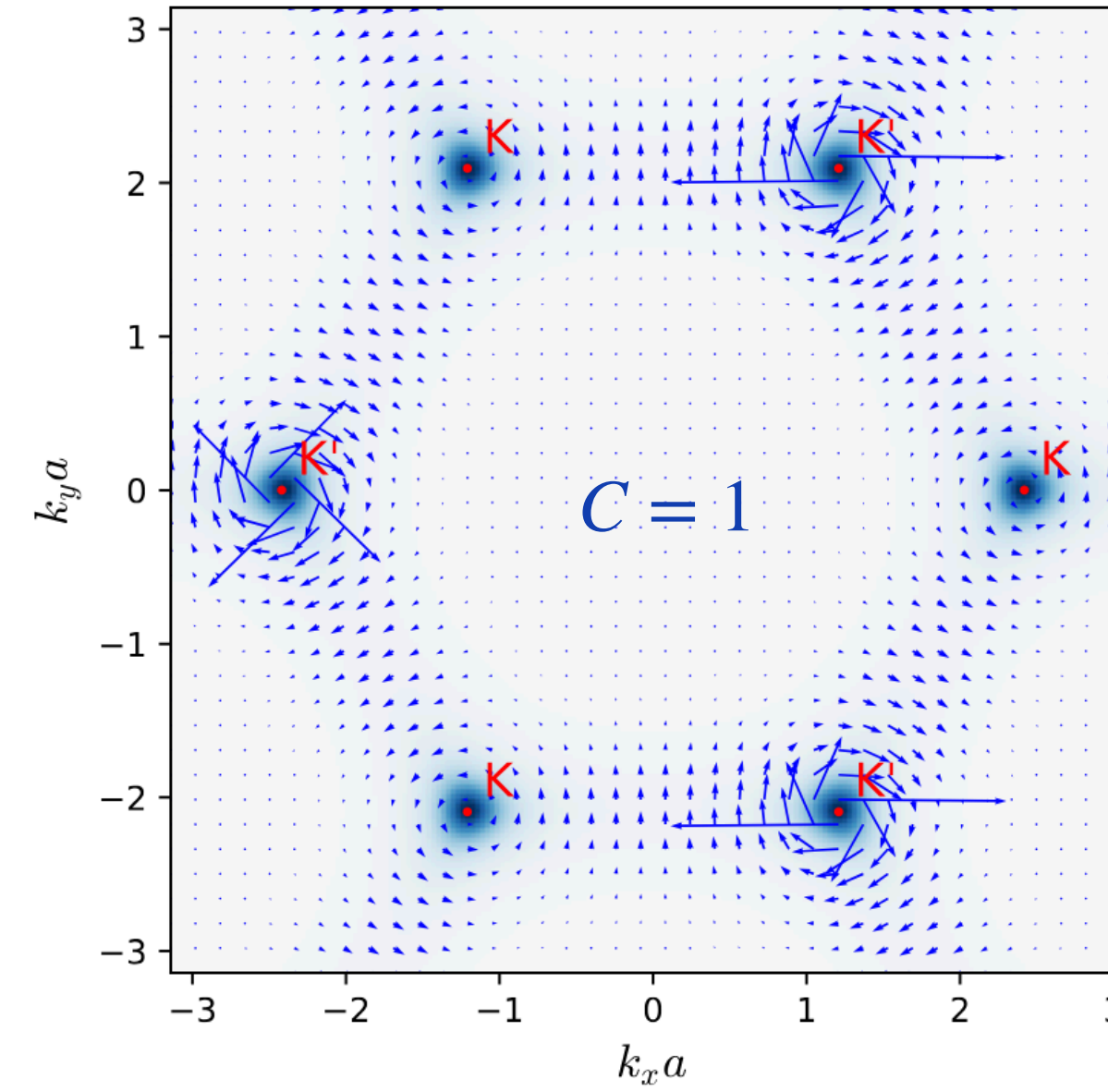
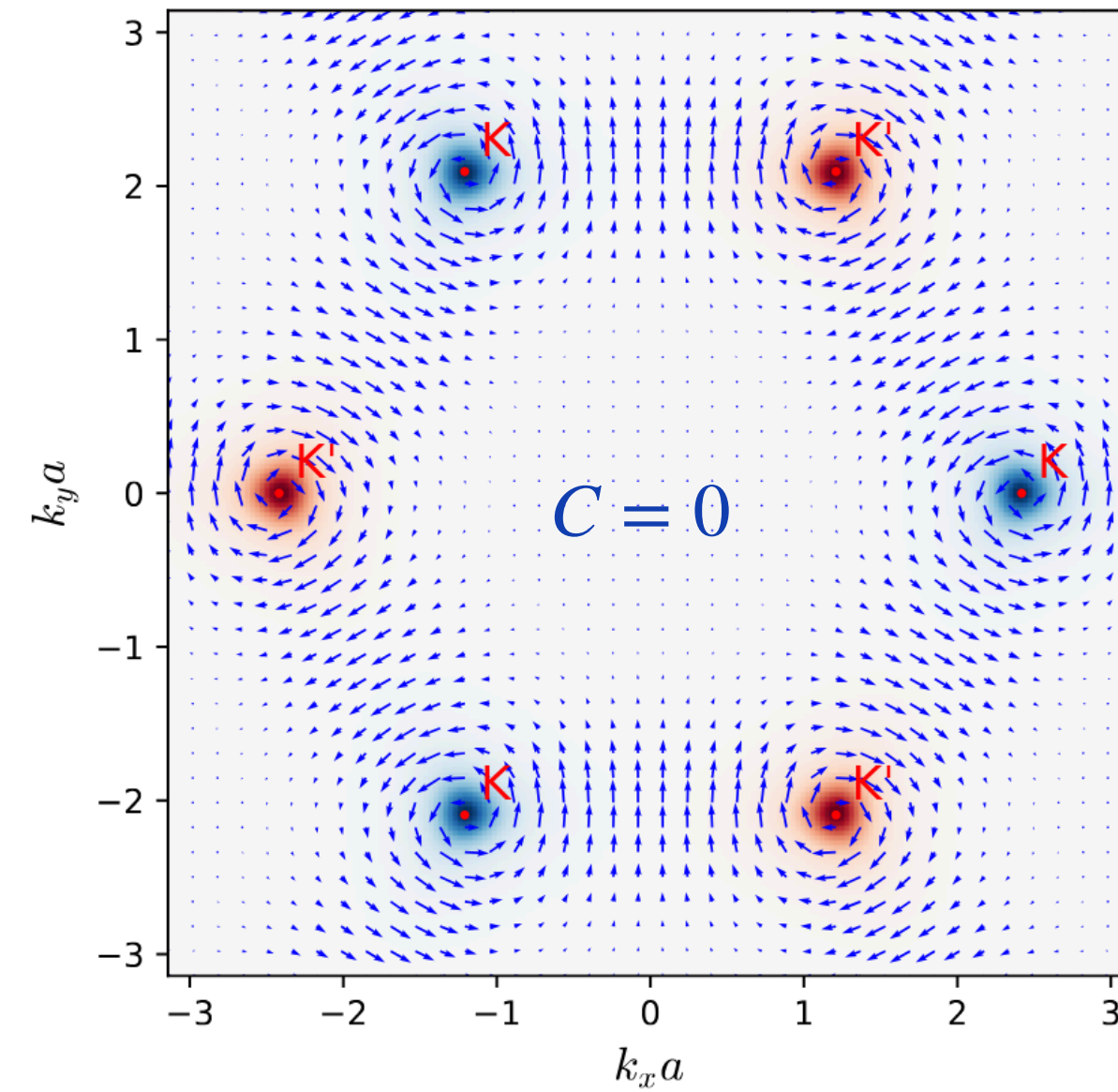


Method: Topological perturbative band theory

- Goal: Discard material details to extract topological invariant (universal physics)
- Step 1: Include moiré field / potential perturbatively, $V_g e^{ig \cdot r}$
- Step 2: Use symmetries to extract invariants from a gap opening points

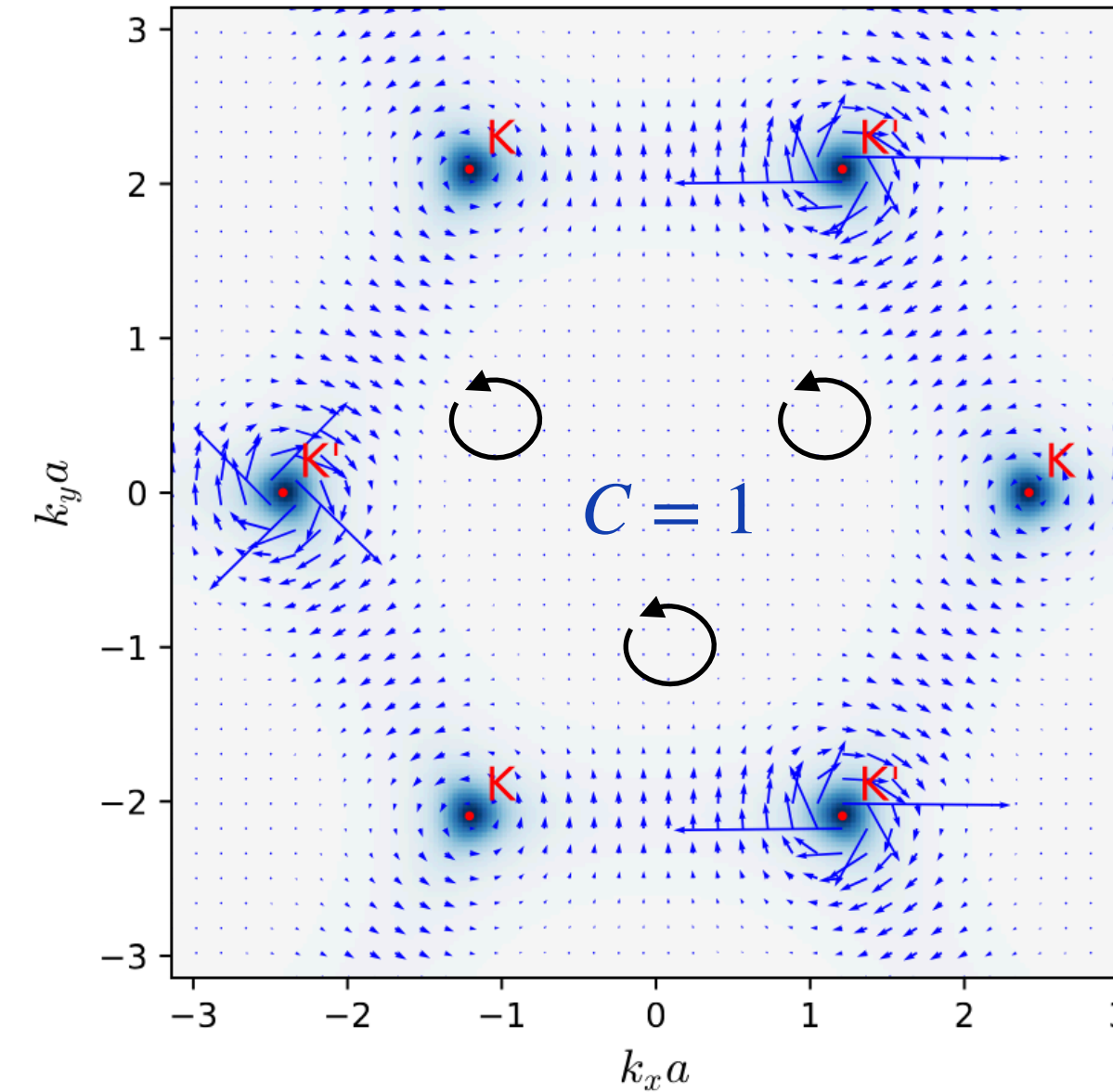
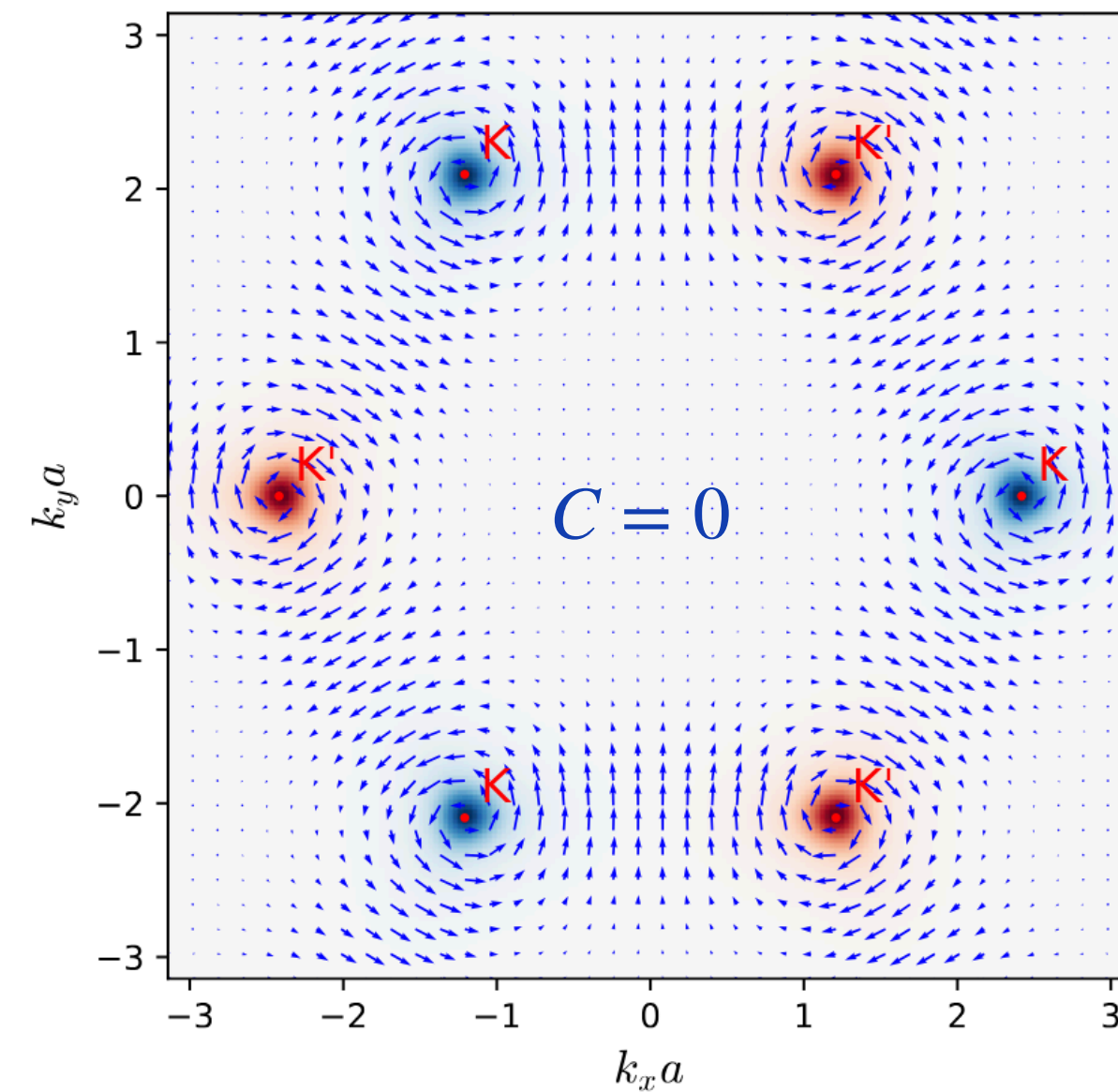


Method: Topological perturbative band theory



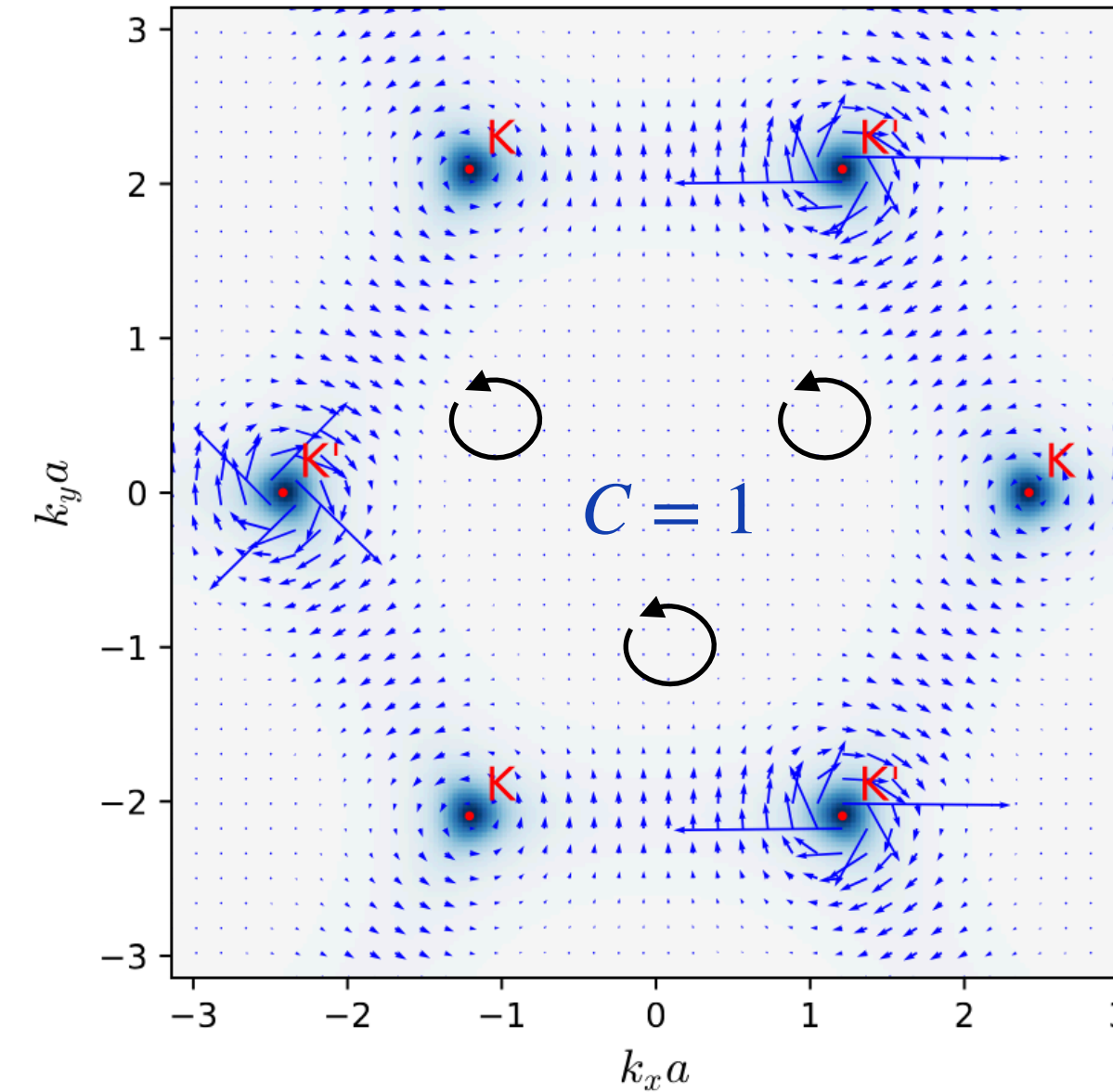
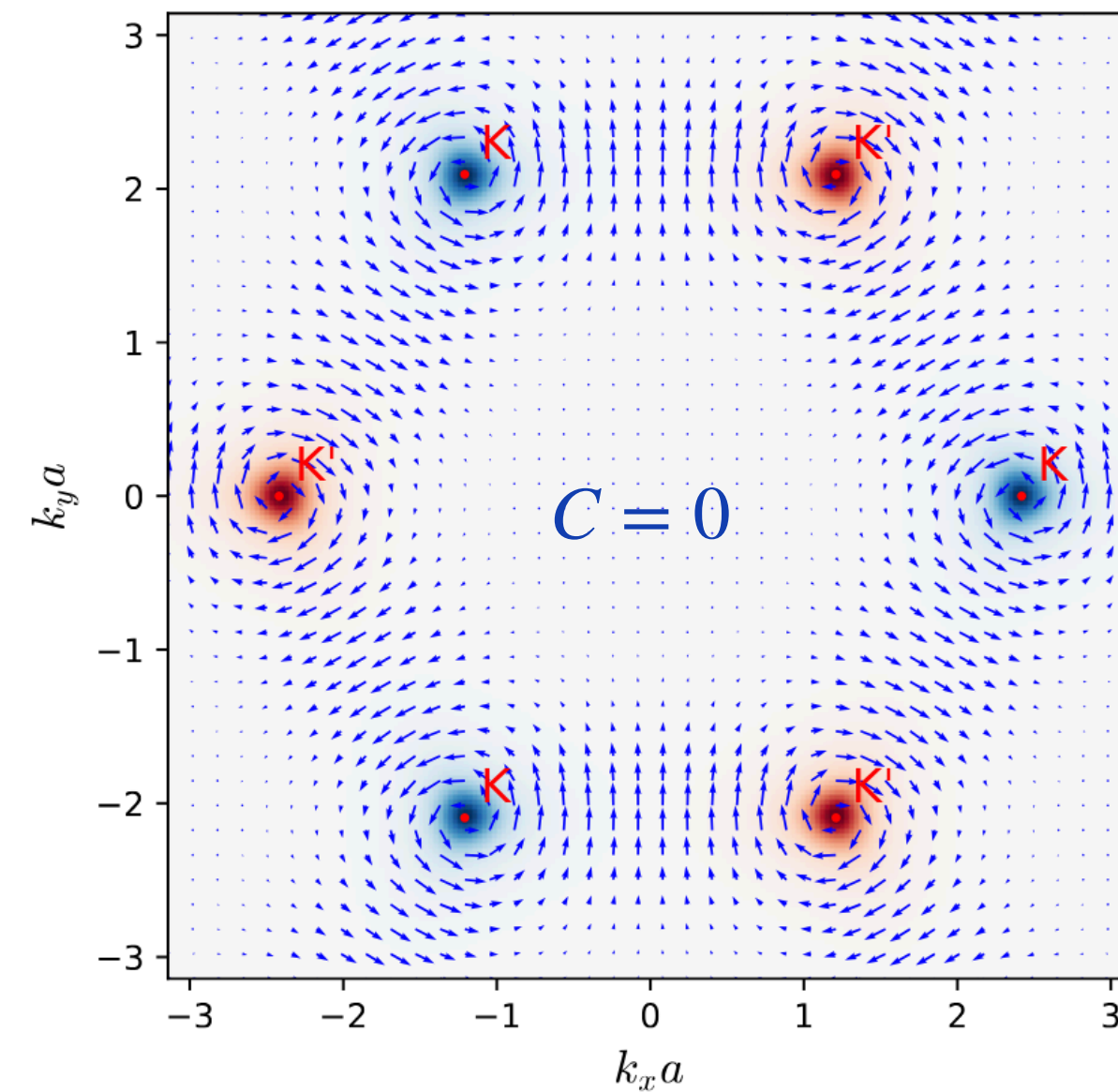
- Chern number = integrated Berry flux = counting vortices of Berry connection with multiplicity

Method: Topological perturbative band theory



- Chern number = integrated Berry flux = counting vortices of Berry connection with multiplicity
- If C3-symmetry: if a vortex arise at random point, appears 3 times: no contribution to Chern number modulo 3
- Only high-symmetry point contribute

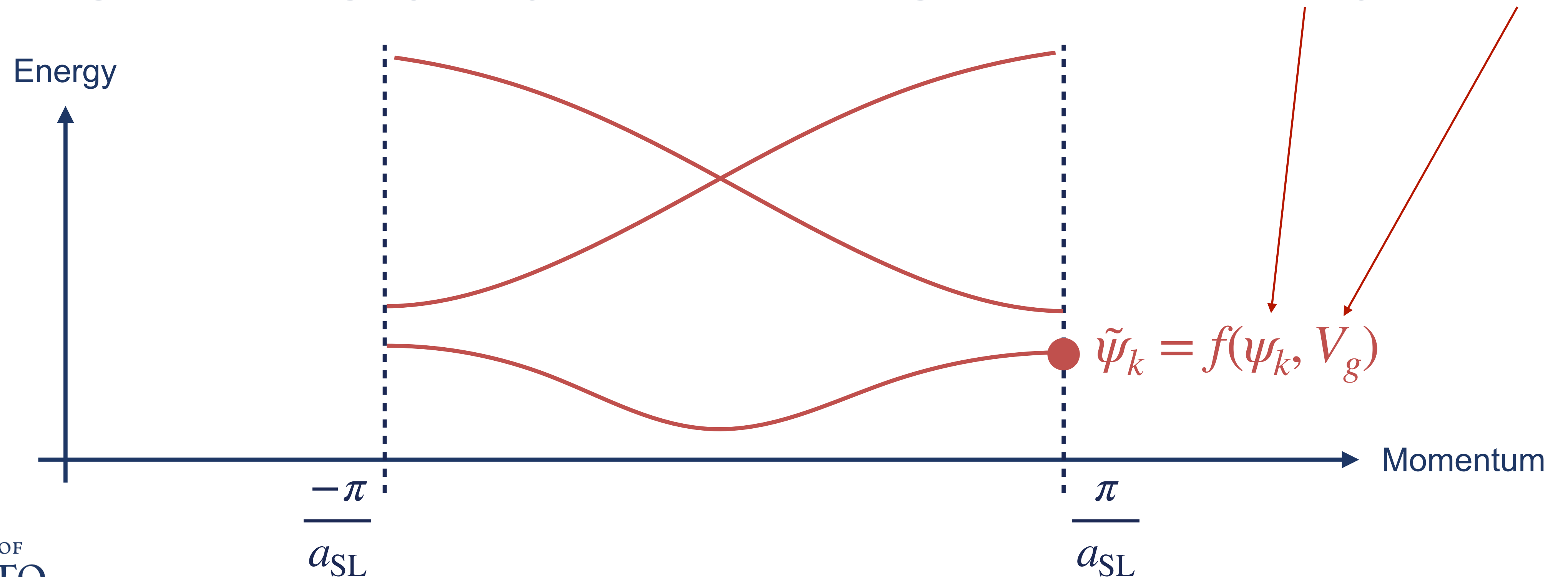
Method: Topological perturbative band theory



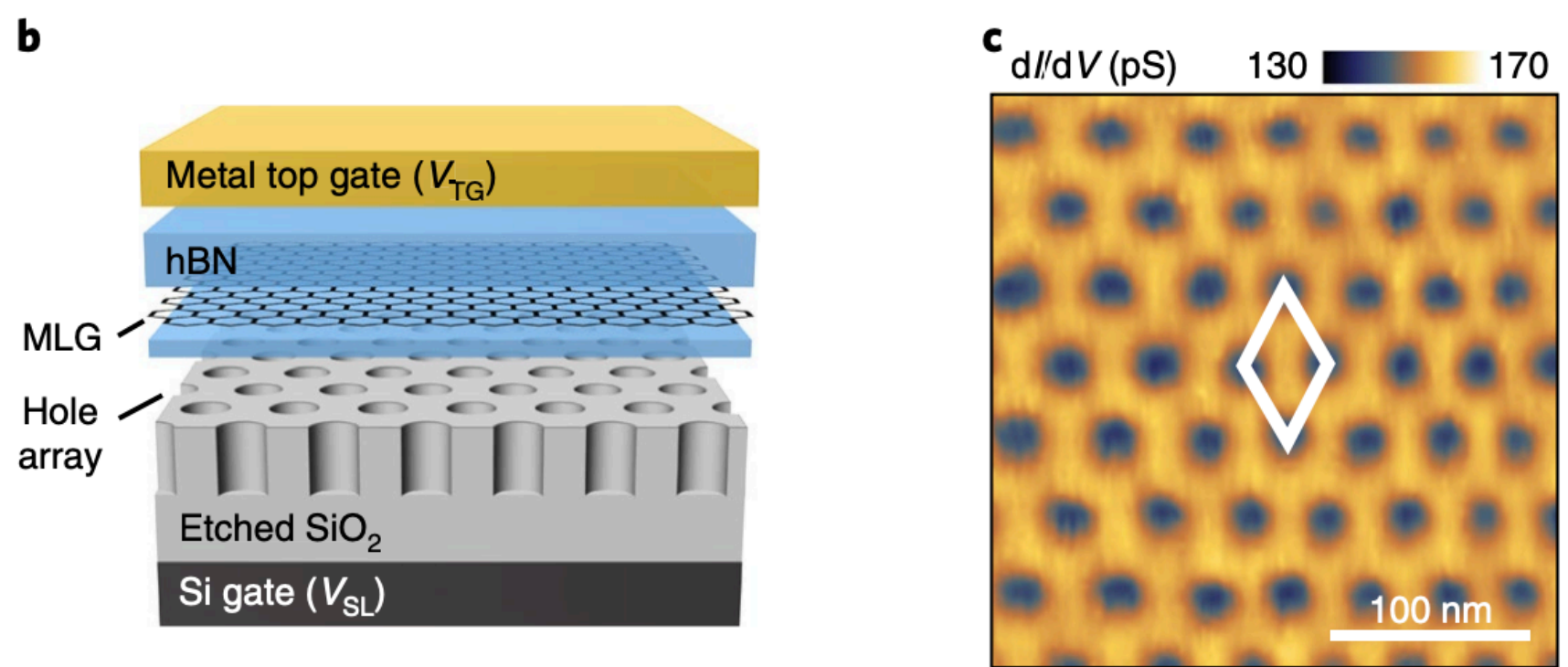
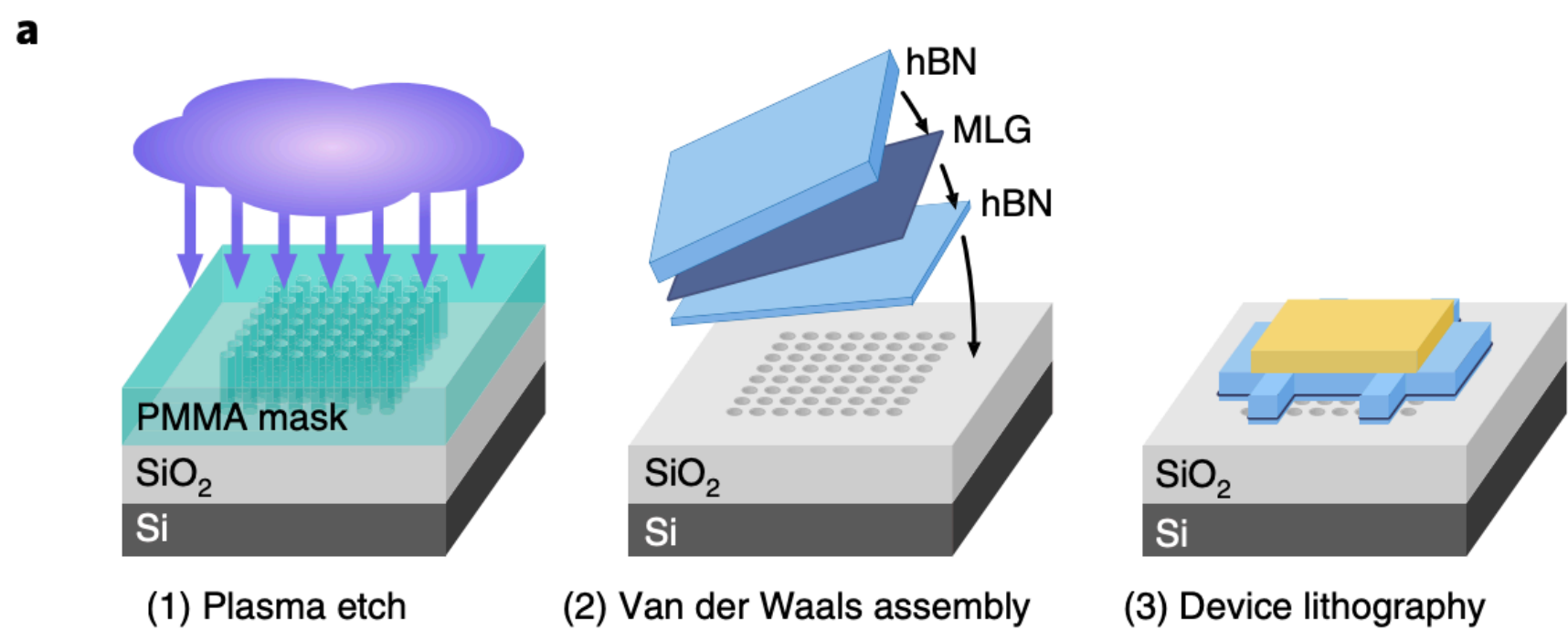
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Method: Perturbative band theory

- Goal: Discard material details to extract topological invariant (universal physics)
- Step 1: Include moiré field / potential perturbatively, $V_g e^{ig \cdot r}$
- Step 2: Obtain eigenvectors at high-symmetry points and infer topological invariants from monolayer & harmonics

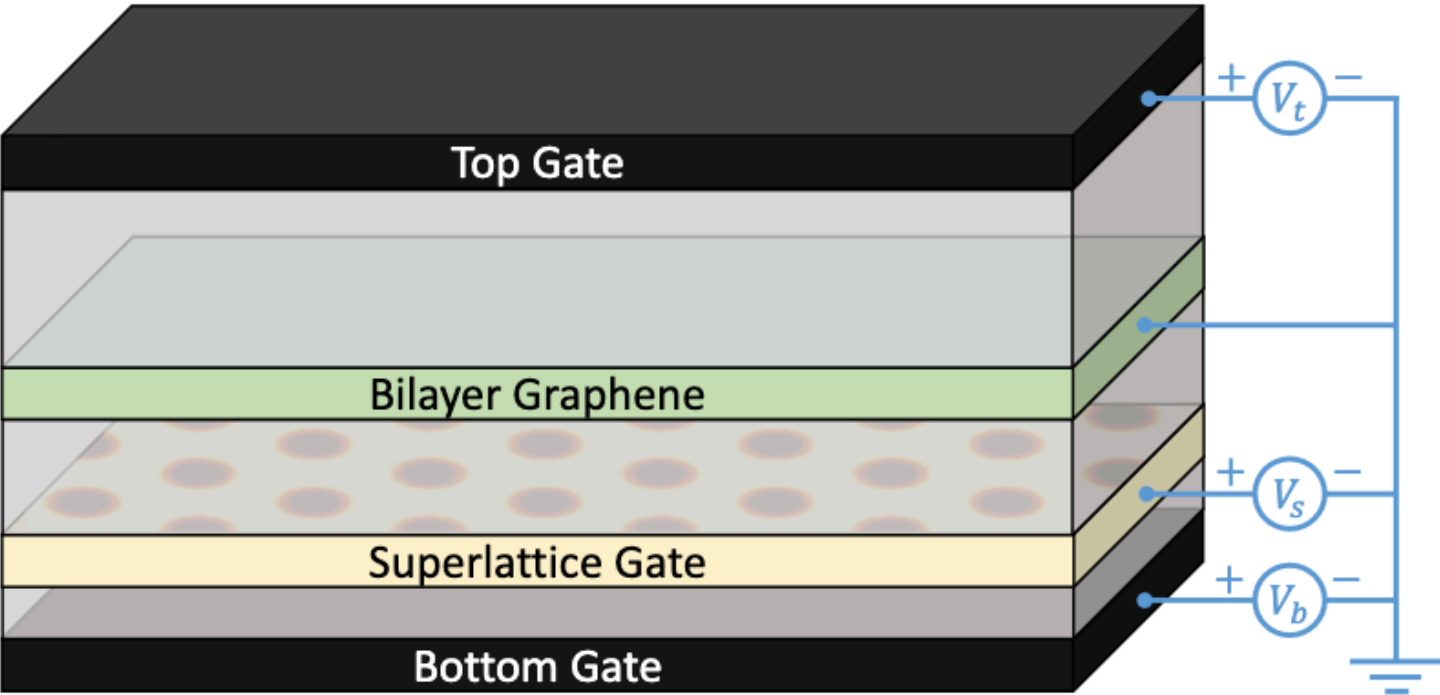


Application 1: Electrostatic superlattices

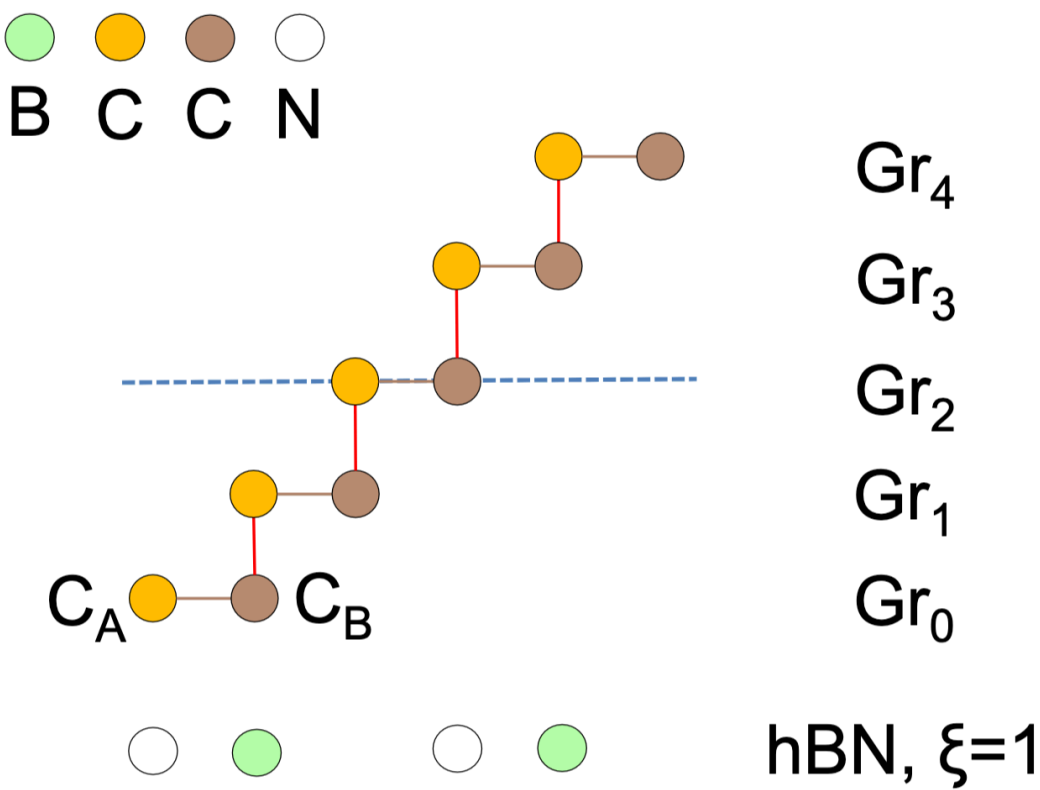


Ruiz *et al.*, Nat. Commun. (2022)

Sun *et al.*, Nano. Lett. (2024)



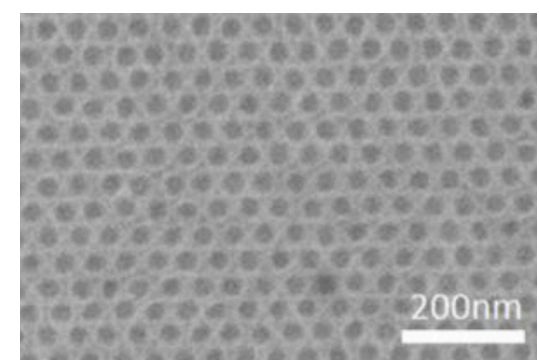
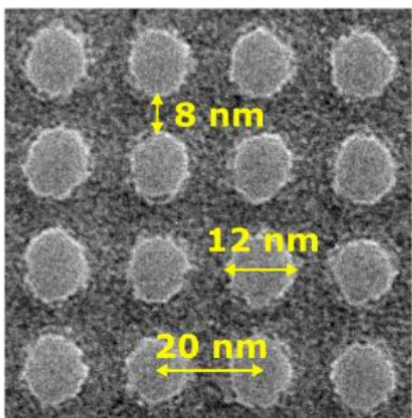
Zheng ... Cano, PRL (2024)



... Bernevig, PRB (2025)

Application 1: Electrostatic superlattices

VC and Cano, PRX (2025)



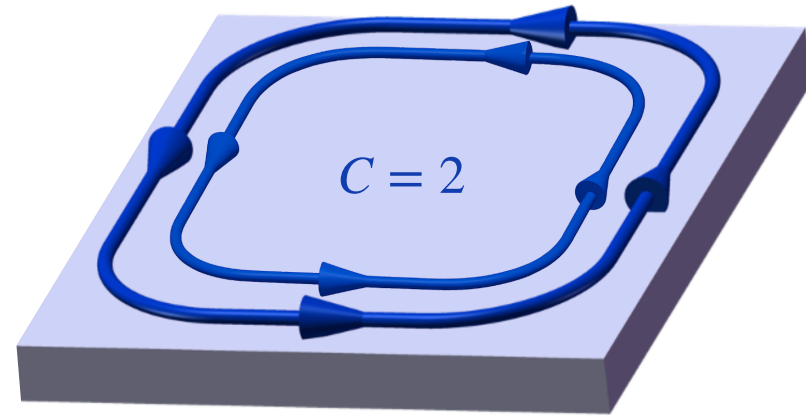
Geometry

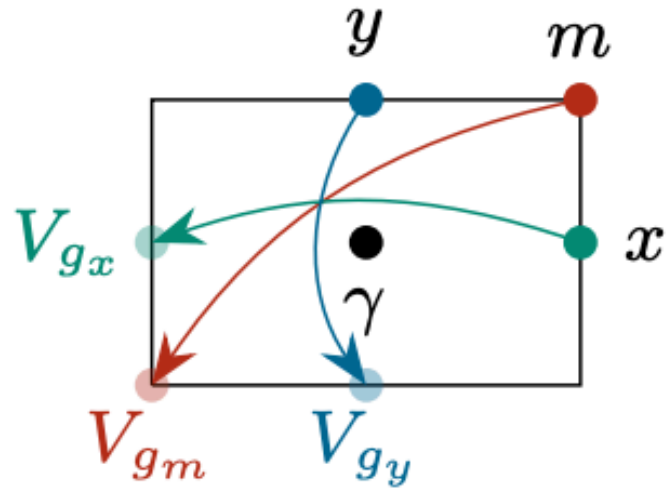
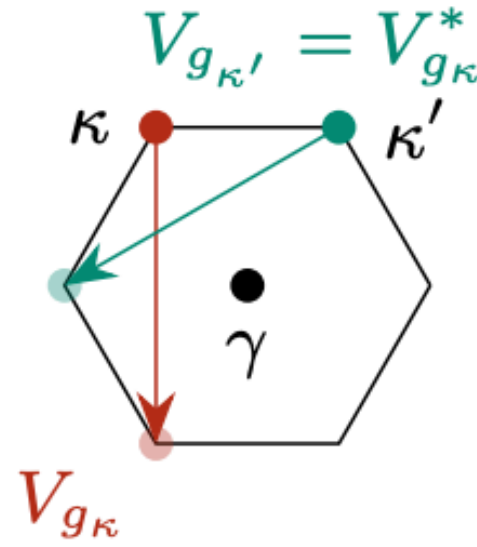
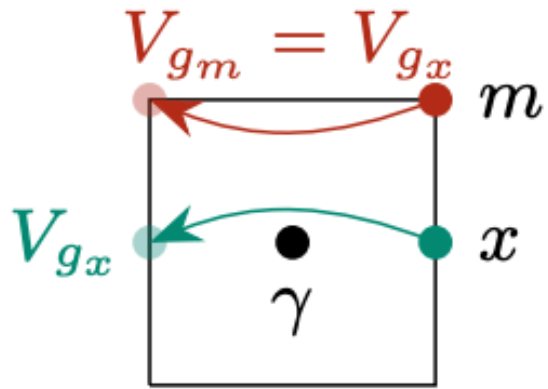
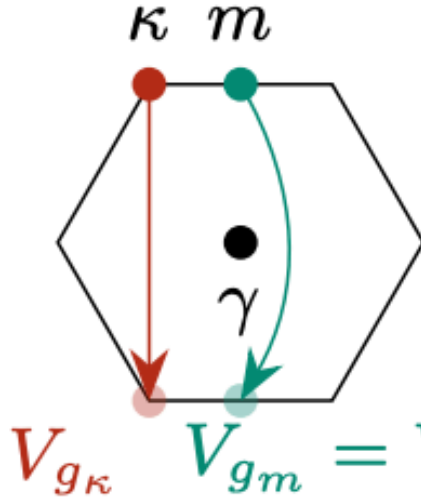
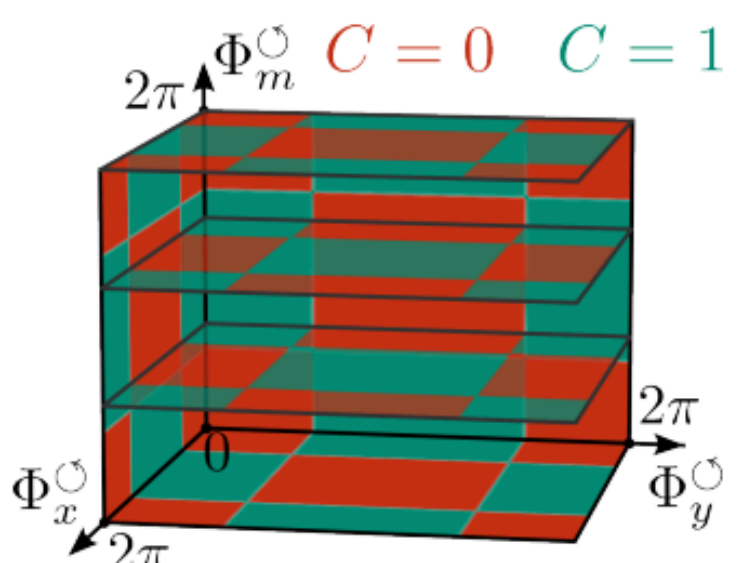
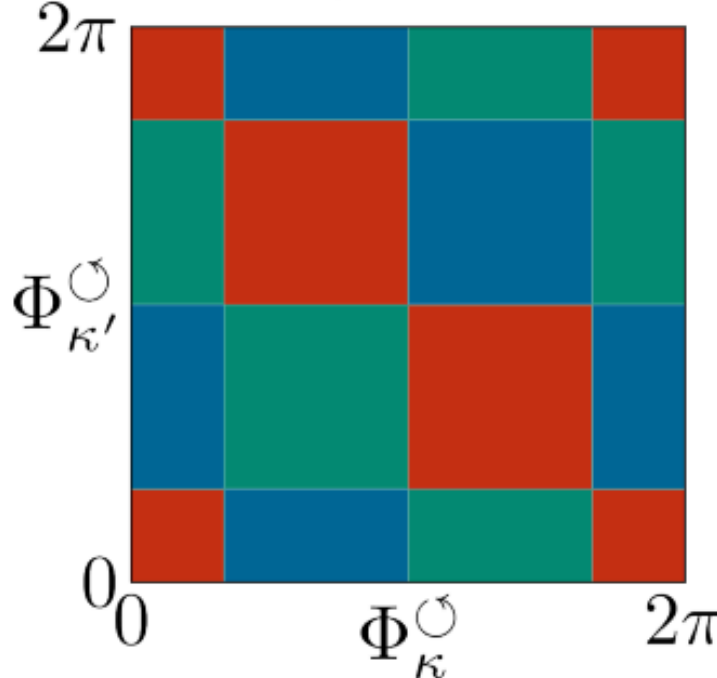
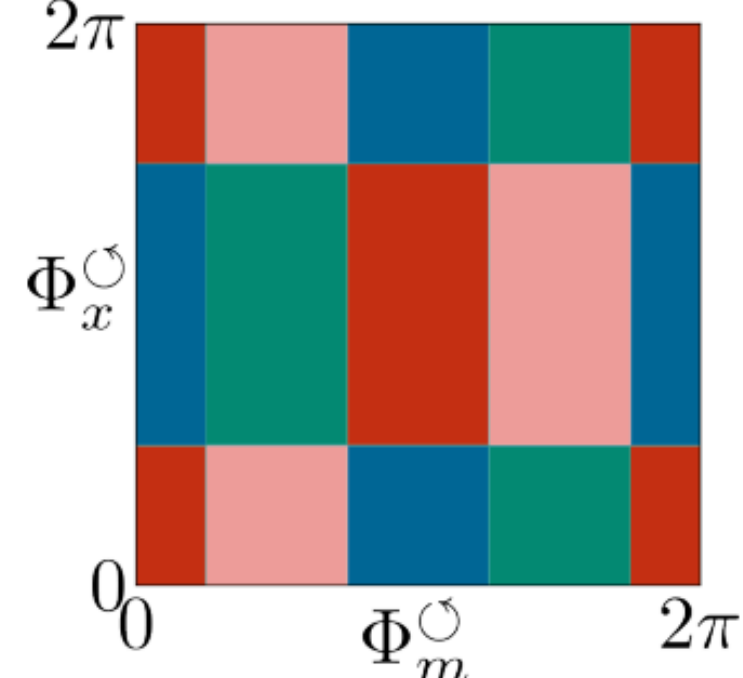
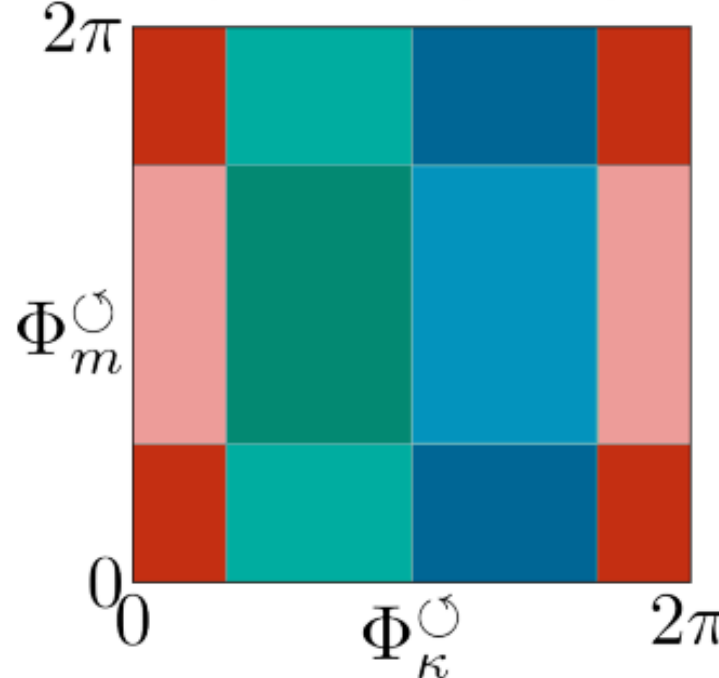
+

few material
coefficients

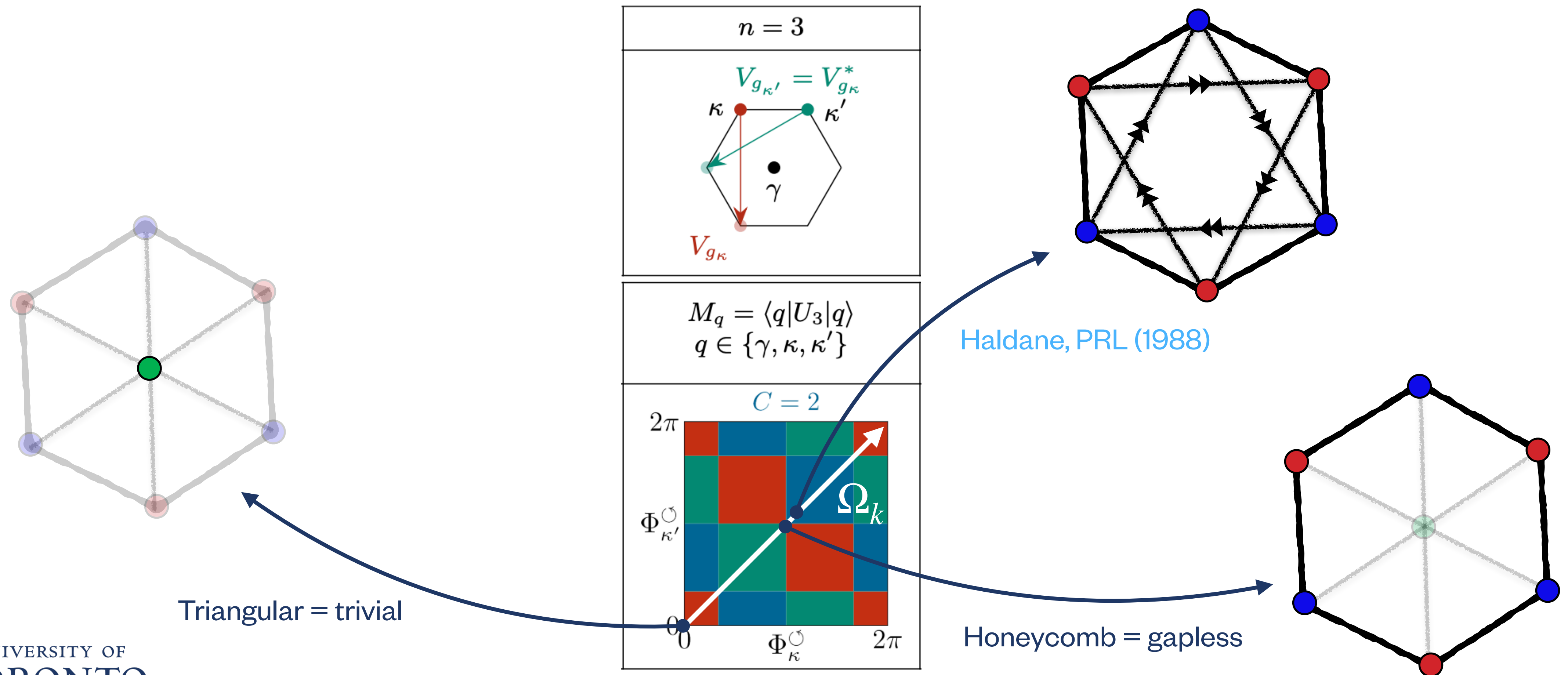
=

Topological
invariant



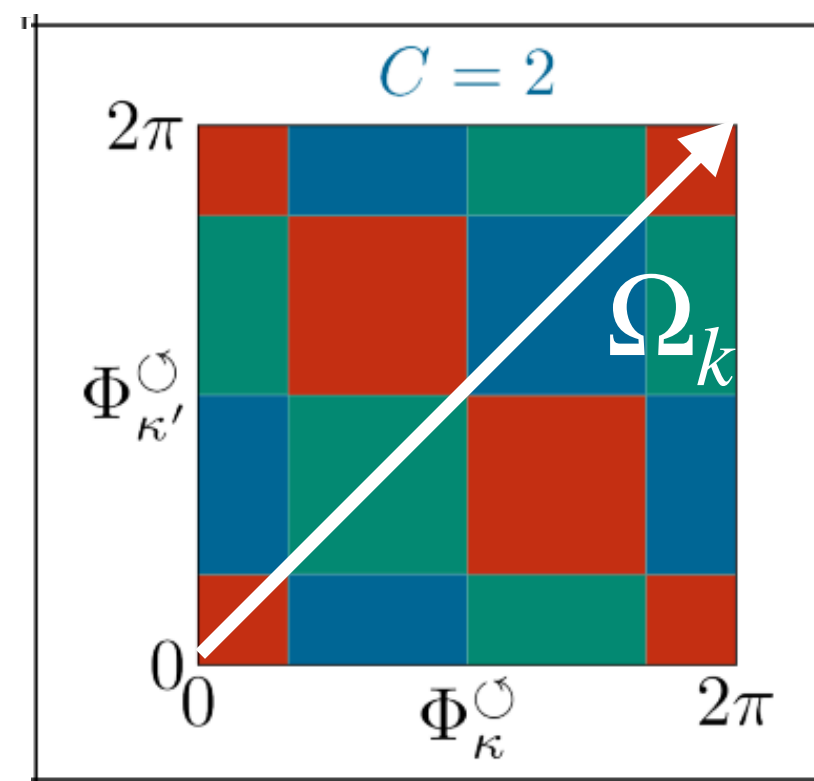
Symmetry group $\mathcal{C}_n$	$n = 2$	$n = 3$	$n = 4$	$n = 6$
Reduced BZ				
Form factors for the general case	$M_q = \langle q U_2 q \rangle$ $q \in \{\gamma, x, y, m\}$	$M_q = \langle q U_3 q \rangle$ $q \in \{\gamma, \kappa, \kappa'\}$	$M_\gamma = \langle \gamma U_4 \gamma \rangle$ $M_m = \langle m U_4 m \rangle$ $M_x = \langle x U_4^2 x \rangle$	$M_\gamma = \langle \gamma U_6 \gamma \rangle$ $M_m = \langle m U_6^3 m \rangle$ $M_\kappa = \langle \kappa U_6^2 \kappa \rangle$
Chern number C_n in the general case as a function of the loop phases $\Phi_q^\odot = p(q) \arg \frac{V_{gq} M_q^*}{M_\gamma^*}$		$C = 2$ 	$C = 3$ 	$C = 4$ $C = 5$ 

Application 1: Electrostatic superlattices

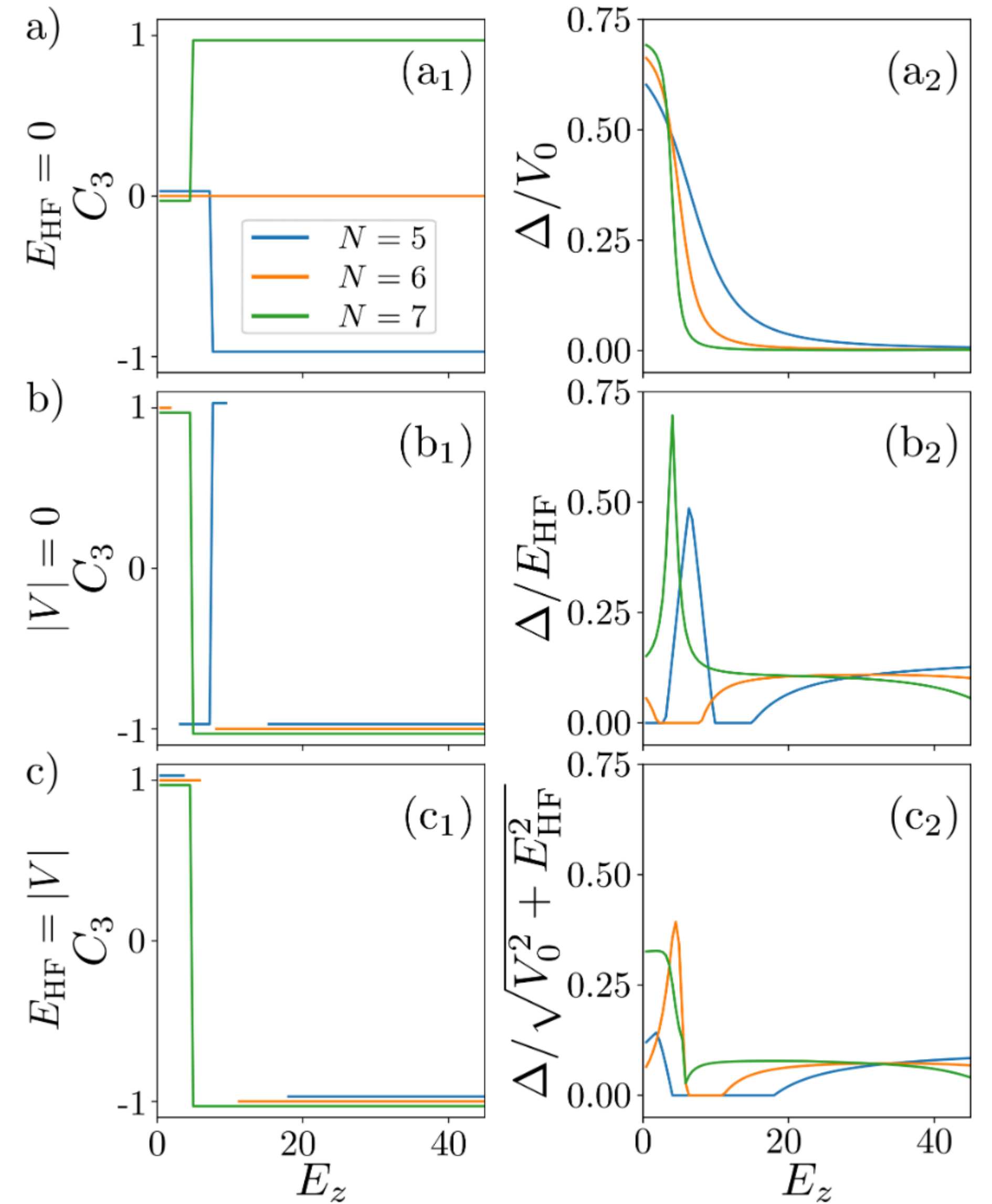


Application 1: Electrostatic superlattices

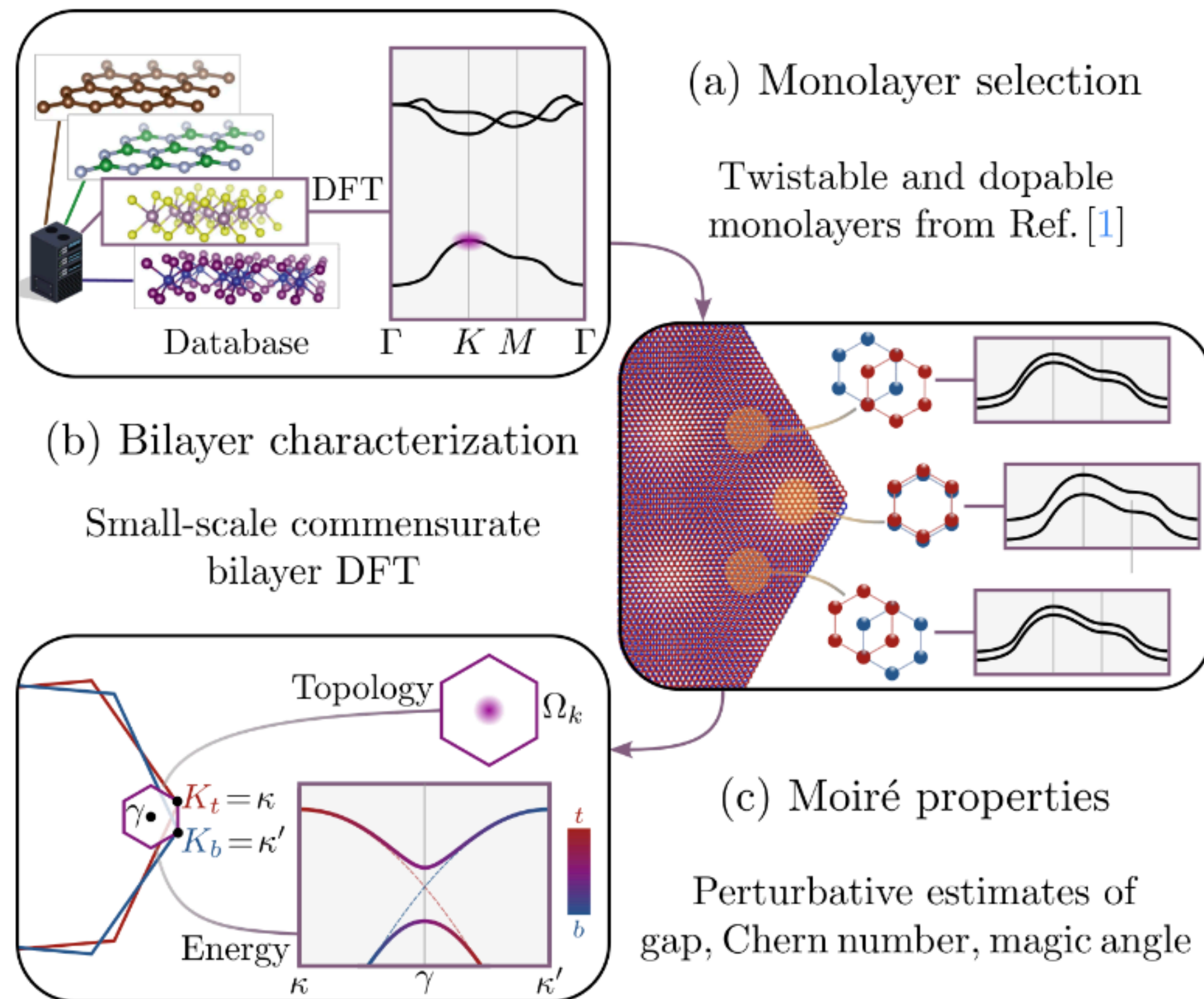
- Note electron and hole with Berry curvature with similar superlattice potential: one will be topological, at least.



- Can include Hartree-Fock potential instead of externally applied one, or combination of both



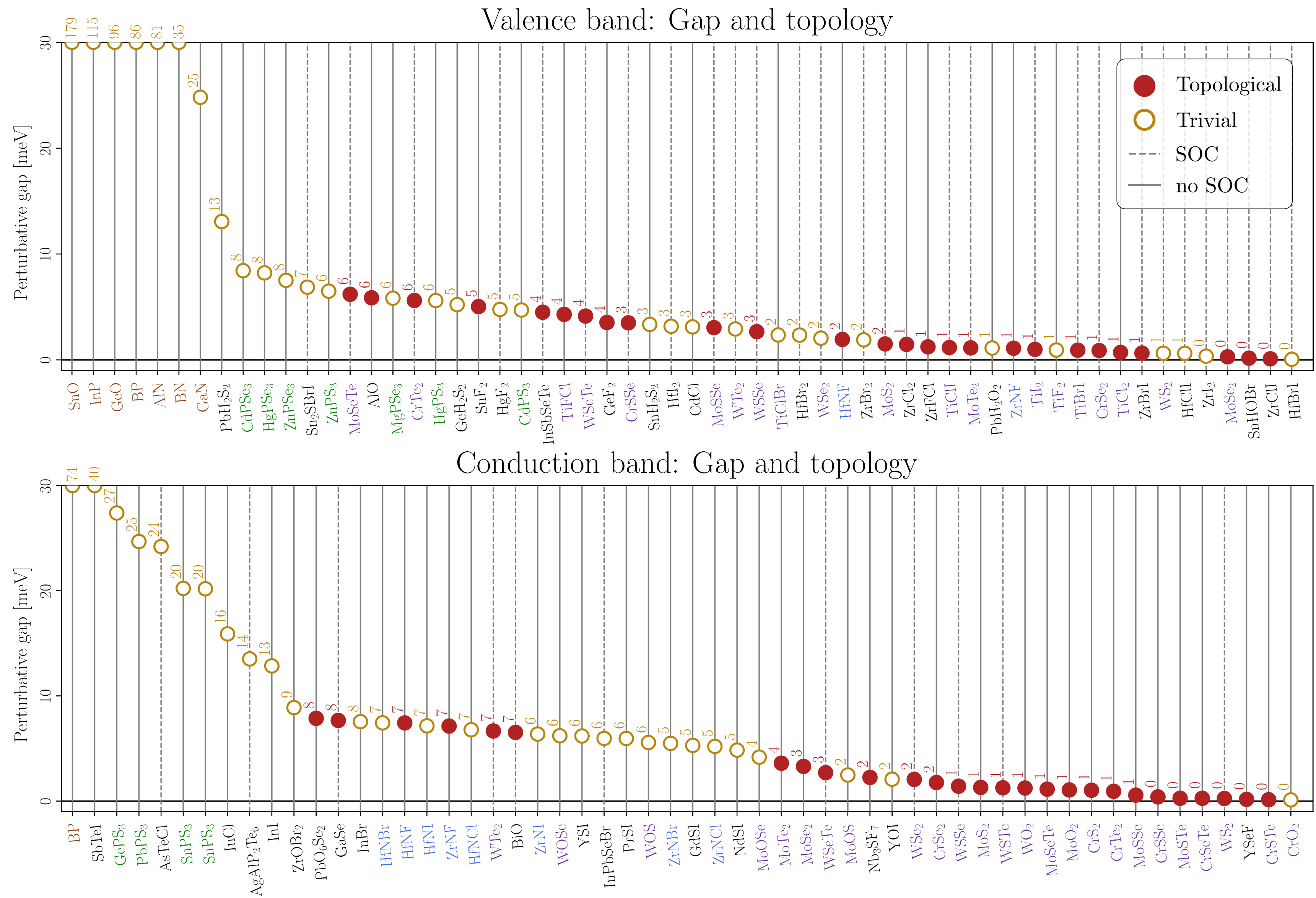
Application 2: twisted bilayers



Same strategy:

- Determine geometry (triangular / honeycomb) of couplings with a handful DFT calculations
- Combine with material coefficients (monolayer)
- Infer gaps and rotation eigenvalues, then Chern

Application 2: a guide to quantum simulations

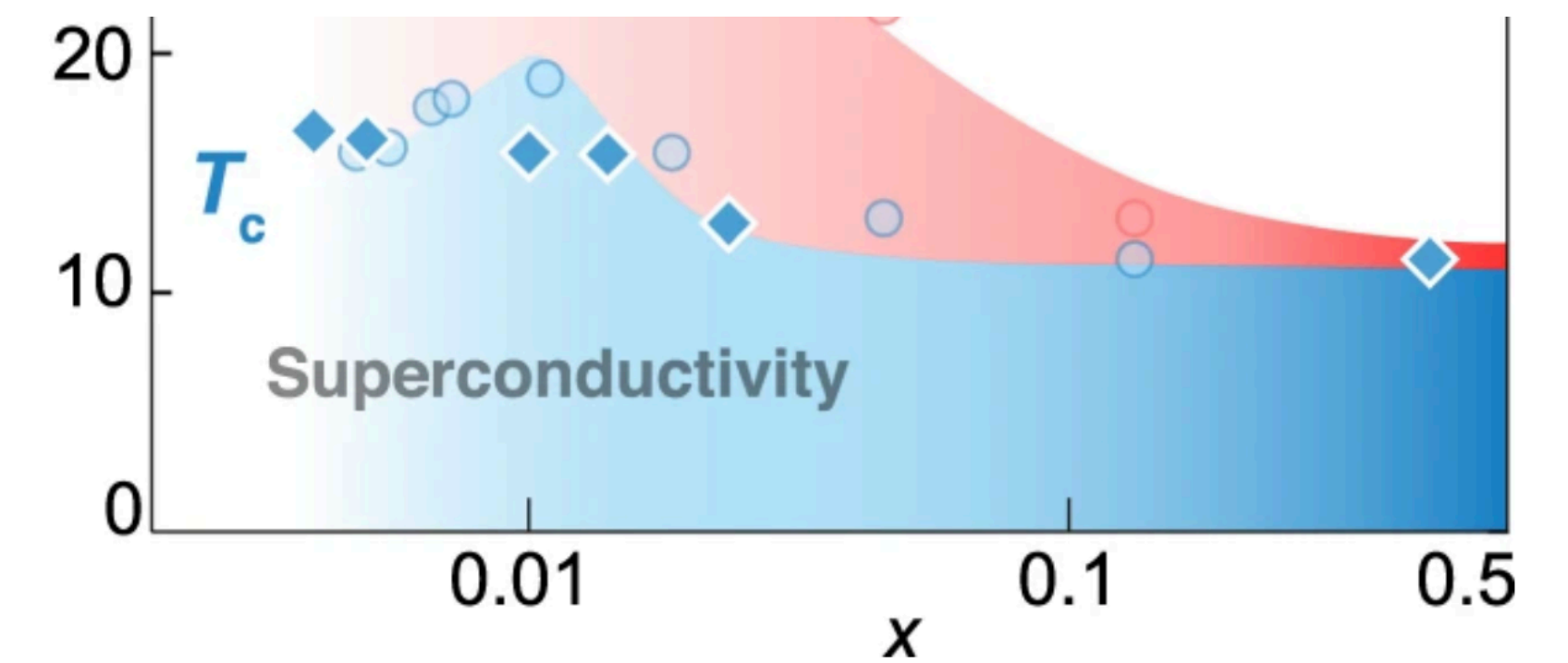
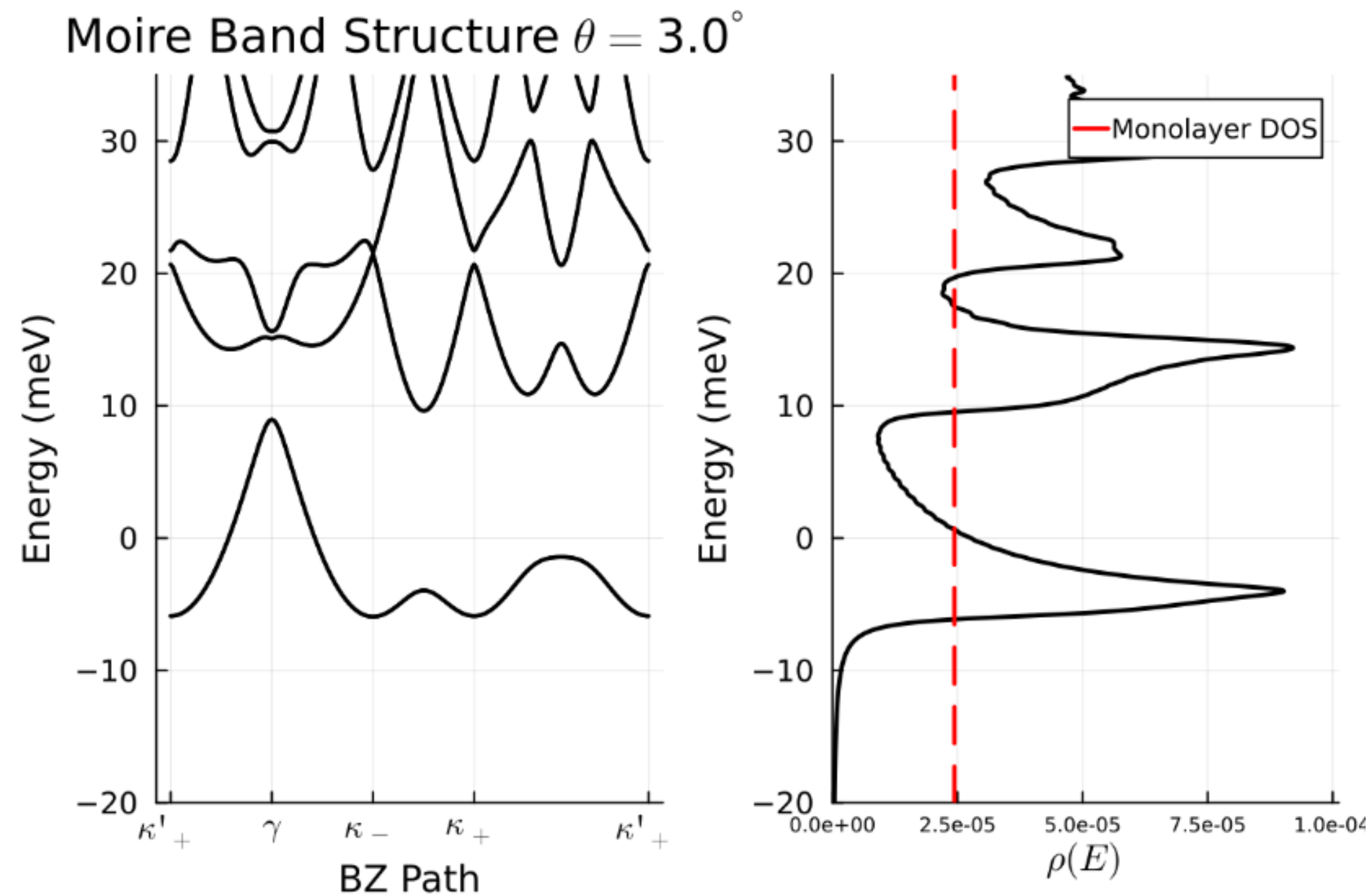


Scan all known semiconductors with C3 symmetry in database to identify topological homo-bilayers

Nakatsuji, Cano, VC, arXiv:2512.15851



Application 2: a guide to quantum simulations



Heyl, ..., Iwasa, *Nat. Commun.* (2022)

ZrNCl superconducts with $T_c \simeq 15K$

Down to concentration $\sim 1e/\text{moiré}$

Increase DOS 5-fold: liquid nitrogen temperatures!

Albert, Hardy, VC, *in preparation*

Outlook

Nakatsuji, Cano, VC, arXiv:2512.15851

- Precise methods for quantitative details are still needed: especially for new candidates identified!
- Extending the classification to other symmetry / systems (systematic manner)
- Method is perturbatively control: know when it fails, which defines θ_{relax} or estimate for θ_{magic}

