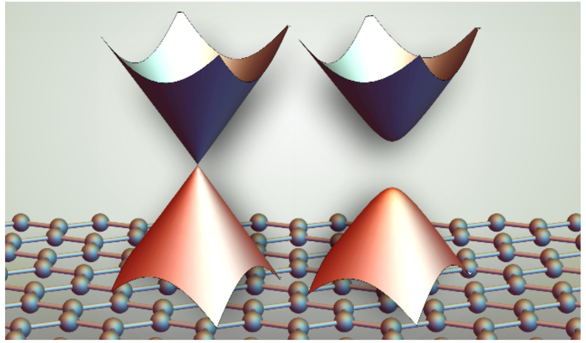


MAX PLANCK INSTITUTE FOR
SOLID STATE RESEARCH

Research Group

Unconventional superconductivity in moiré transition metal dichalcogenides

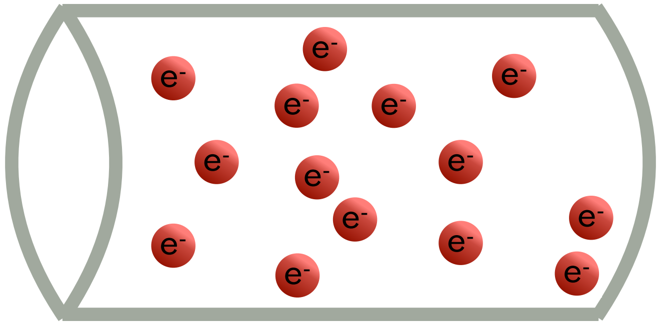
Laura Classen

Nico Gneist, Michael Scherer (Bochum)
Lennart Klebl, Ammon Fischer, Dante Kennes (RWTH Aachen)

ERG, June 2022

Correlated phases in quantum materials

- Collective phases of interacting electron systems?



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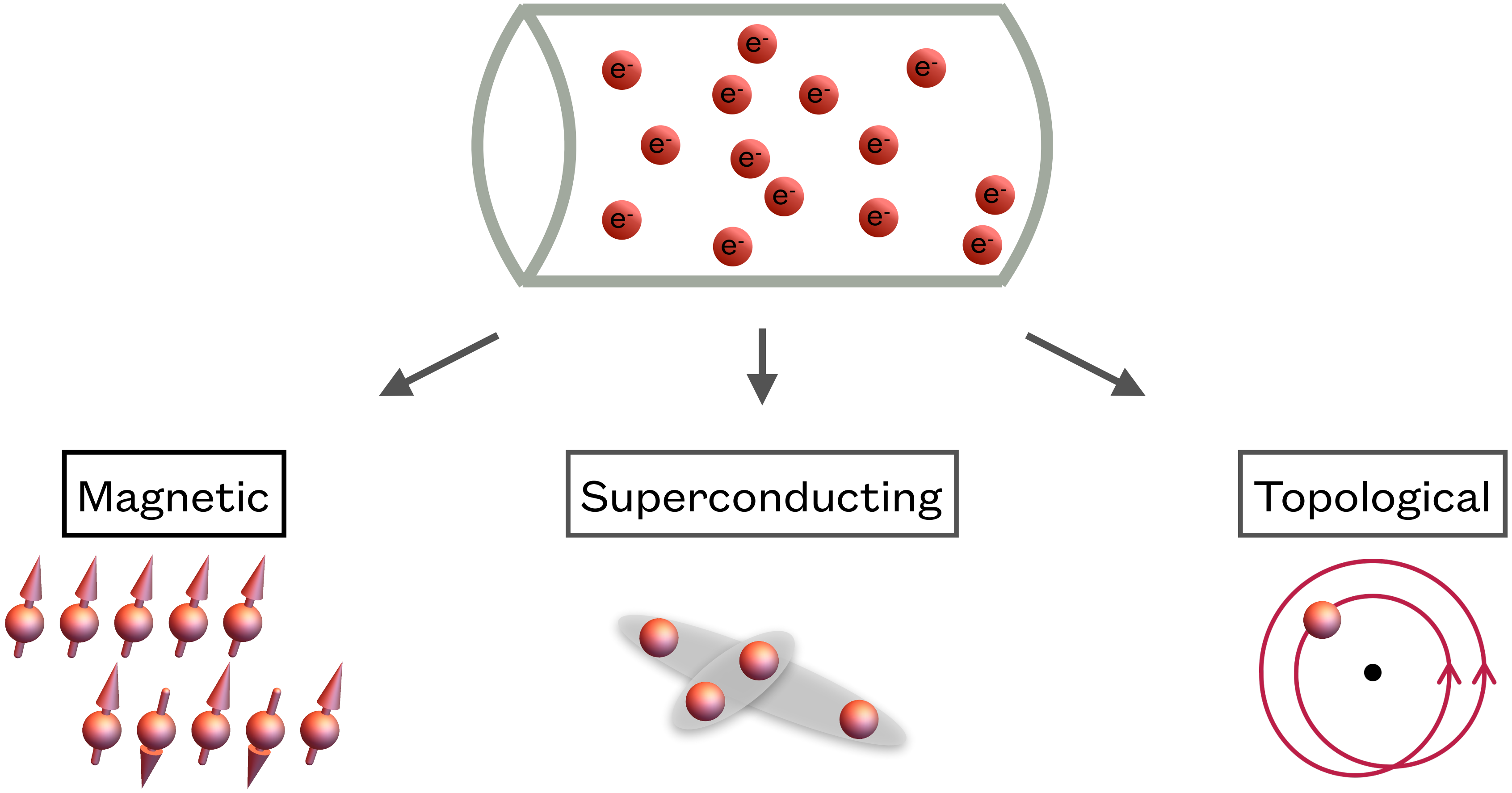

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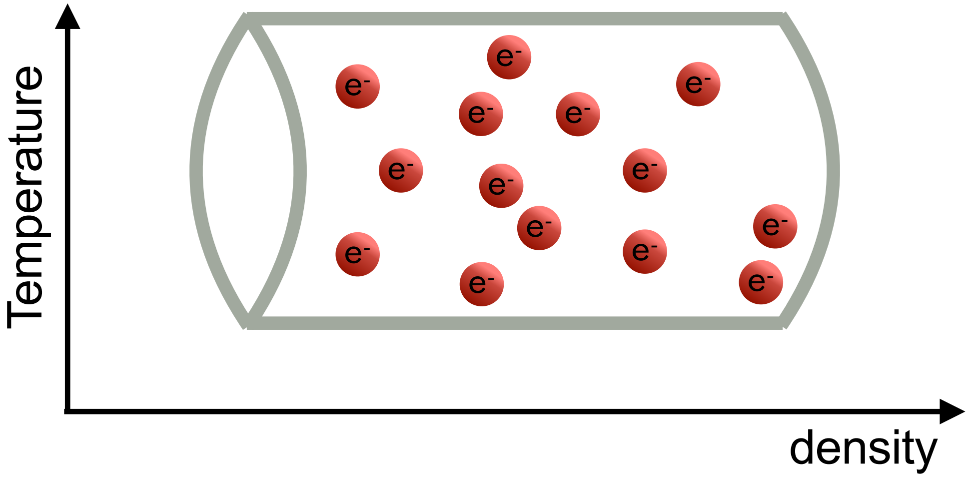
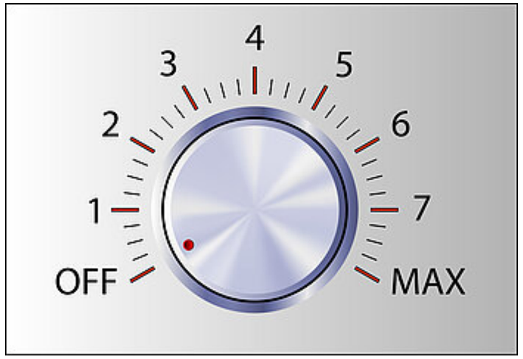


- Tuning knobs: temperature, density, external fields, ….



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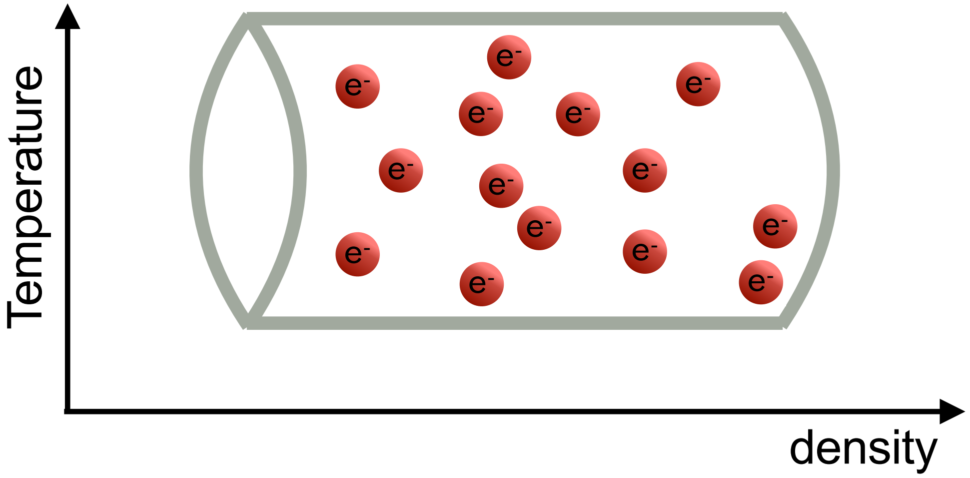
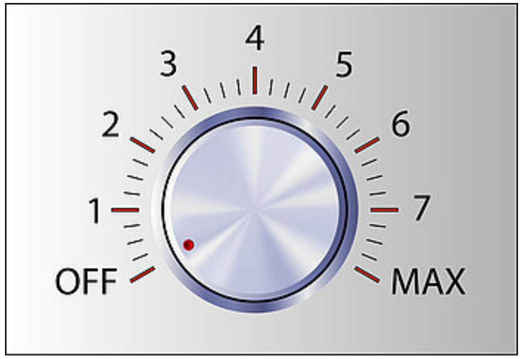


- Tuning knobs: temperature, density, external fields, ….

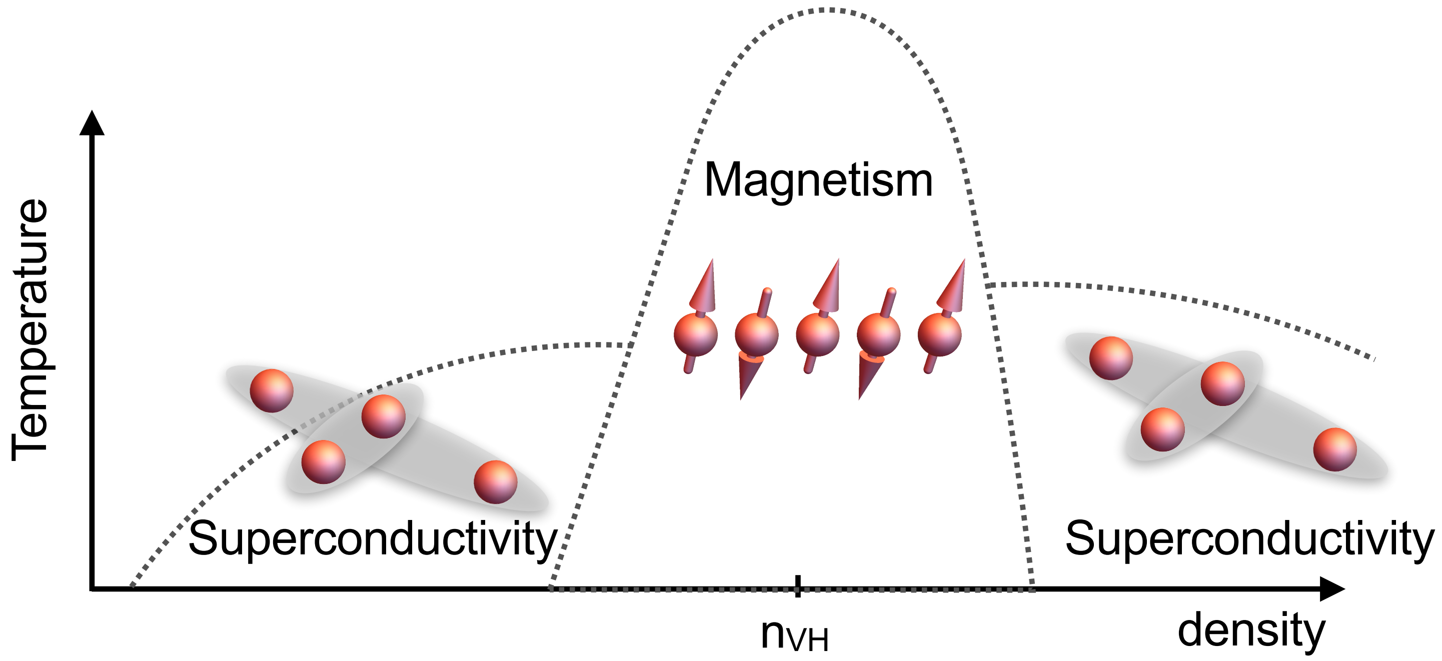
many different (classes of) materials!

High-Tc superconductors, quantum magnets,
Dirac materials, low-dimensional systems, ….



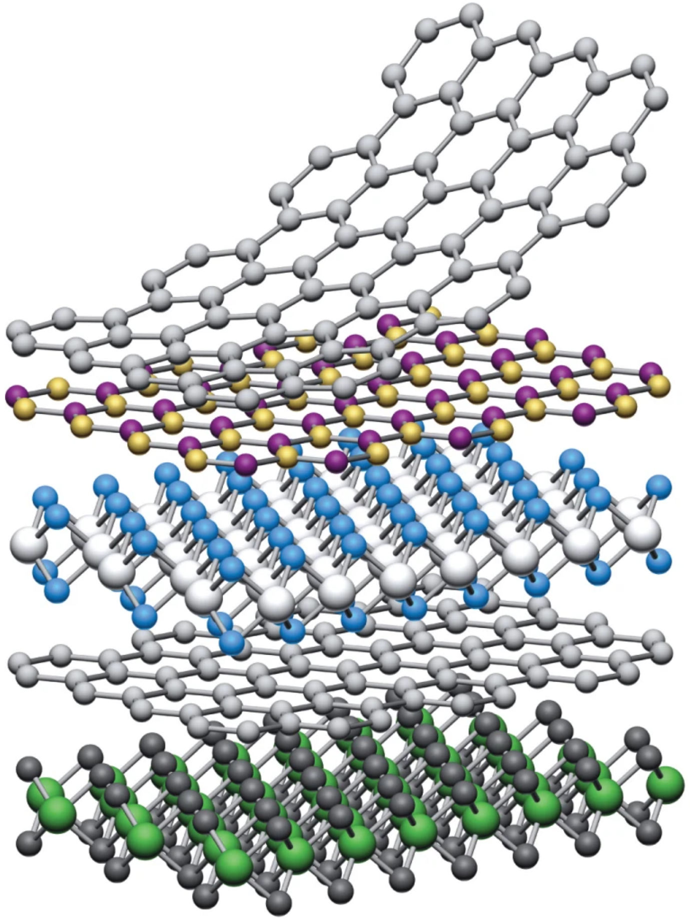
Outline

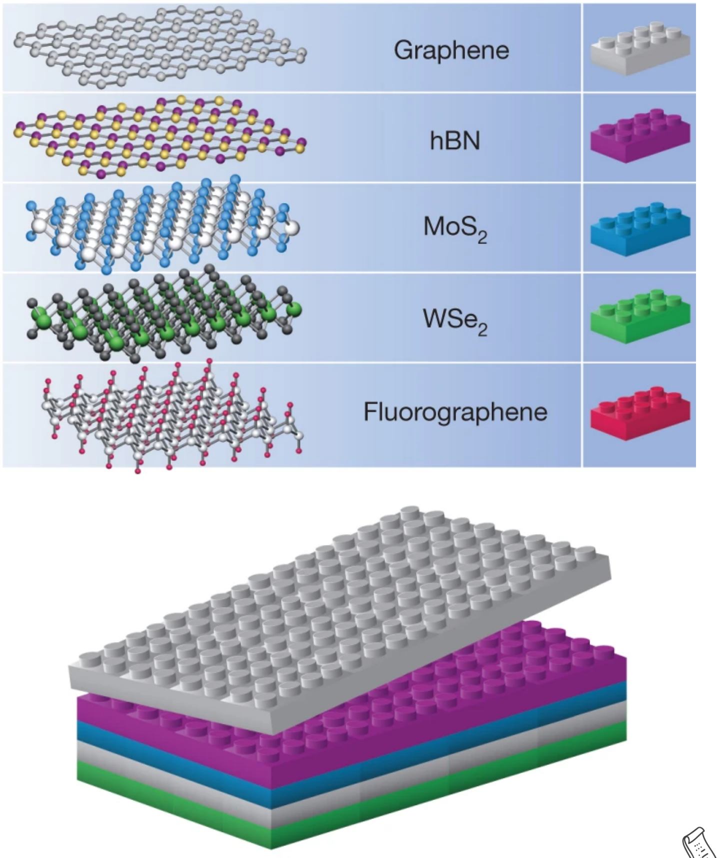
- Correlated physics in 2D moiré materials
- Simulate triangular-lattice Hubbard model
- FRG: superconductivity from repulsive interactions/interplay of orders



2D Materials

- Designer heterostructures from stacking and twisting 2D materials

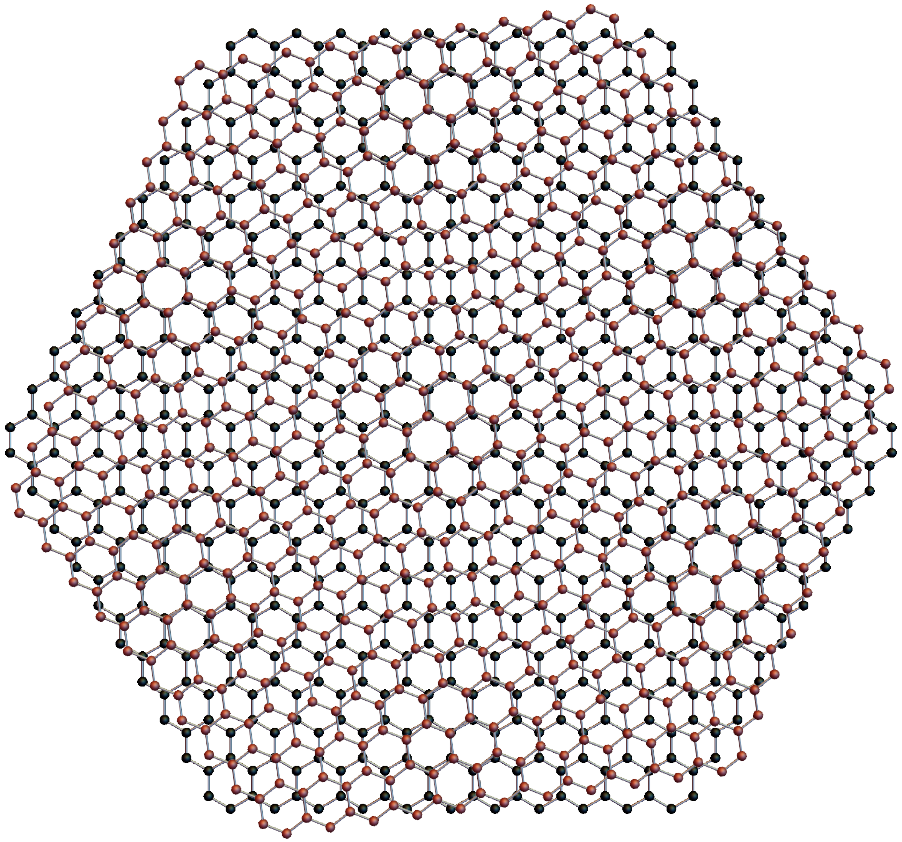




Geim & Grigorieva, Nature (2013)

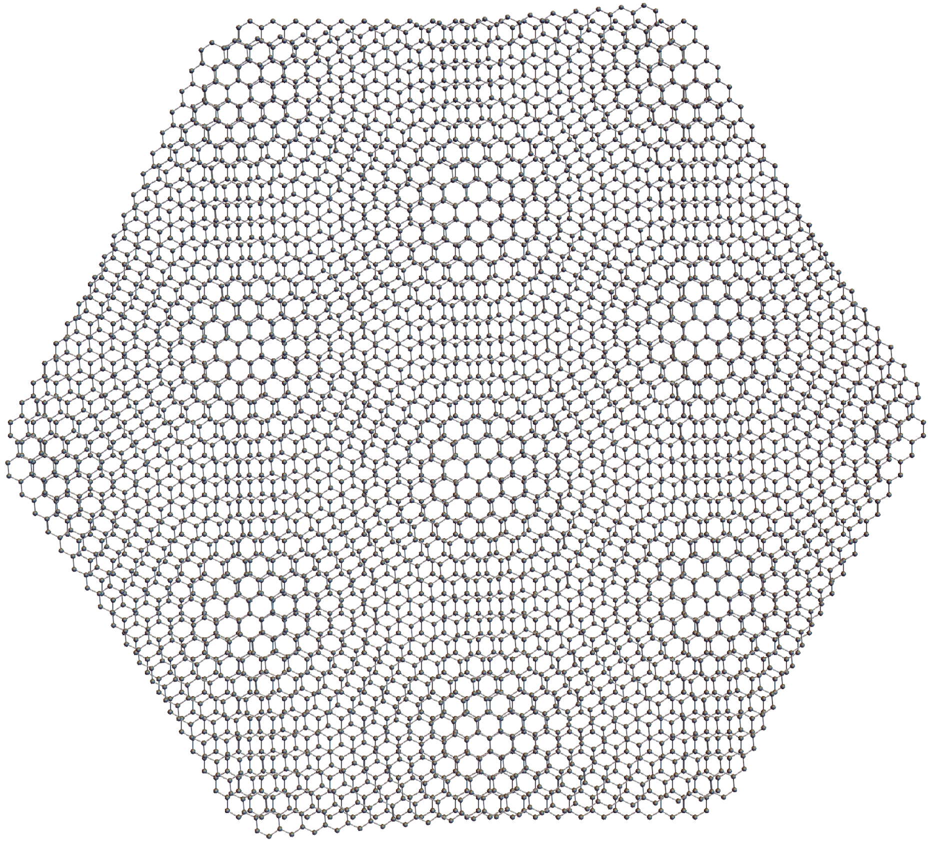
Twisted bilayer graphene

- Graphene: carbon atoms on honeycomb lattice (Dirac fermions, weakly correlated)

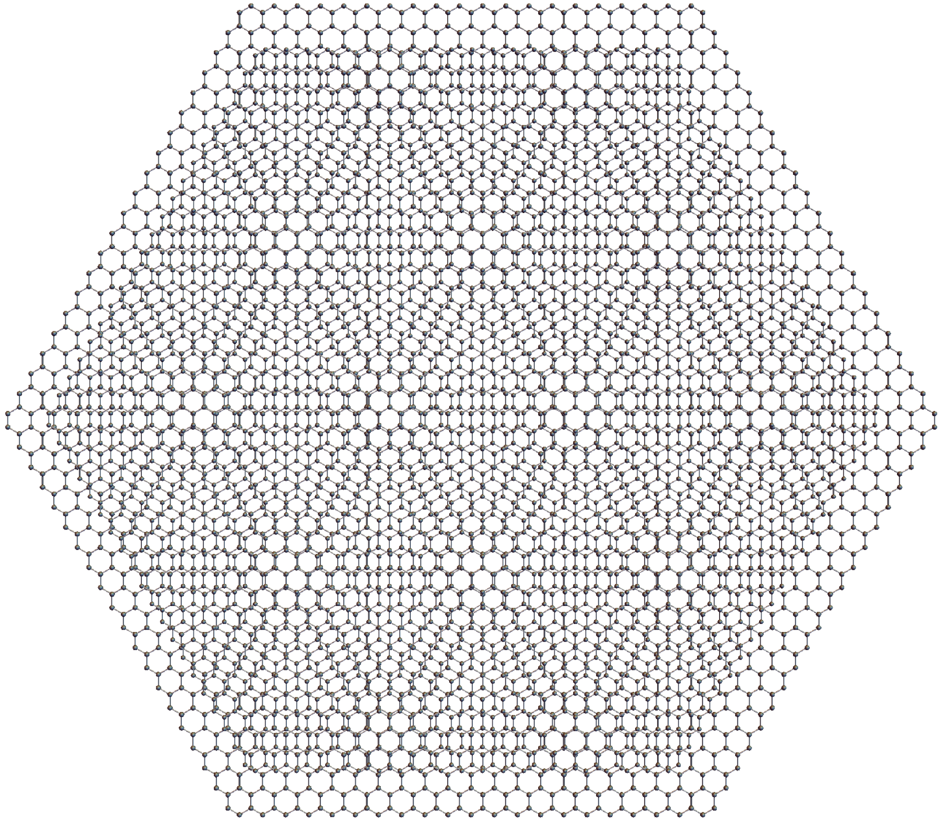


Moiré materials

- Overlay two periodic structures with small mismatch → **moiré** pattern (superlattice)



rotation by $\theta = 5°$

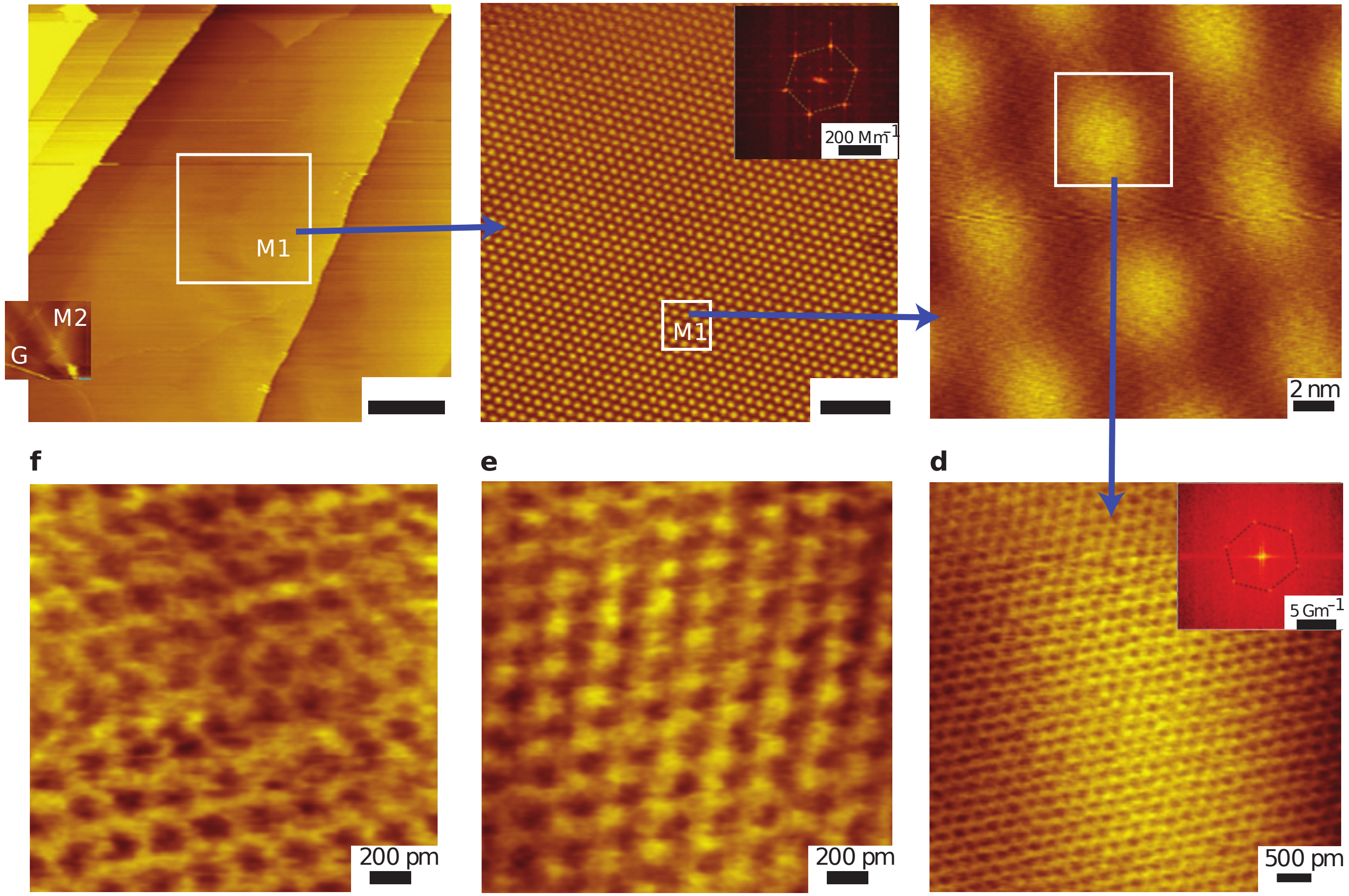


$\theta = 0°$ but different lattice constants

Twisted bilayer graphene

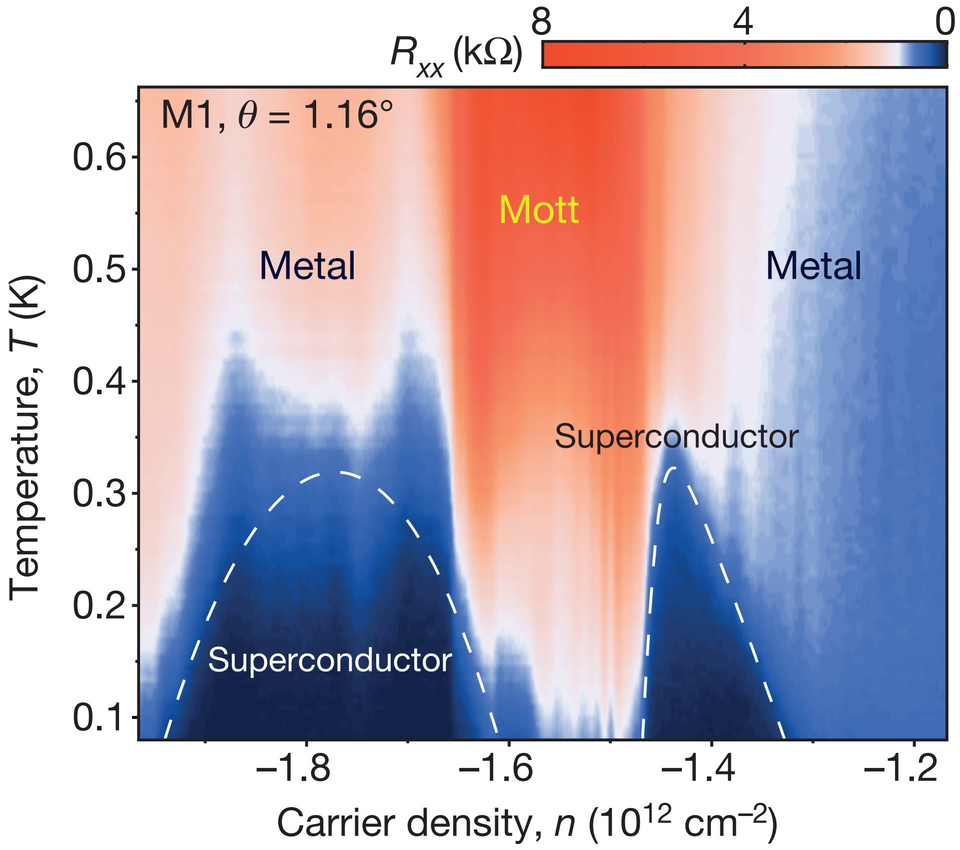
- Scanning tunneling microscopy image of two graphene layers with relative rotation of $1.8°$

Li *et al.*, Nature Physics (2010)

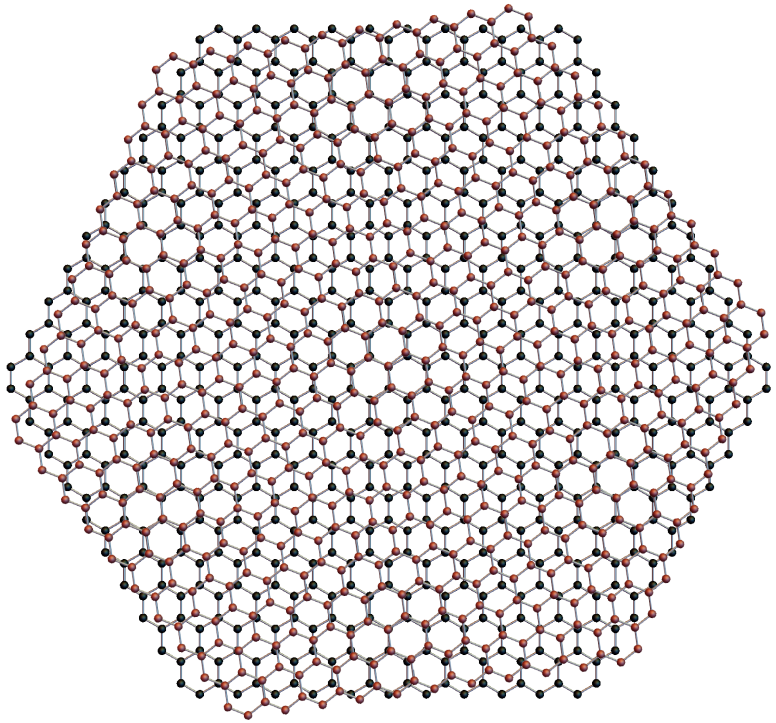


Magic angle twisted bilayer graphene

- Strong interactions arise: correlated insulators and superconductors around $\theta^\circ \sim 1$



Cao *et al.*, Nature (2018)



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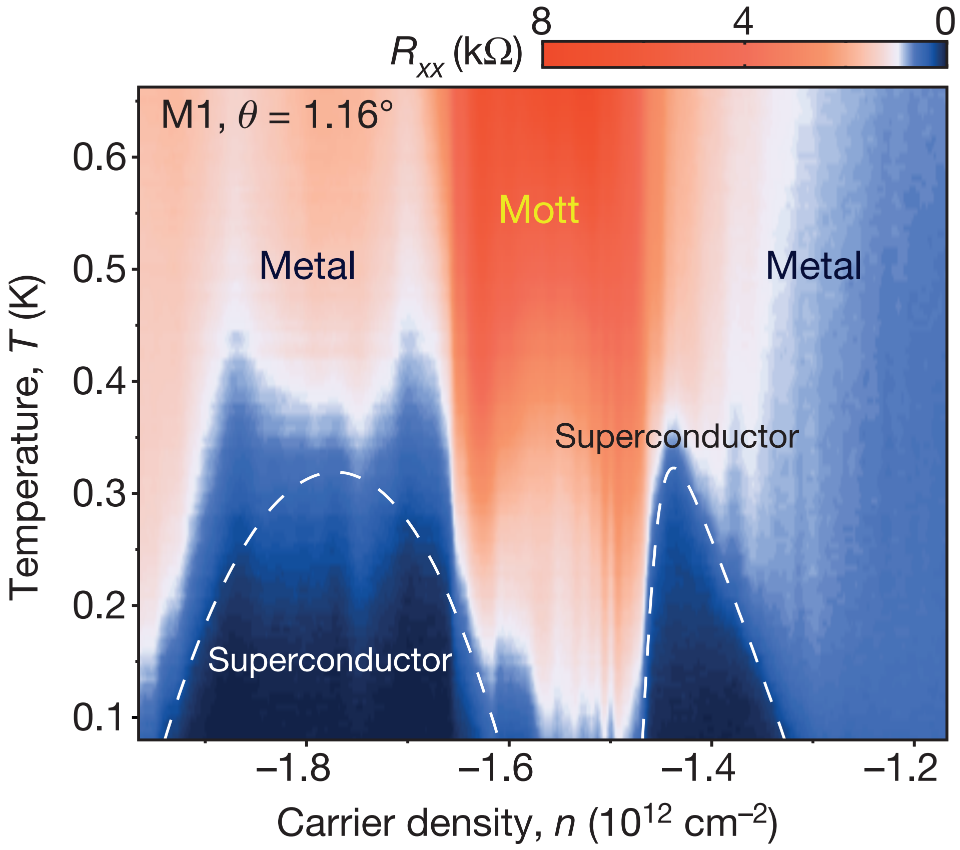
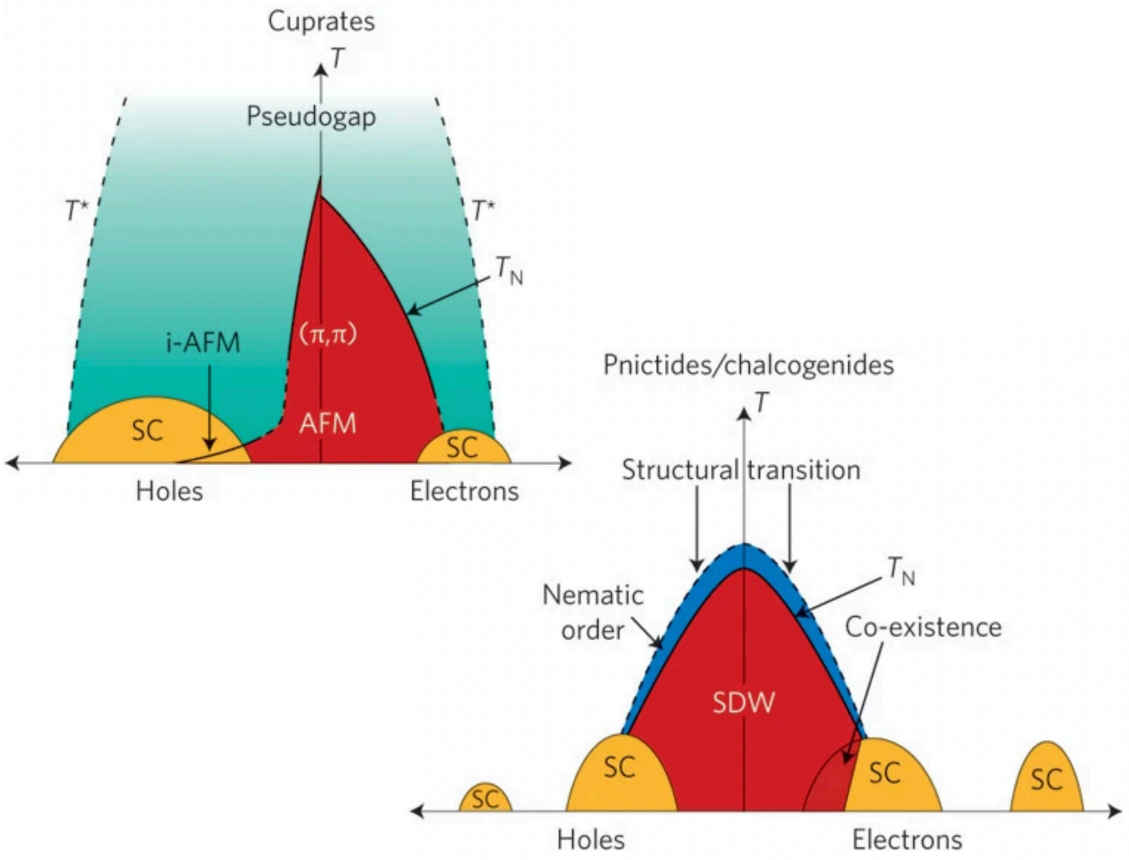


Cao *et al.*, Nature (2018)



Basov, Chubukov, Nature Physics (2011)

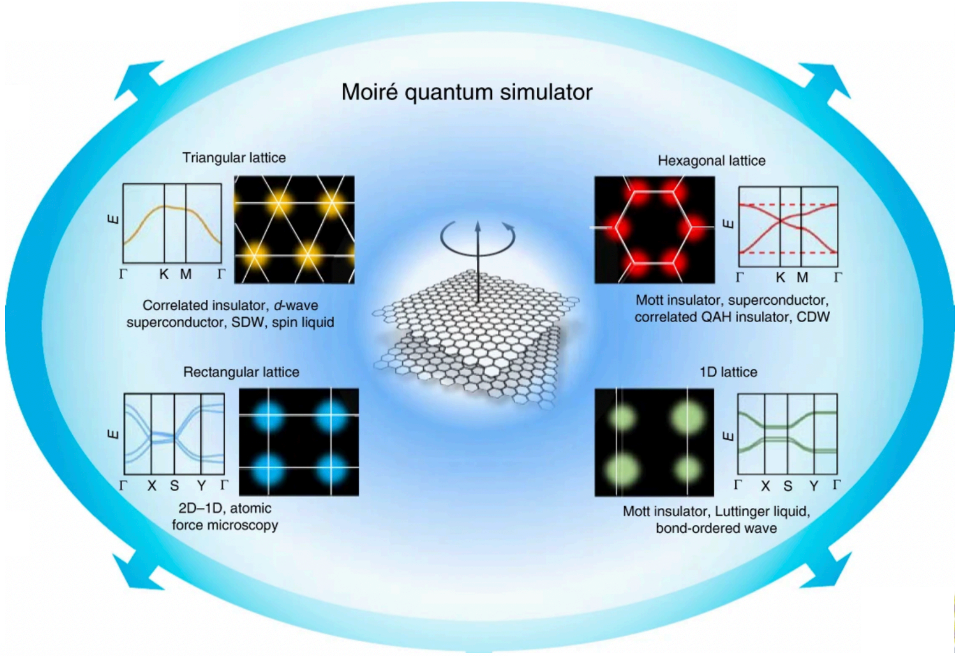
Moiré materials as "quantum simulators"

- Correlated phases in many other 2D heterostructures
- Moiré potential quenches kinetic energy

  → New platform for study of correlated physics
- High degree of control:
  stacking, twisting, gating, screening layers, light-matter interaction

  → Quantum simulation between cold atoms and solid state materials

Kennes et al, Nature Physics (2021)



Transition metal dichalcogenides →

Article

Simulation of Hubbard model physics in WSe_2/WS_2 moiré superlattices

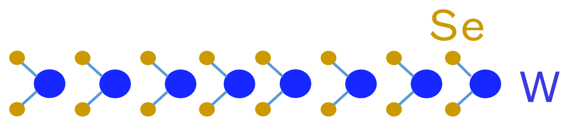
https://doi.org/10.1038/s41586-020-2085-3

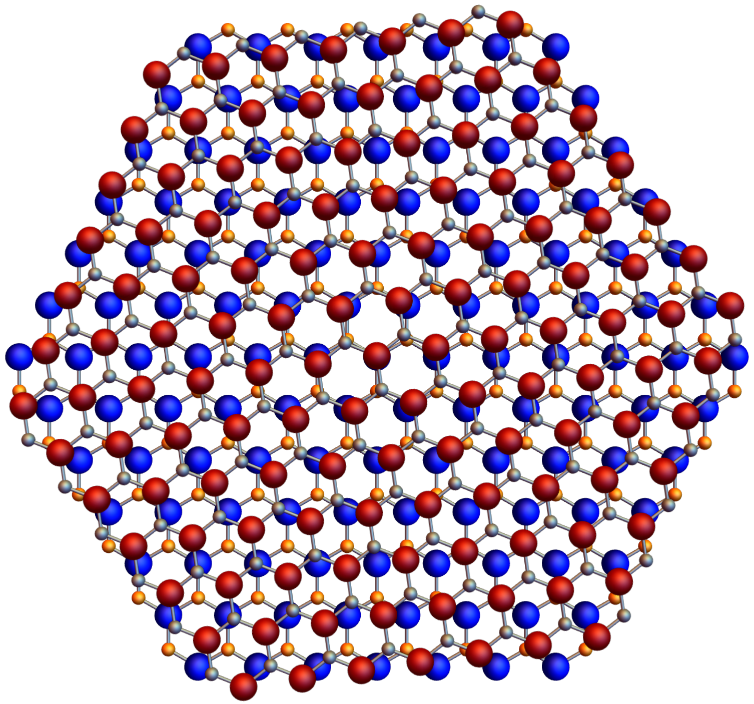
Received: 18 August 2019

Yanhao Tang[1], Lizhong Li[1], Tingxin Li[1], Yang Xu[1], Song Liu[2], Katayun Barmak[3], Kenji Watanabe[4], Takashi Taniguchi[4], Allan H. MacDonald[5], Jie Shan[1,6,7] & Kin Fai Mak[1,6,7]

Transition metal dichalcogenides (TMDs)

- Also form 2D materials (3 atom thick)



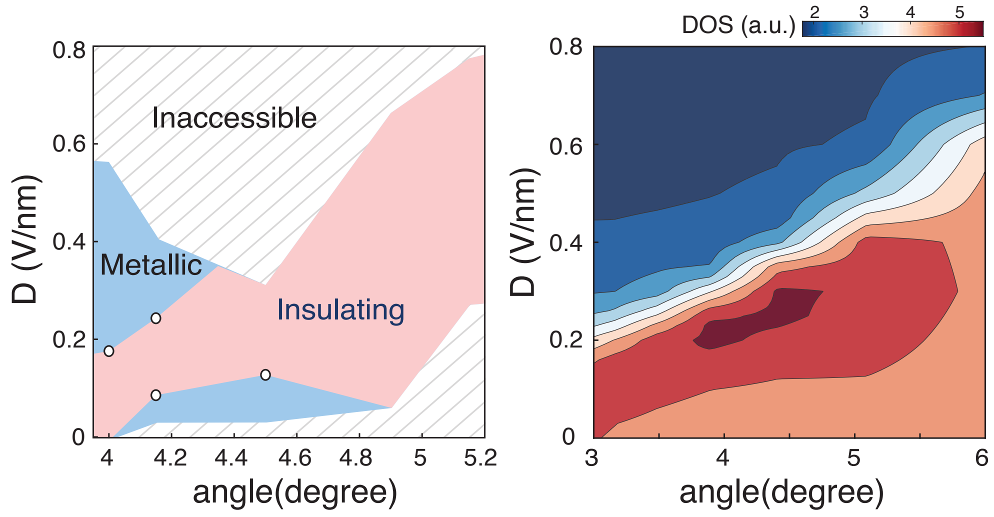


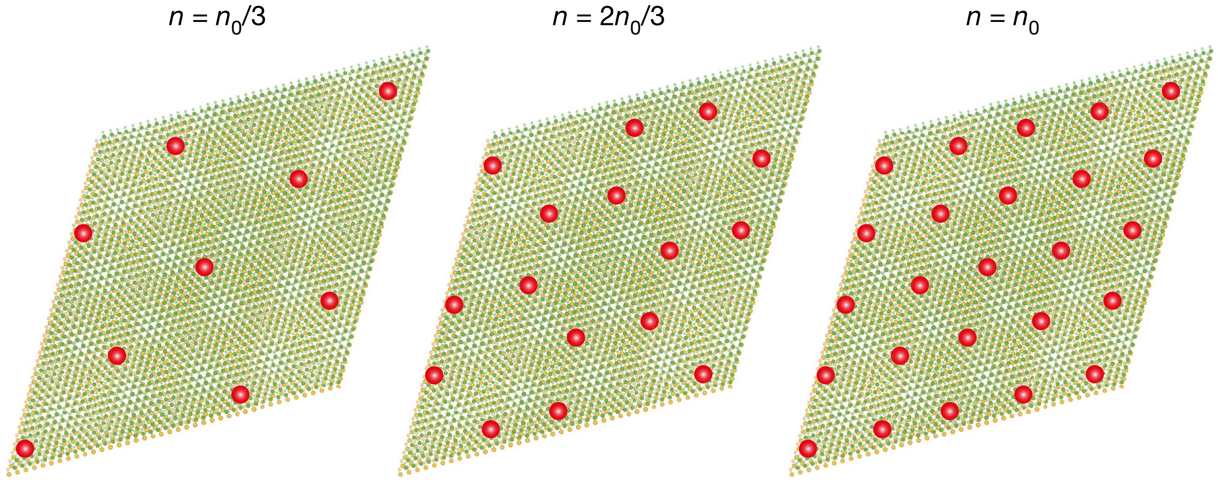
MX_2
M=Transition metal
X=Chalcogen

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg	3	4	5	6	7	8	9	10	11	12	Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La - Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac - Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

Correlated states in moiré TMDs

- "Magic continuum" of angles
- Also correlated insulators reported
  - "Cooperation" between insulator at 1/2 filling & (Van Hove) peak in density of states
  - Wigner crystals & stripe phases at fractional fillings → interactions of **extended** range





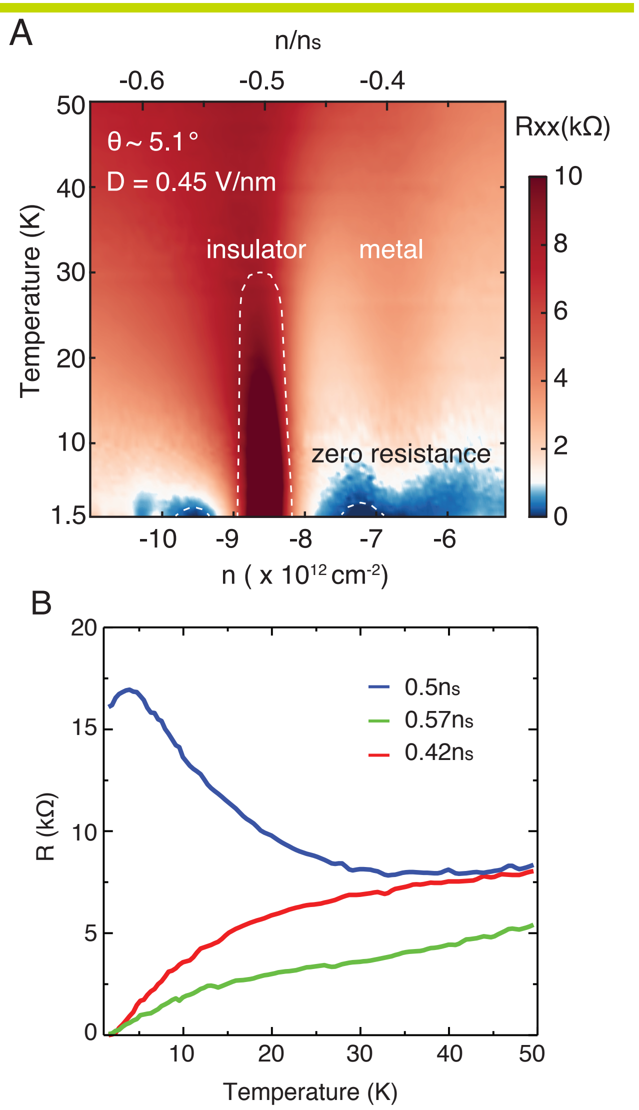
Wang et al, Nature Mat. (2020)
Regan *et al.*, Nature (2020)
Xu *et al.*, Nature (2020)
Jin *et al.*, Nature Materials (2021)
…

Superconductivity (?)

- Evidence for zero-resistance state in tWSe2
  Wang et al, Nature Mat. (2020)

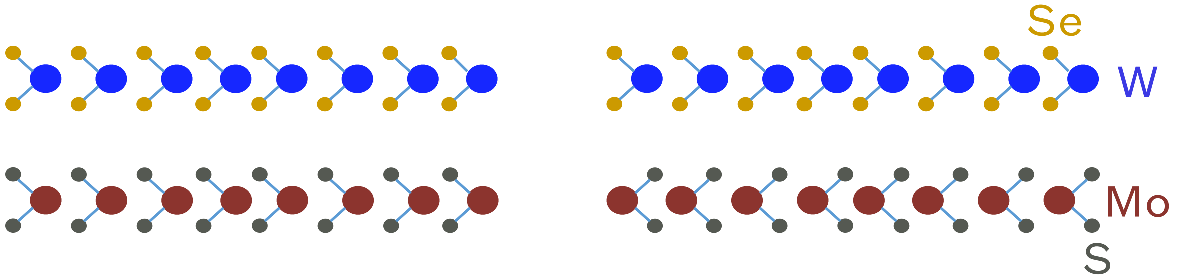
- Is superconductivity exclusive for graphene systems?
- Conventional vs. electronic mechanism?

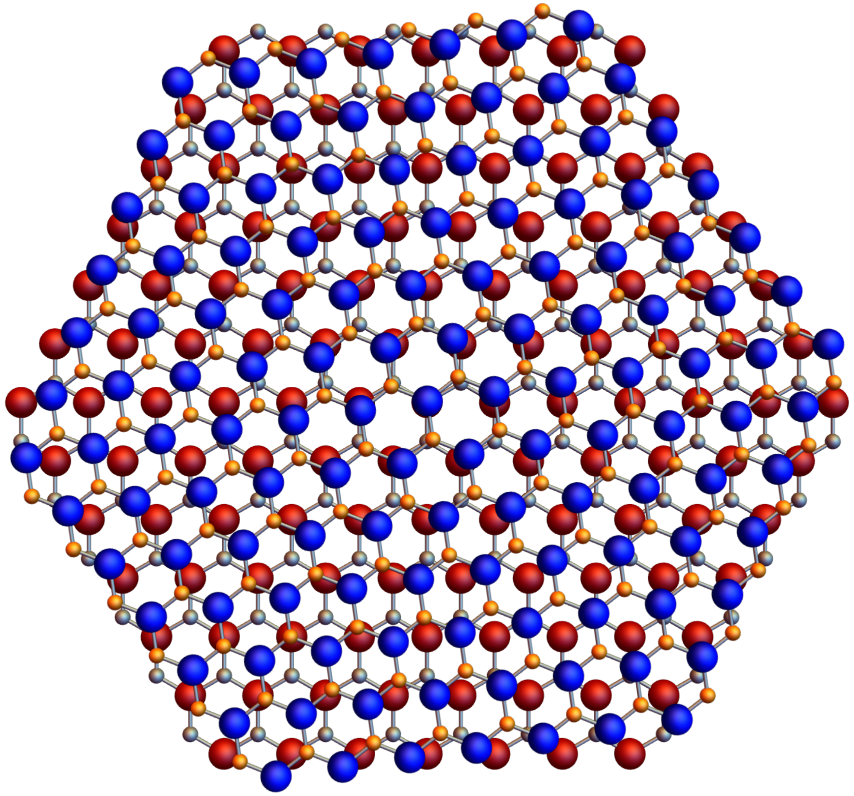
- Theoretical viewpoint:
  - SC not exclusive [here: Van Hove scenario]
  - If unconventional: hexagonal symmetry guarantees interesting SC states
    [2D irreps for p-,d- wave → nematic or topological SC]

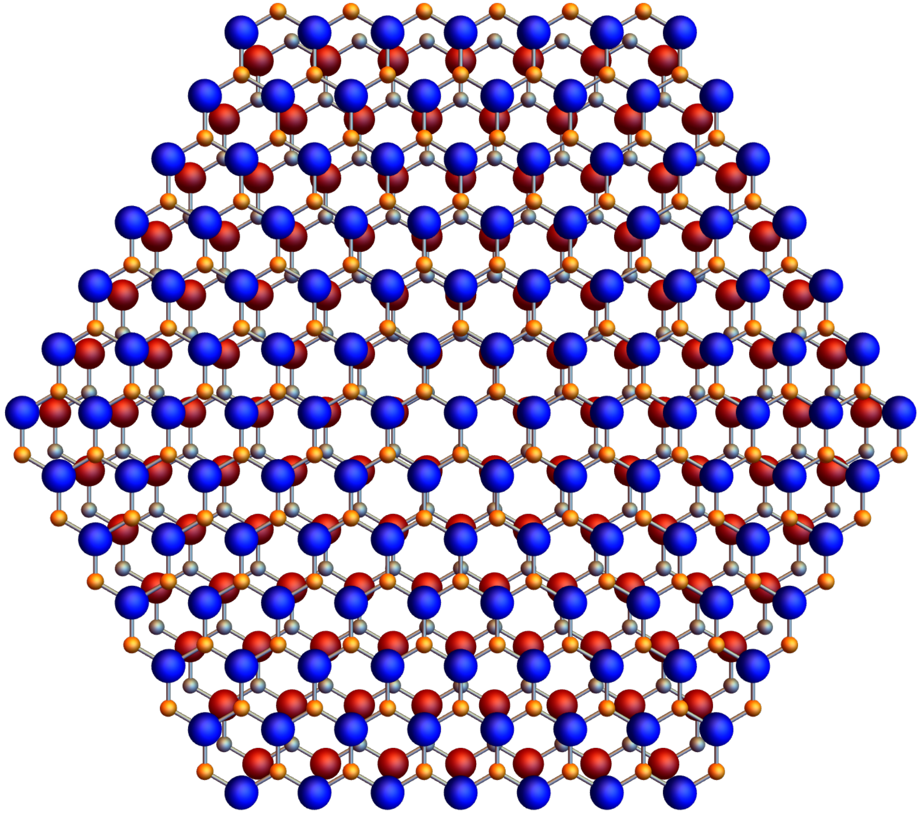


Moiré transition metal dichalcogenides

- Homo- vs hetero-bilayers
- AA vs AB stacking (0° vs 180°)



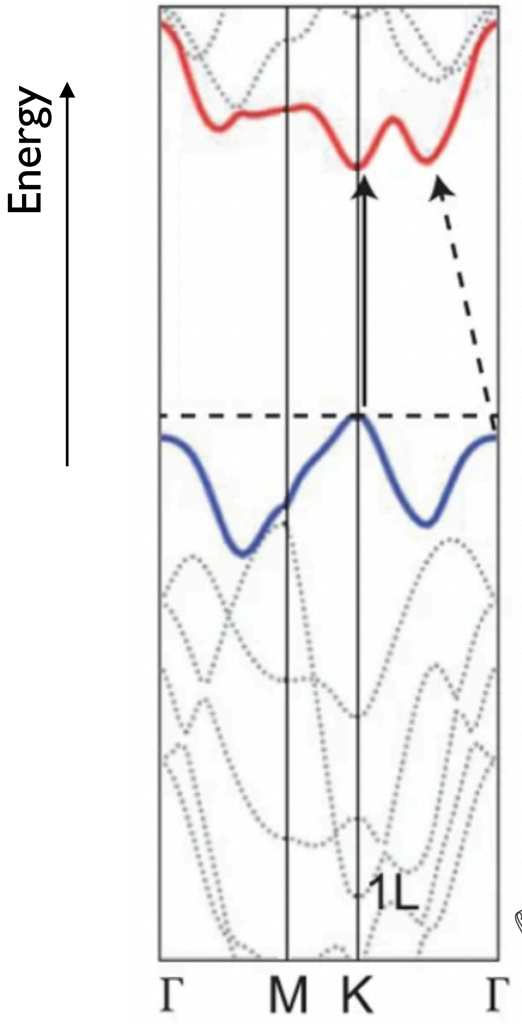




Moiré transition metal dichalcogenides

- Valence-band maxima near K, K’
- Spin-valley locking: $(K, \uparrow)$ and $(K', \downarrow)$
- Band gap depends on material

Band structure of WSe2



Chhowalla et al Nature Chem. (2013)

Moiré transition metal dichalcogenides

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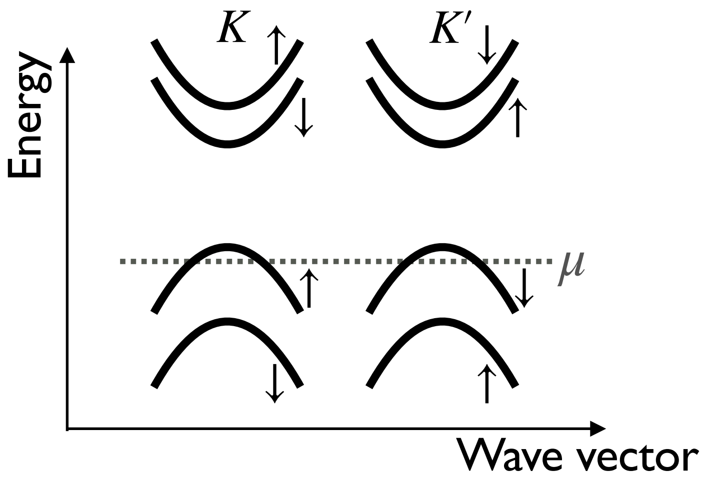
Schematic band structure WSe2



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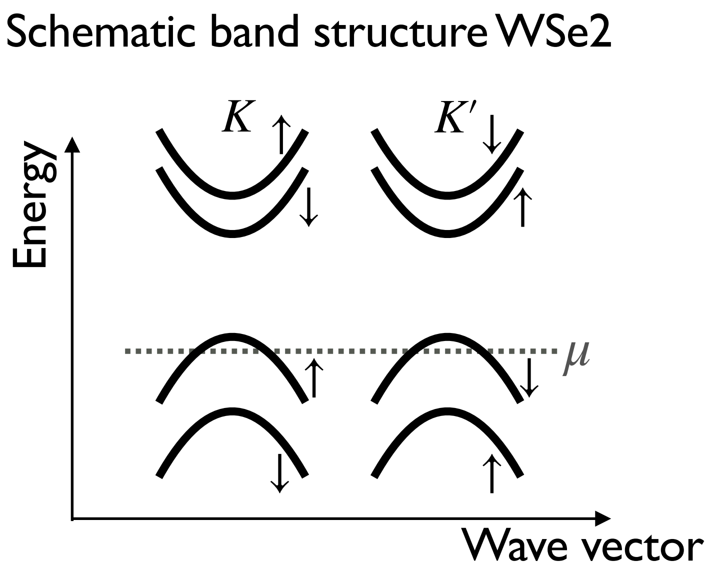
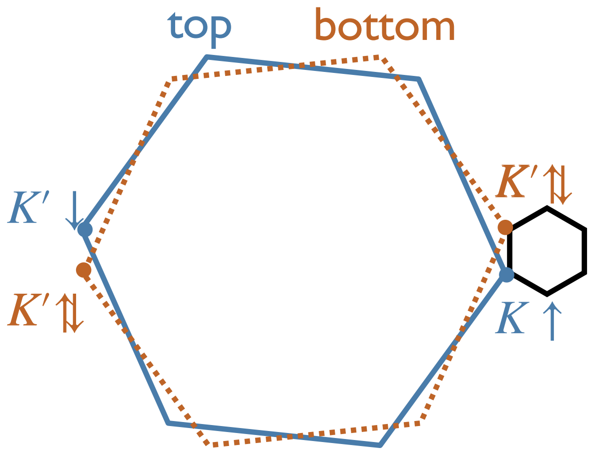
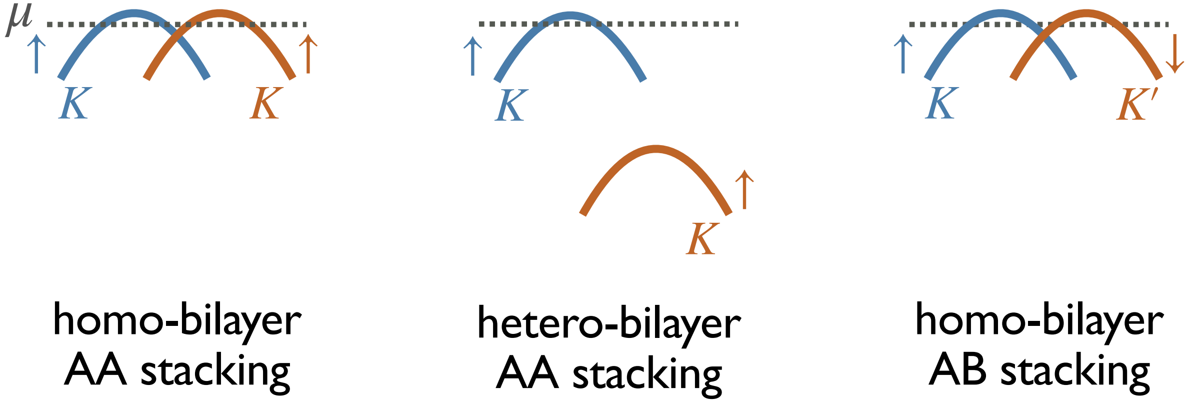


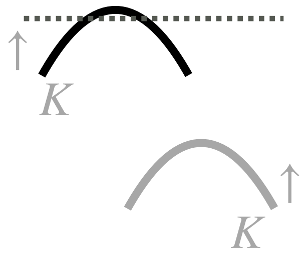
- Differences in set-up for moiré bands:

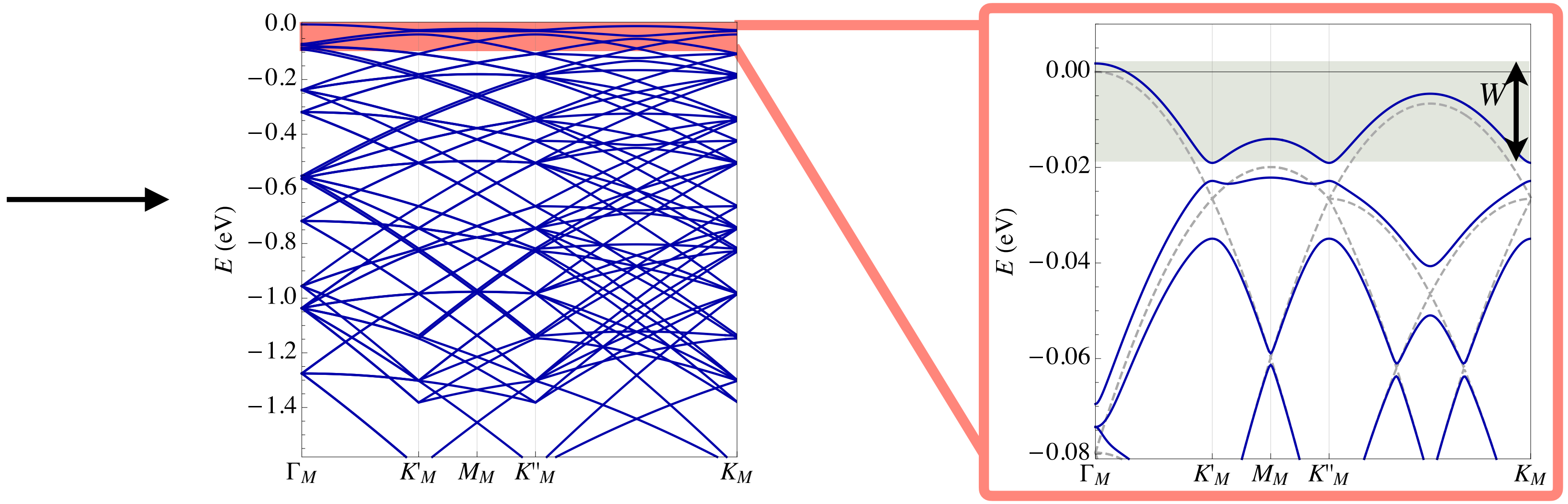




Simulate triangular-lattice Hubbard models

- Add moiré potential: $\Delta(\mathbf{r}) = \sum_{\mathbf{G}} V(\mathbf{G})\, e^{i\mathbf{G}\cdot\mathbf{r}}$
- Huge increase of unit cell → bands folded back into reduced zone





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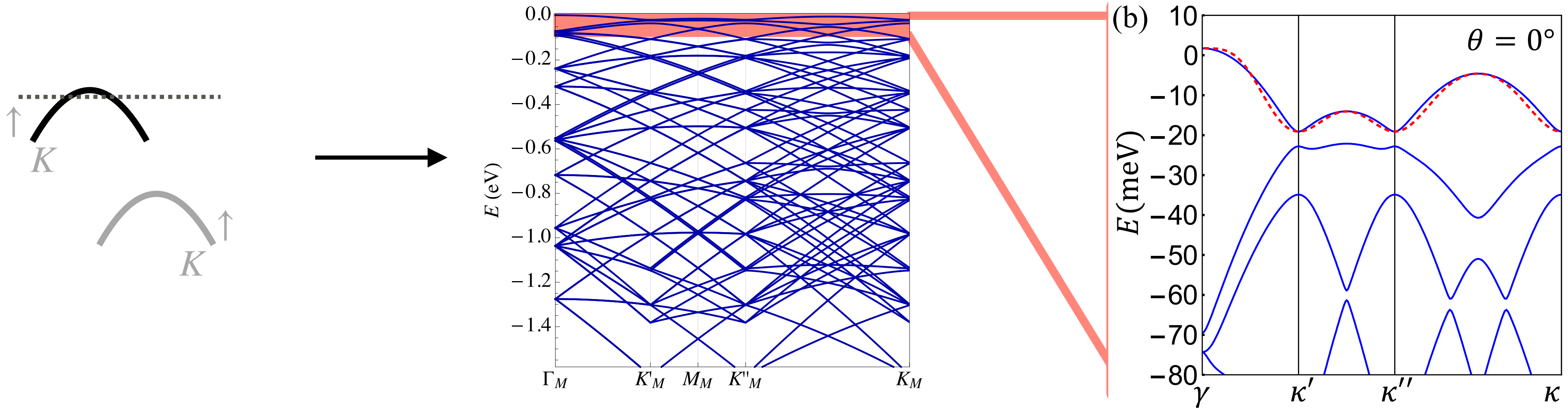
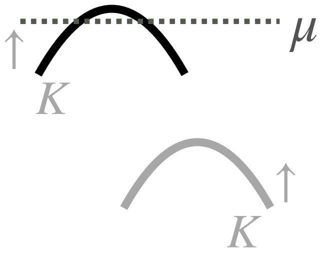


- Highest valence band: well described by triangular lattice Hubbard model

Wu, Lovorn, Tutuc, MacDonald, PRL (2018)

Simulate triangular-lattice Hubbard models

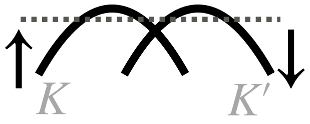
hetero-bilayer
AA stacking



Triangular-lattice Hubbard model with SU(2) between $(K\uparrow)$ & $(K'\downarrow)$

Wu, Lovorn, Tutuc, MacDonald, PRL (2018)

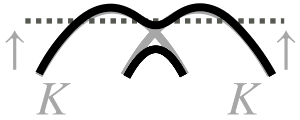
homo-bilayer
AB stacking



- Inter-layer hopping suppressed due to spin conservation
- SU(4) triangular-lattice Hubbard model
  $(K\uparrow$ top$)$, $(K'\downarrow$ top$)$, $(K\uparrow$ bot.$)$, $(K'\downarrow$ bot.$)$

Wu, Lovorn, Tutuc, Martin, MacDonald, PRL (2019)
Zhang Sheng, Vishwanath, PRL (2021)

homo-bilayer
AA stacking



- Displacement field breaks SU(2) between $(K\uparrow)$ & $(K'\downarrow)$ and tunes energy states

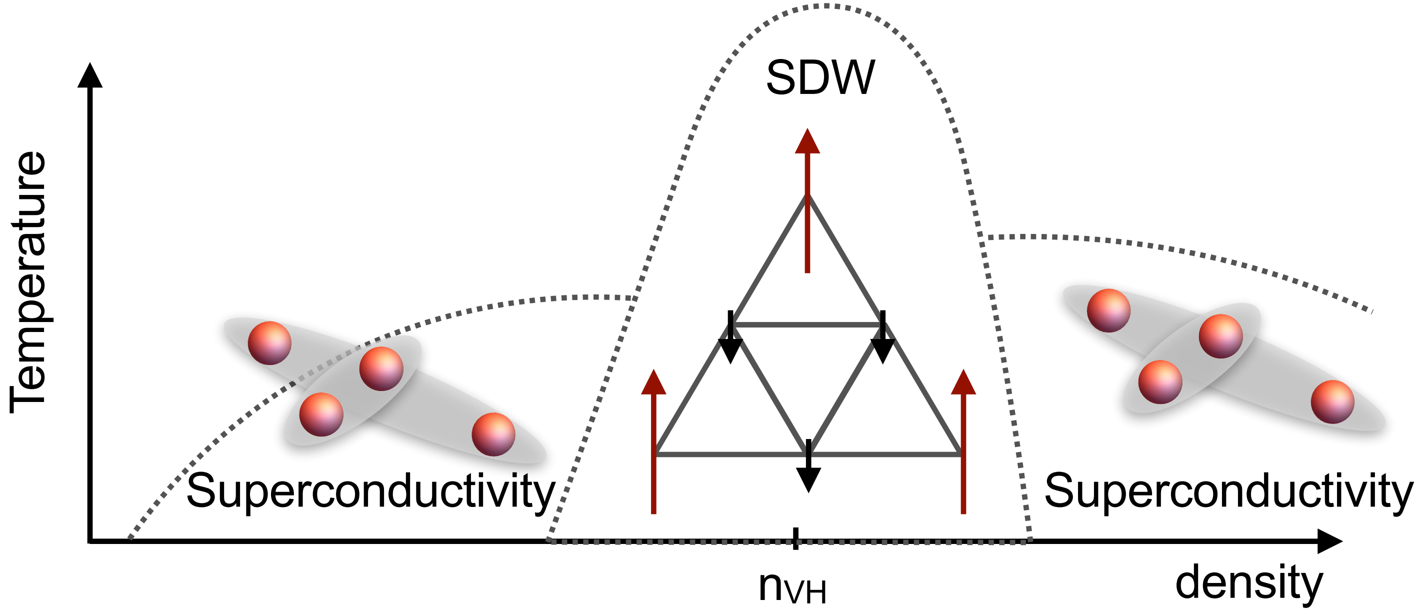
Pan, Wu Das Sarma, PRR (2020)
Zang, Wang, Cano, Millis, PRB (2021)

Interplay of orders for triangular lattice

- Two ordering tendencies at special filling:
  - Van Hove singularity
  - Nested Fermi surface

Honerkamp, PRB (2003)
Raghu et al, PRB (2010)
Nandkishore et al, Nat. Phys. (2012)
Chern, Batista PRL (2012)
Nandkishore et al, PRB (2014)

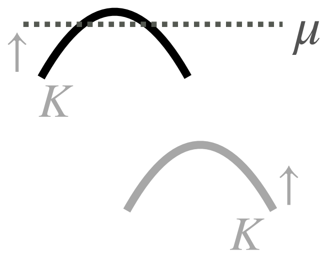
  - Magnetism: spin-density-wave
  - Unconventional superconductivity



➡ Change for moiré models?

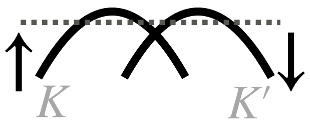
Effects on interplay of orders

hetero-bilayer
AA stacking



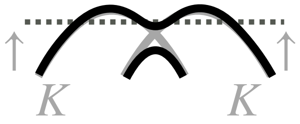
- Effect of longer-ranged Coulomb repulsion?
  - M. Scherer, D. Kennes, LC, arXiv:2108.11406
  - N. Gneist, LC, M. Scherer, arXiv:2203.01226

homo-bilayer
AB stacking



- Effect of more flavours in SU(4)?
  - Classen, Honerkamp Scherer, PRB 99, 195120 (2019)

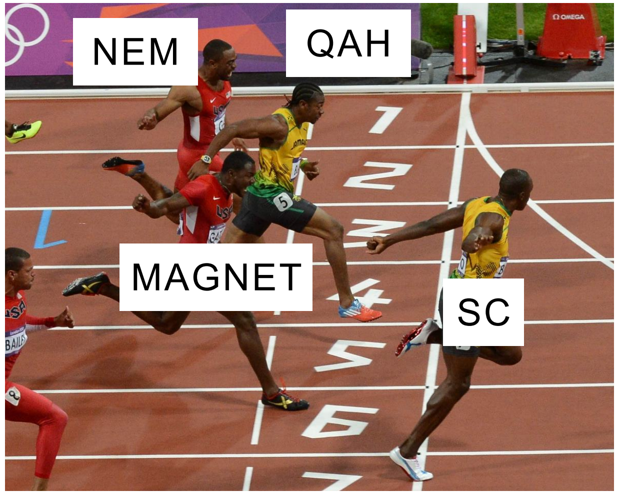
homo-bilayer
AA stacking



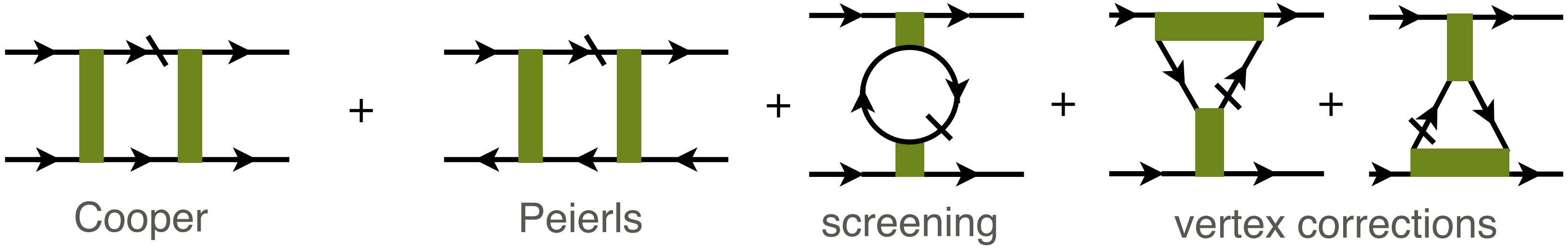
- Effect of Fermi surface geometry and Van Hove location?
  - L. Klebl, A. Fischer, LC, M. Scherer, D. Kennes arXiv:2204.00648

Competing orders from FRG

- Functional RG: discovery tool for ordering tendencies
- Calculate static 2-particle correlation function $V(p_1, p_2, p_3)$ dressed by interactions
  neglect $\geq$ 6-point vertex, self-energy feedback, frequency-dependence
- Unbiased, momentum-resolved!



$$\frac{d}{d\Lambda} V^{\Lambda}(k_1, k_2, k_3, k_4) =$$

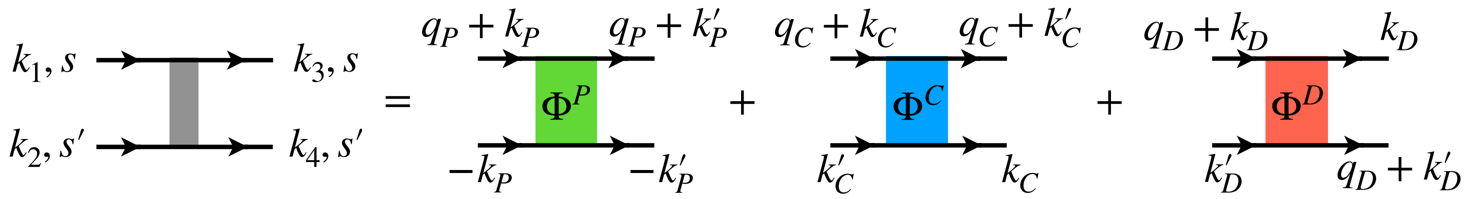


Metzner, Salmhofer, Honerkamp, Meden, Schönhammer, Rev. Mod. Phys. (2012)

Momentum resolution

- 3 schemes: Fermi-surface patching, TUFRG, momentum-mesh (+ non-SU(2) symmetry)
- Channel decomposition:

$$V = \Phi^P + \Phi^C + \Phi^D$$

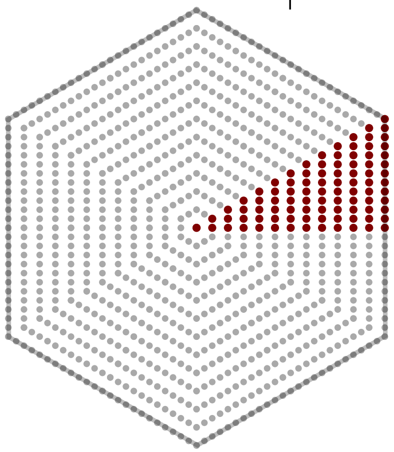


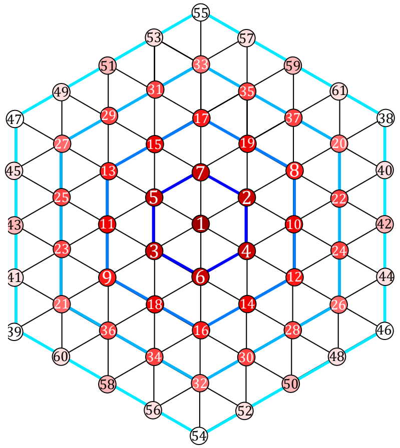
- TUFRG:

$$\Phi^X(q,k,k') = \sum_{l,l'} X^{l,l'}(q) f_l(k) f^*_{l'}(k')$$

Channel X	P	C	D
Interaction type	Pairing	Magnetic	Density
Transfer momentum q_X	$\boldsymbol{k}_1 + \boldsymbol{k}_2$	$\boldsymbol{k}_1 - \boldsymbol{k}_4$	$\boldsymbol{k}_1 - \boldsymbol{k}_3$
Momentum k_X	$-\boldsymbol{k}_2$	$\boldsymbol{k}_4$	$\boldsymbol{k}_3$
Momentum k'_X	$-\boldsymbol{k}_4$	$\boldsymbol{k}_2$	$\boldsymbol{k}_2$

- High-resolution of transfer momenta q
- Form-factor expansion for k,k' $f_l(k) = e^{i\mathbf{k}\cdot\mathbf{R}_l}$





Karrasch et al, J. Phys. Cond. Mat. (2008)
Husemann, Salmhofer, PRB (2009)
Lichtenstein et al, Comp. Phys. Com. (2017)

AA hetero-bilayer

- SU(2) Hubbard model

$$H = \sum_{i,j}\sum_{\sigma} t_{i-j} c^\dagger_{i,\sigma} c_{j,\sigma} - \mu \sum_{i\sigma} c^\dagger_{i,\sigma} c_{i\sigma} + \frac{U}{2}\sum_{i,\sigma,\sigma'} n_{i\sigma} n_{i\sigma'} + \sum_{\sigma,\sigma'}\sum_{i,j} V_{i-j} n_{i\sigma} n_{j\sigma'} \qquad n_{i\nu} = c^\dagger_{i\nu} c_{i\nu}$$

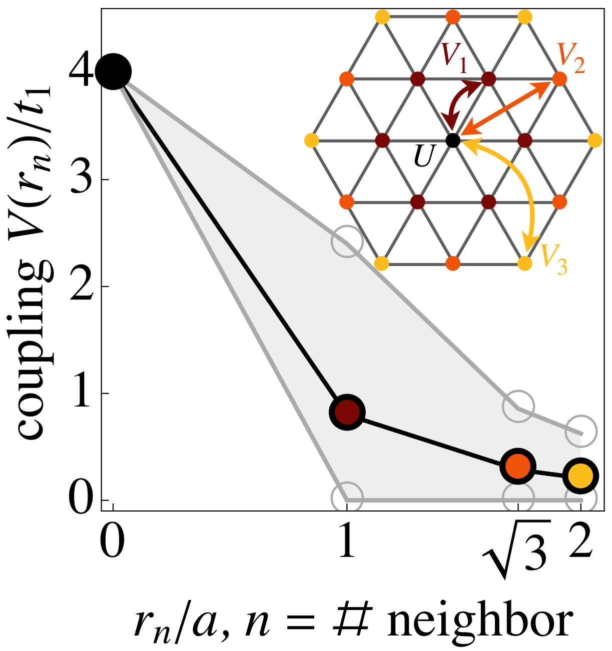
- **Longer-ranged** interactions important! Up to V_3.

- Overall strength tunable, e.g., substrate engineering

- Specifically: WSe2/MoS2

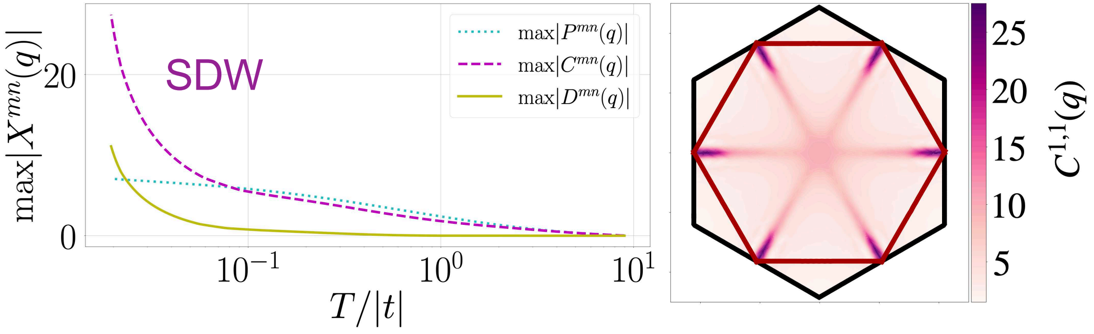
$\theta = 0:\ t_1 \approx 2.5\,\mathrm{meV}, t_2 \approx 0.5\,\mathrm{meV}, t_3 \approx 0.25\,\mathrm{meV}$

Wu, Lovorn, Tutuc, MacDonald, PRL (2018)

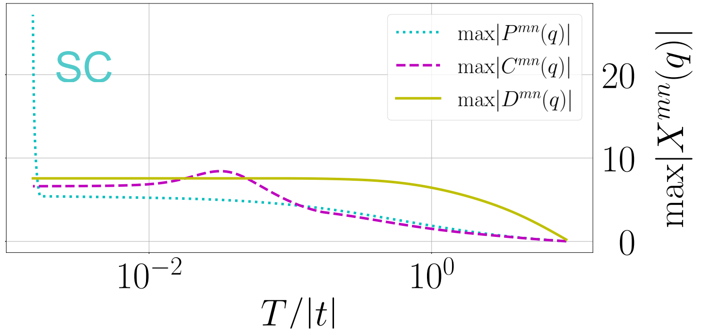


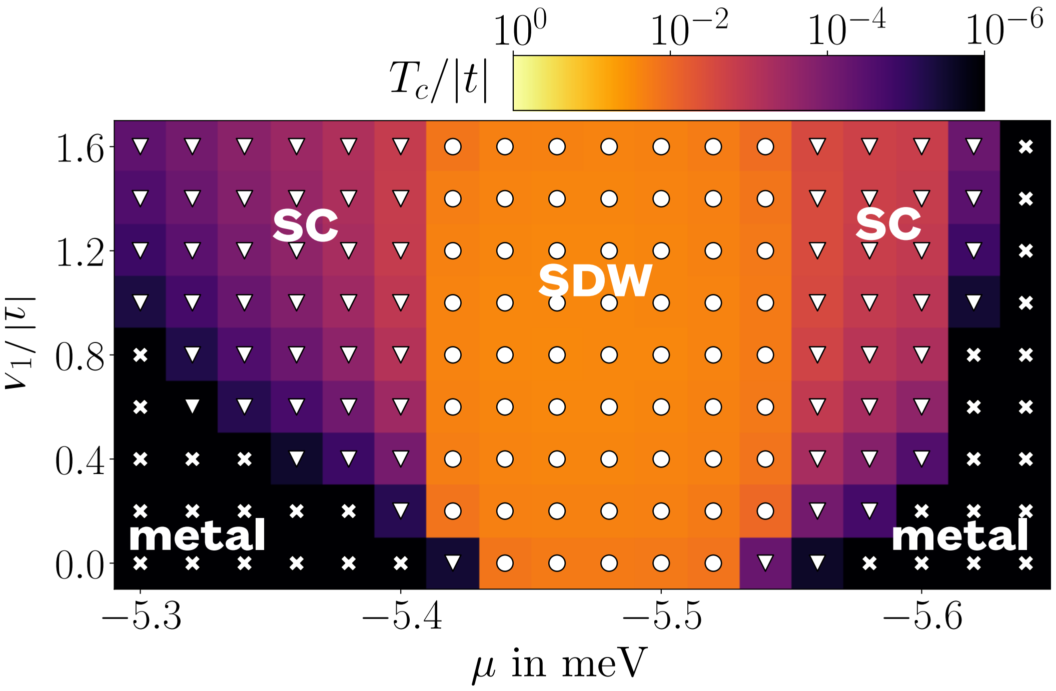
AA hetero-bilayer

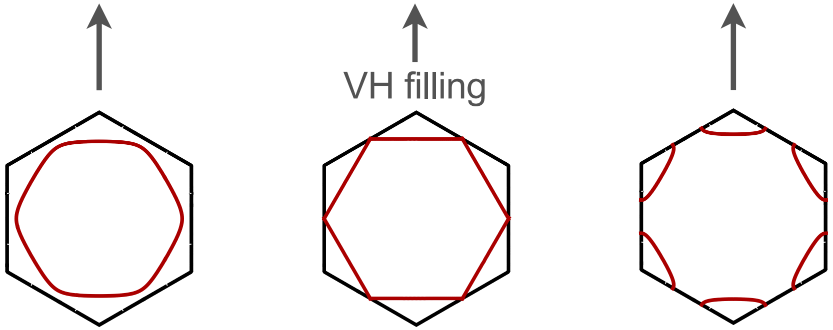
- Spin density wave instability:



- Longer-ranged interactions stabilise unconventional pairing state

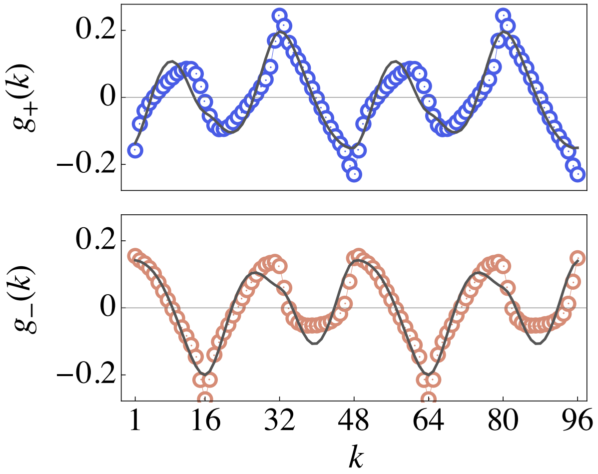


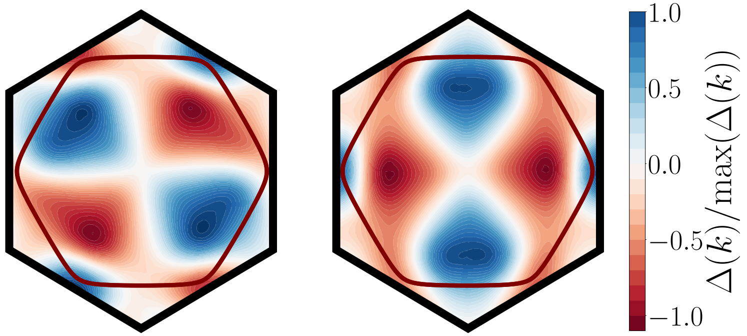




Pairing symmetry

- SC gap: $\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} V_{pair}(\mathbf{k}, \mathbf{k}') \frac{\Delta(\mathbf{k}')}{2\xi_{\mathbf{k}'}} \tanh \frac{\xi_{\mathbf{k}'}}{2T_c}$
- Fitted well by 2nd nearest-neighbour harmonics of irrep E_2 of lattice symmetry C_{6v} → "g-wave"
- 2 degenerate solutions (symmetry!)





Superconducting state

- 2 degenerate pairing solutions → gap $\Delta(\mathbf{k}) = \Delta_1 g_1(\mathbf{k}) + \Delta_2 g_2(\mathbf{k})$
- Which linear combination realised in ground state?
- Minimize Landau free energy

$$\mathscr{L} = \alpha(|\Delta_1|^2 + |\Delta_2|^2) + \beta(|\Delta_1|^2 + |\Delta_2|^2)^2 + \gamma|\Delta_1^2 + \Delta_2^2|^2$$

Superconducting state

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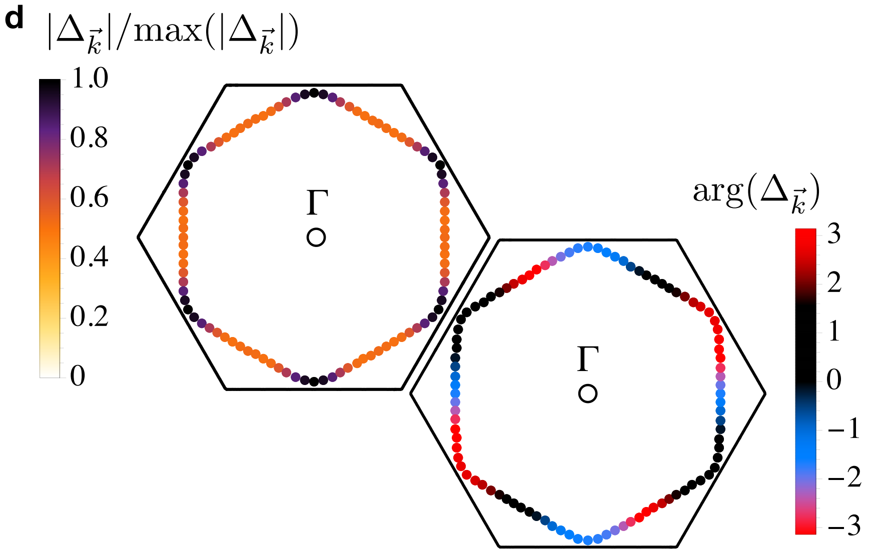
  $$\mathscr{L} = \alpha(|\Delta_1|^2 + |\Delta_2|^2) + \beta(|\Delta_1|^2 + |\Delta_2|^2)^2 + \gamma|\Delta_1^2 + \Delta_2^2|^2$$

- FRG data as input to calculate α, β, γ

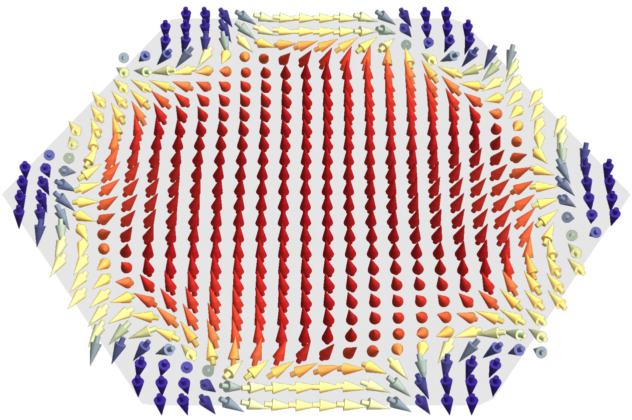
  $\Rightarrow\ \Delta(\mathbf{k}) = \Delta_1[g_1(\mathbf{k}) \pm i g_2(\mathbf{k})]$
- $|\Delta(\mathbf{k})|$ has no nodes, arg $\Delta(\mathbf{k})$ winds 4 times



Topological superconductivity

- Spontaneous breaking of time-reversal: $g_1 + ig_2$ vs $g_1 - ig_2$
- "Skyrmion" number $\mathcal{N} = \frac{1}{4\pi}\int_{\mathrm{BZ}} d^2k\, \mathbf{m} \cdot \left(\frac{\partial \mathbf{m}}{\partial k_x} \times \frac{\partial \mathbf{m}}{\partial k_y} \right)$

  based on "pseudo-spin" $\mathbf{m} = \frac{(\mathrm{Re}\Delta_{\mathbf{k}}, \mathrm{Im}\Delta_{\mathbf{k}}, \xi_{\mathbf{k}})}{\sqrt{\xi^2 + \Delta_{\mathbf{k}}^2}}$



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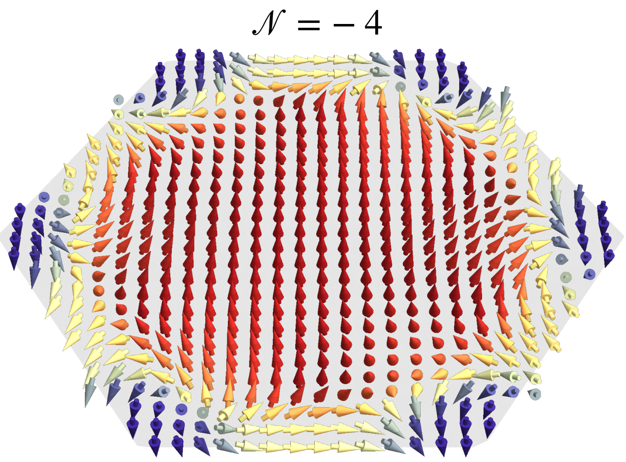
- $\left.\begin{array}{l} g + ig : \mathcal{N} = 4 \\ d + id : \mathcal{N} = 2 \end{array}\right\}$ same symmetry under C_6, different topology



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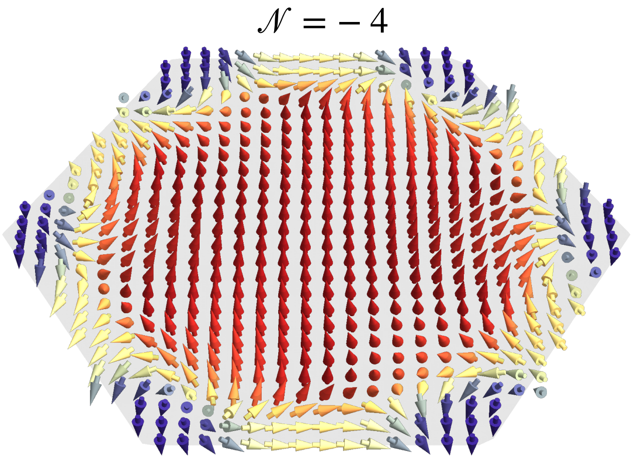
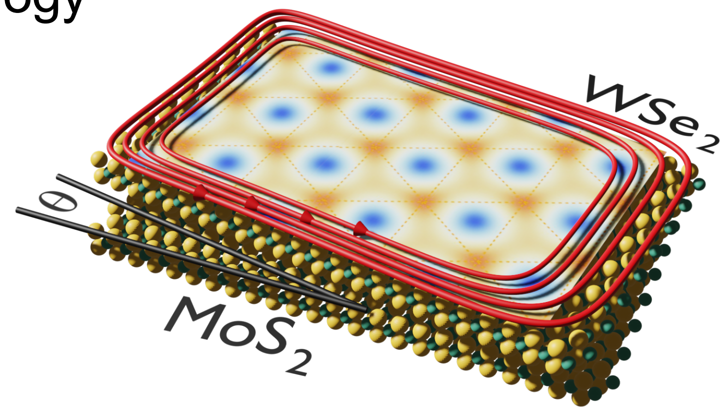


- $\left.\begin{array}{l} g + ig : \mathcal{N} = 4 \\ d + id : \mathcal{N} = 2 \end{array}\right\}$ same symmetry under C_6, different topology

- $\mathcal{N}$ chiral edge modes → enhanced, quantized response
  - Spin Hall conductance $\sigma^s_{xy} = \mathcal{N}\hbar/(8\pi)$
  - Thermal Hall conductance $\kappa = \mathcal{N}\pi k_B^2/(6\hbar)$



AB homobilayer

- SU(4) Hubbard model

$$H = -t\sum_{\langle i,j\rangle}\sum_{\alpha}(c^\dagger_{i\alpha}c_{j\alpha} + h.c.) + U\sum_i\left(\sum_\alpha n_{i,\alpha}\right)^2 + J\sum_{\langle i,j\rangle}\sum_x (c_i^\dagger T^x c_i)(c_j^\dagger T^x c_j)$$

SU(4) generators

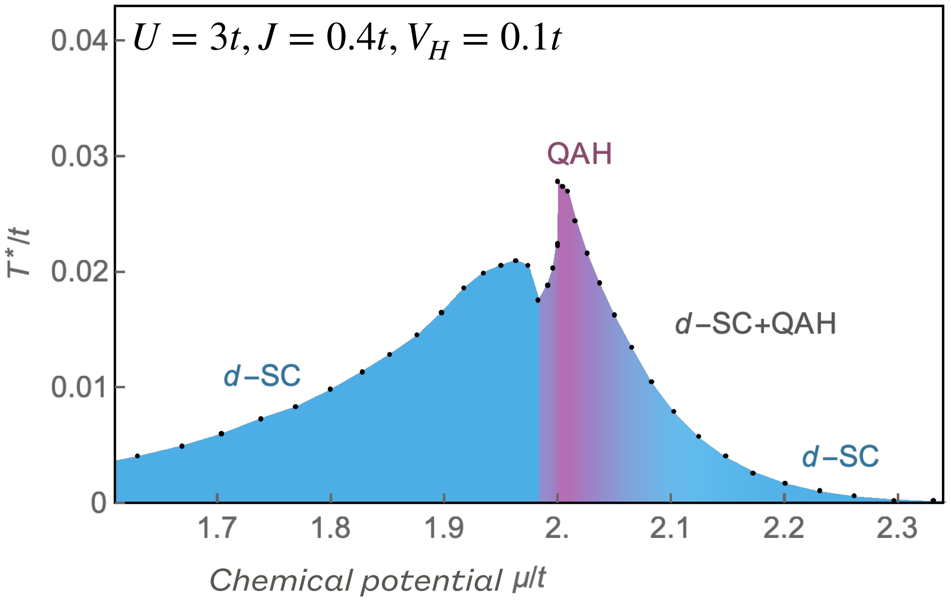
$$\alpha \in \{(K\uparrow t), (K'\downarrow t), (K\uparrow b), (K'\downarrow b)\}$$

- Include exchange coupling J

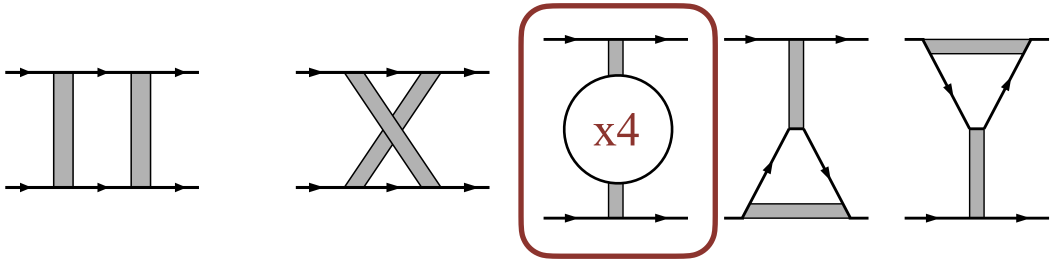
- Also tested robustness regarding Hund's coupling SU(4) → SU(2) x SU(2)

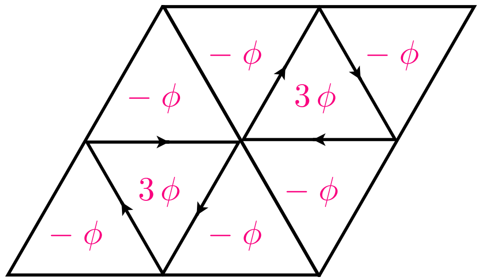
AB homobilayer

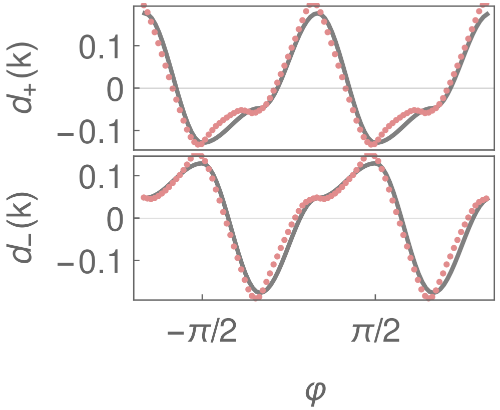
- Main ordering tendencies:
  - QAH: interaction-induced quantum anomalous Hall state (same as iCDW: loop currents)
  - d-wave superconductivity



- QAH instead of SDW due to more flavours







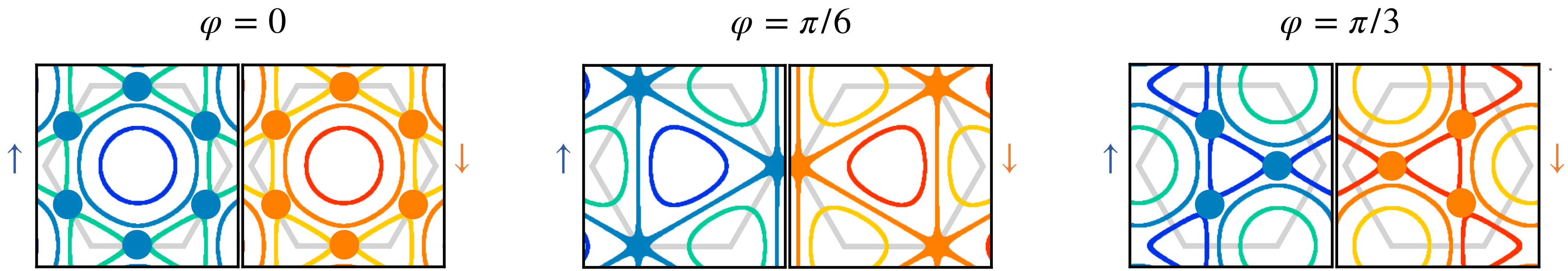
See also Lin, Nandkishore PRB(2019)

AA homobilayer

- Hubbard model with SU(2) breaking from displacement field

$$H = -\sum_{\langle i,j \rangle} \sum_{\sigma} |t| e^{i\sigma\varphi} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{U}{2} \sum_{i,\sigma,\sigma'} n_{i\sigma} n_{i\sigma'}$$

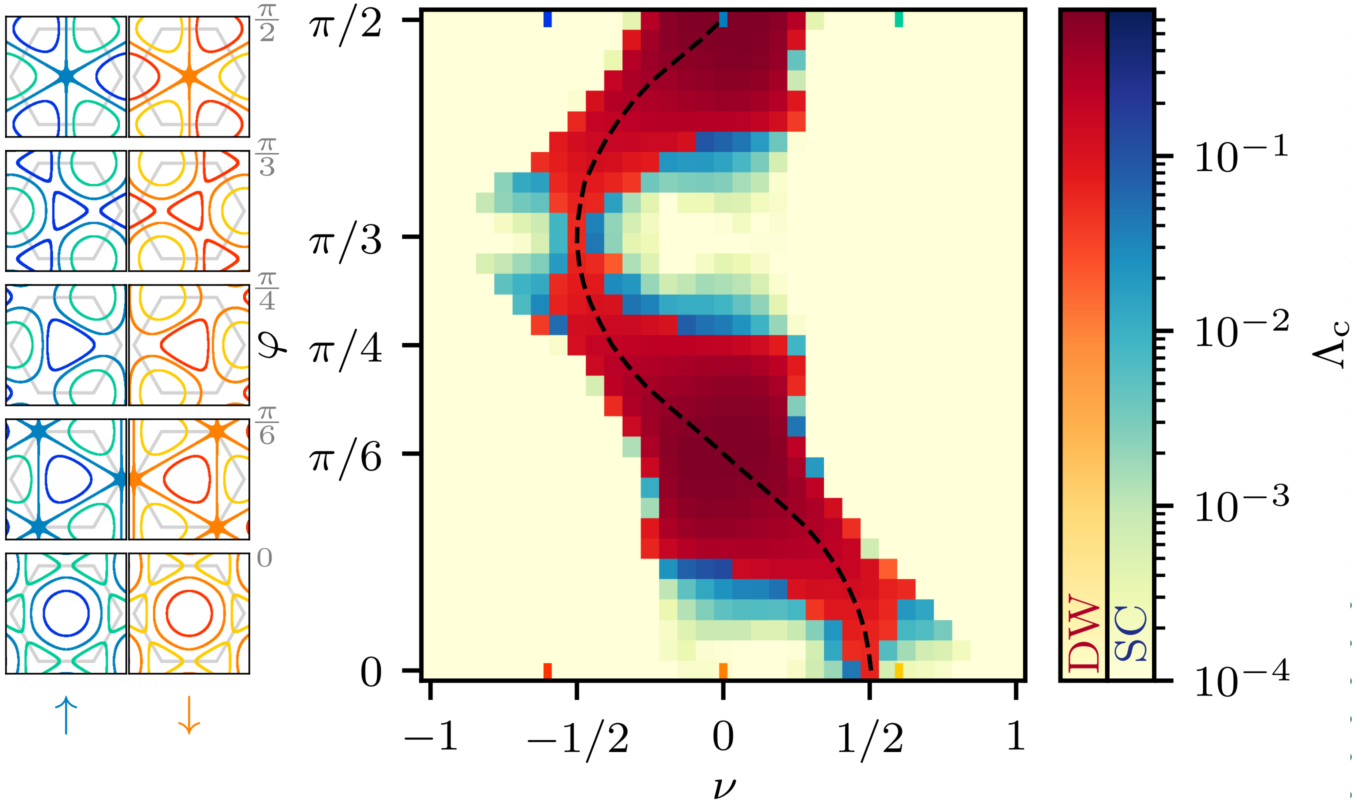
- Displacement field yields Peierls phase $\varphi \in [0, \pi/3]$
- Tunable Van Hove singularities → rich phase diagram of symmetry-broken phases



Pan, Wu Das Sarma, PRR (2020); Zang, Wang, Cano, Millis, PRB (2021)

AA homobilayer

- Density-wave instabilities follow Van Hove singularity
- Fluctuations mediate pairing in vicinity



AA homobilayer

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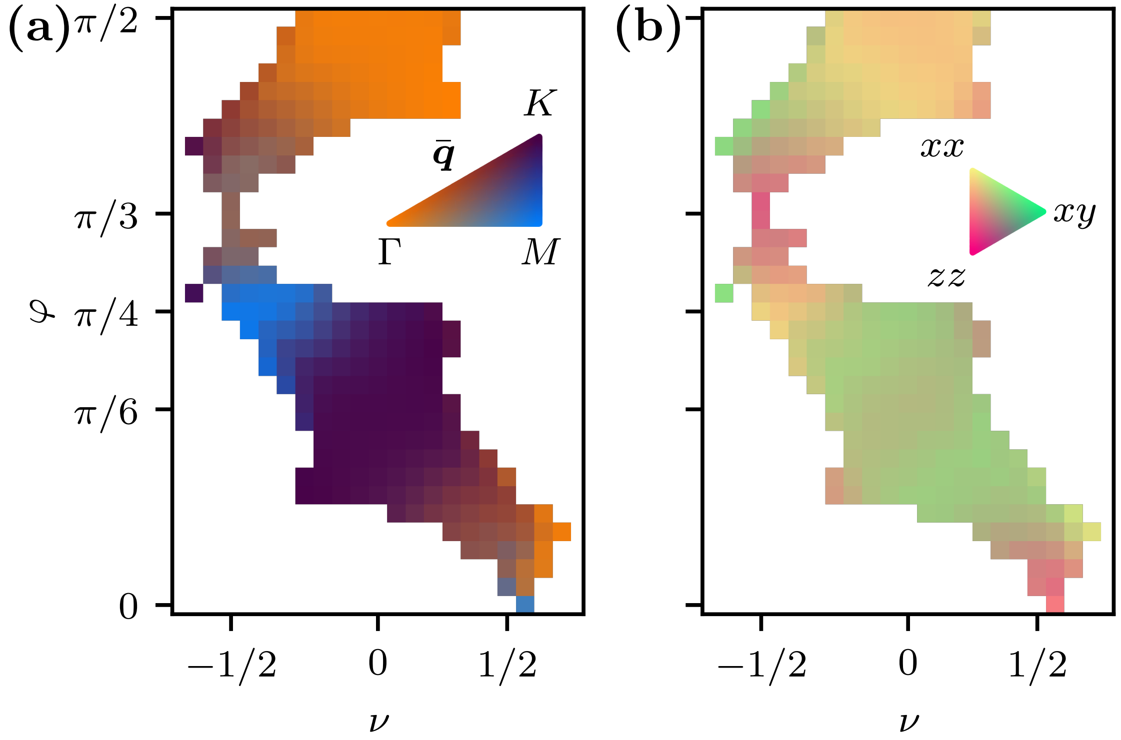
- (Incommensurate) wave vectors of DWs follow Fermi surface nesting:

  3 stripes → $120°$ spiral → FM



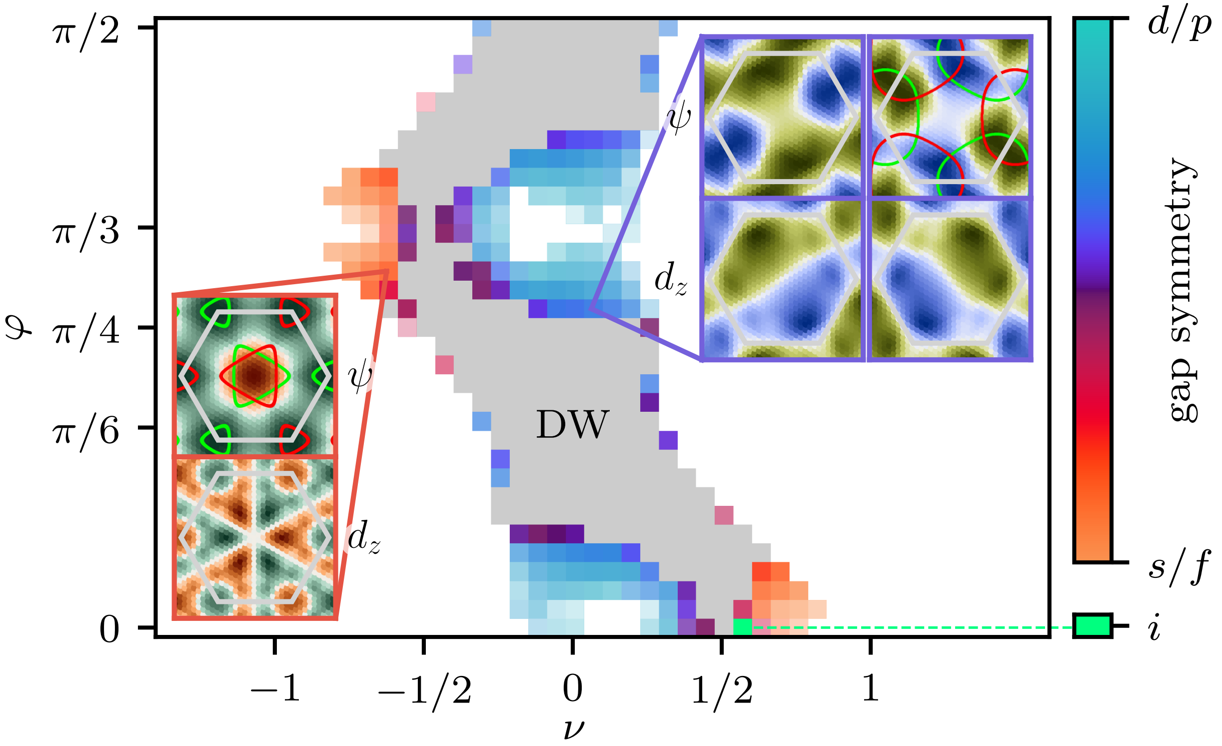
AA homobilayer

- Density-wave instabilities follow Van Hove singularity
- Fluctuations mediate pairing in vicinity

- (Incommensurate) wave vectors of DWs follow Fermi surface nesting:

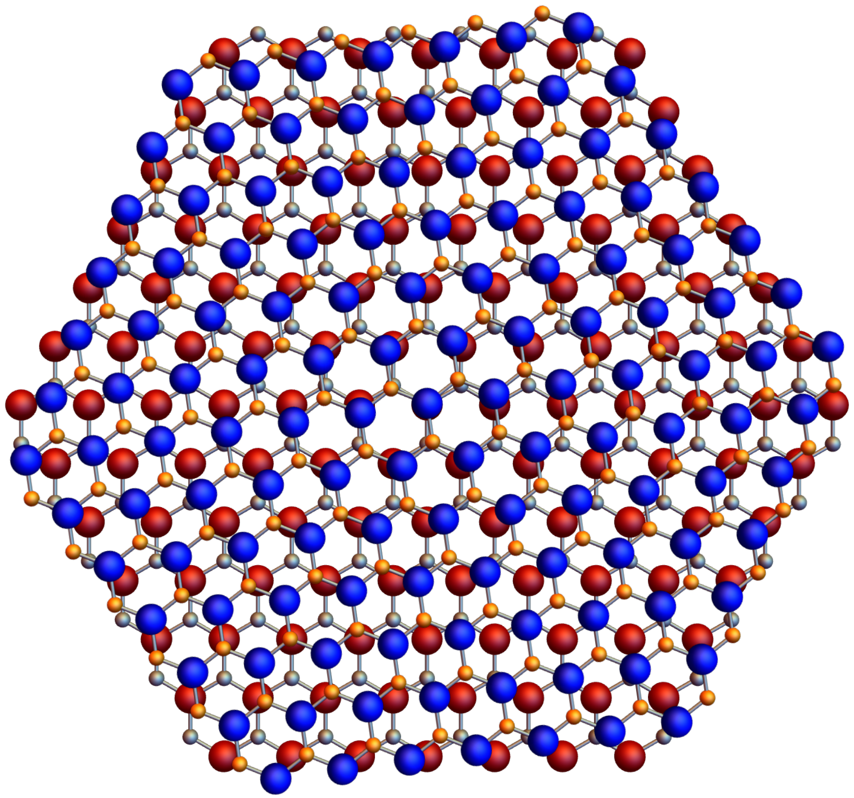
  3 stripes → 120° spiral → FM

- Pairing symmetry: mixed s/f or p/d (p+ip/d+id)
- Mainly determined by filling (i.e. Fermi surface): maximise gap



Summary

- Study correlated phases and mechanism for superconductivity
- Moiré materials: stacked and twisted 2D materials
- Moiré transition metal dichalcogenides as "simulators" for triangular-lattice Hubbard model
- FRG to investigate interplay of orders → unbiased method with high enough momentum resolution



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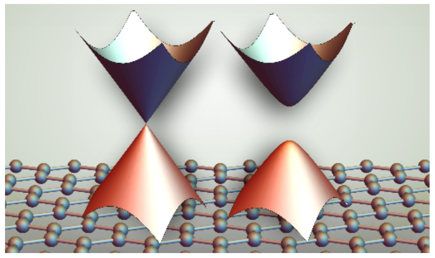
Thank you!

Nico Gneist, Michael Scherer (Bochum)
Lennart Klebl, Ammon Fischer, Dante Kennes (RWTH Aachen)



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