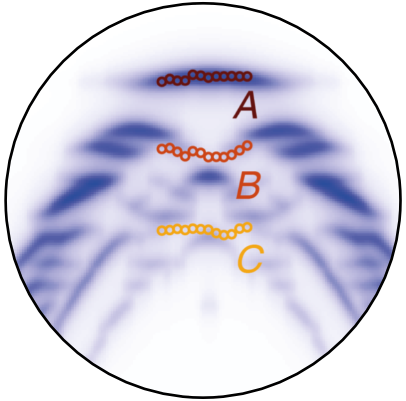
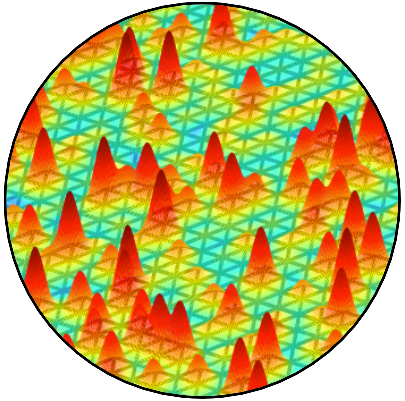
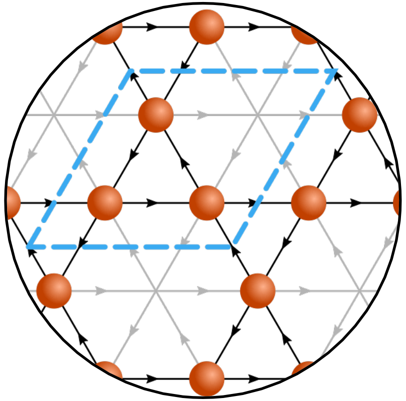
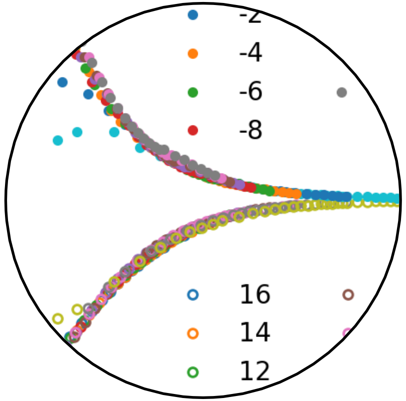


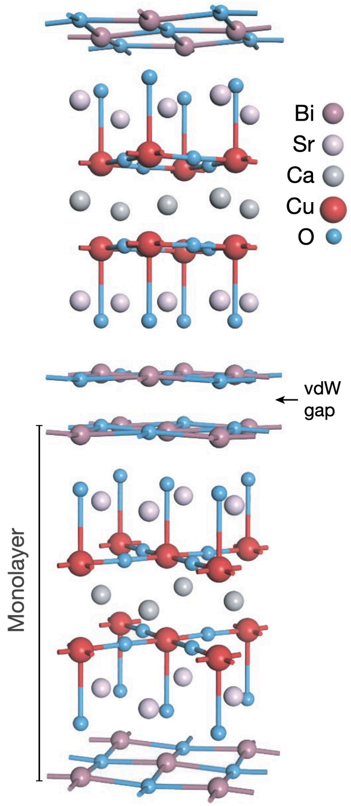




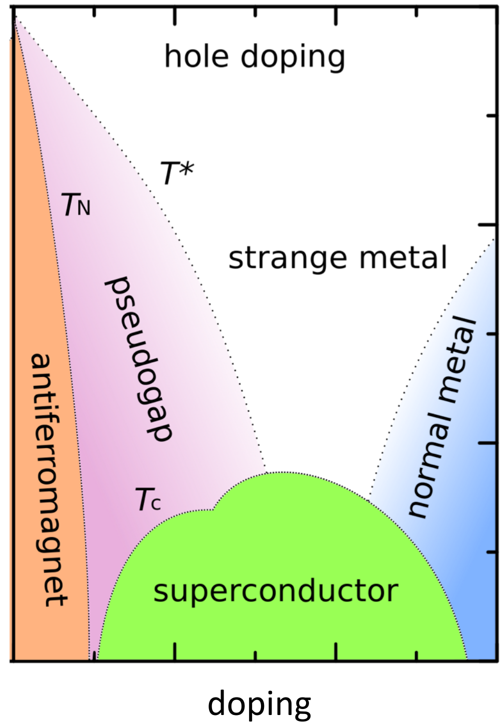
Forget graphene: more exotic moiré physics with TMDs

Louk Rademaker

Friday 7 October 2022, LPS Orsay

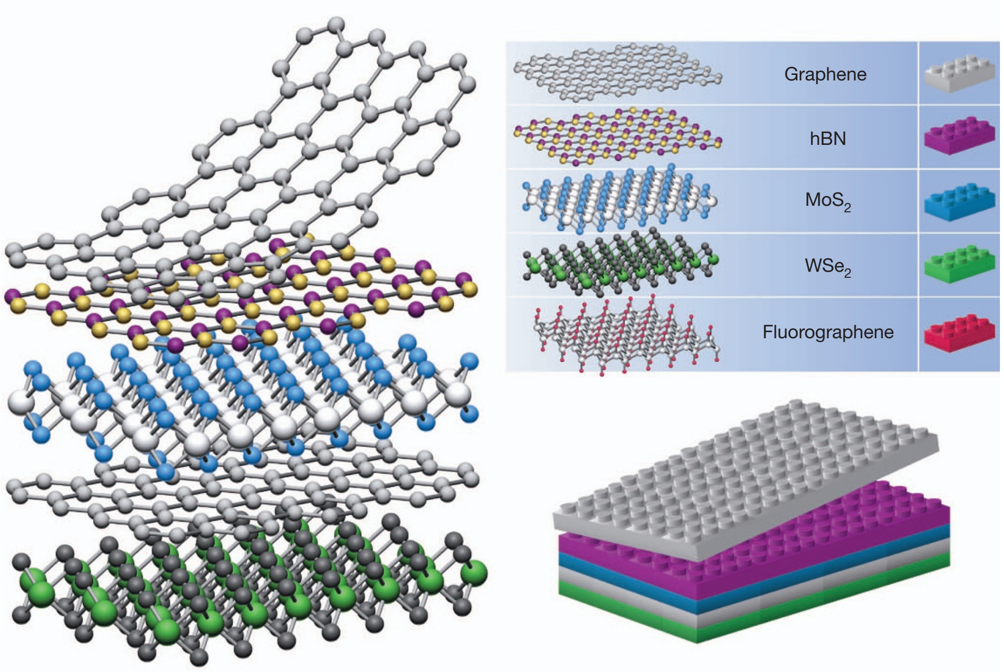
Strong correlations!





Van der Waals – moiré materials

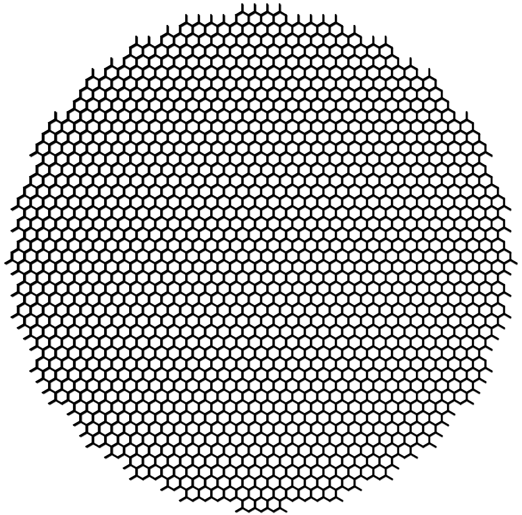
Van der Waals heterostructures: Atomic ‘LEGO’



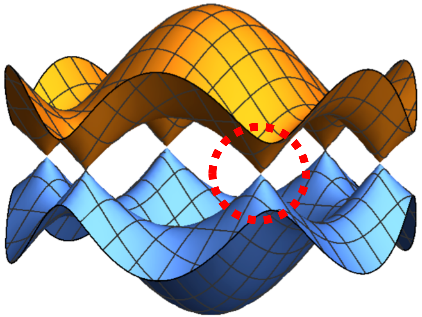
Ref: Geim Nature 2013

Moiré pattern

Twist or Lattice mismatch



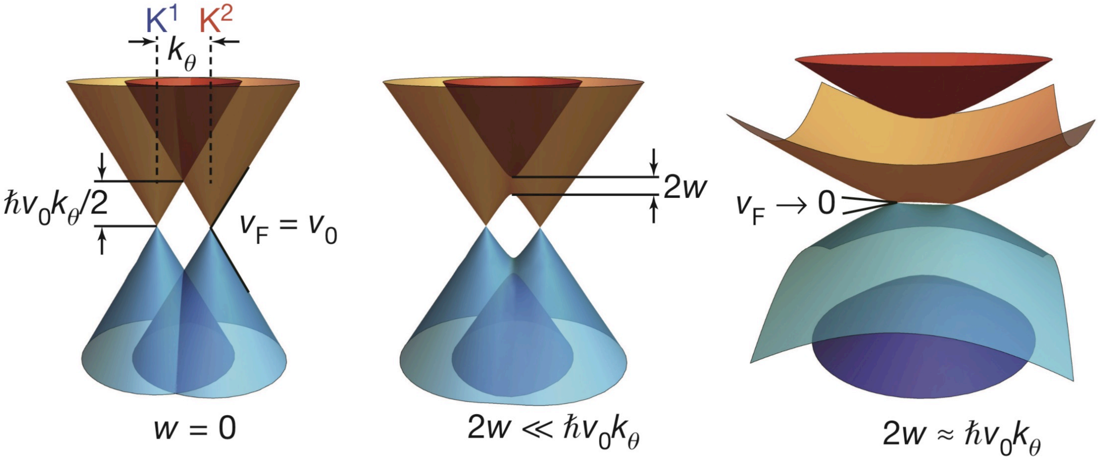
Monolayer graphene



Dirac cone dispersion of **massless** electrons

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

Twisted Bilayer Graphene (tBG)

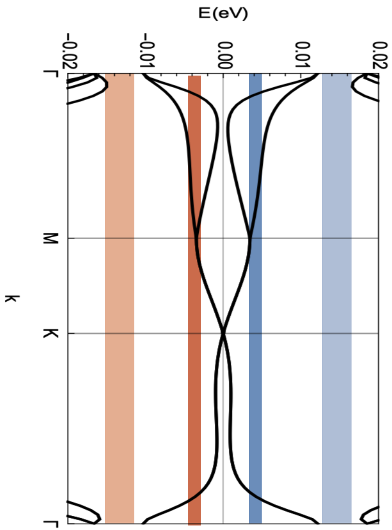


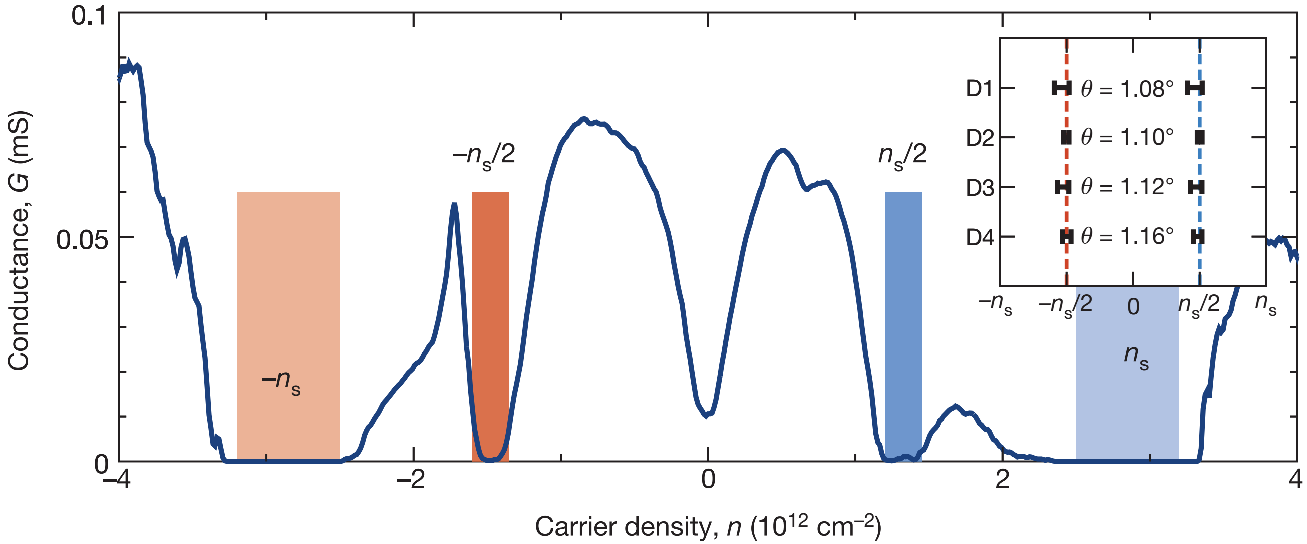
Dirac cones of each layer are **close** **+** Interlayer **hopping** **=** Topological **Flat bands**

'Magic Angle' tBG

Ref: Bistritzer PNAS 2011; Cao Nature 2018

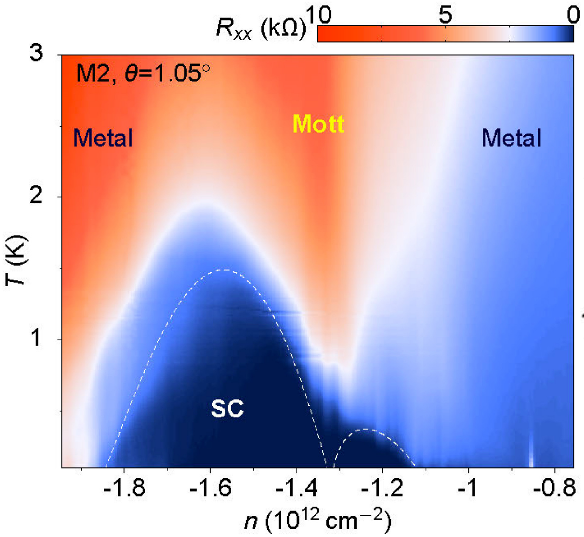
Correlated insulator

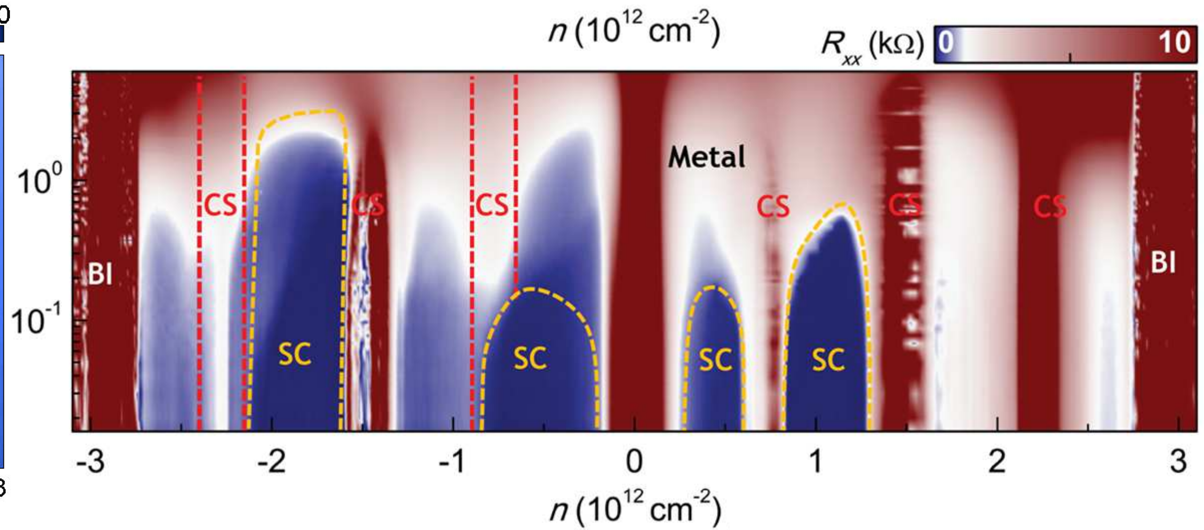




Ref: Rademaker PRB ‘18, Cao Nature ’18

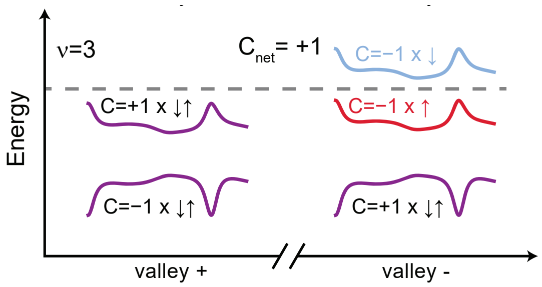
Superconductivity

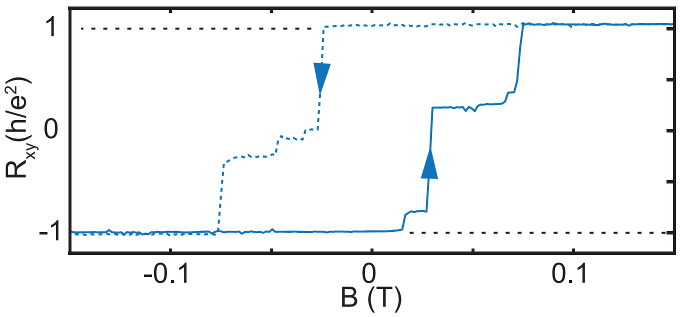




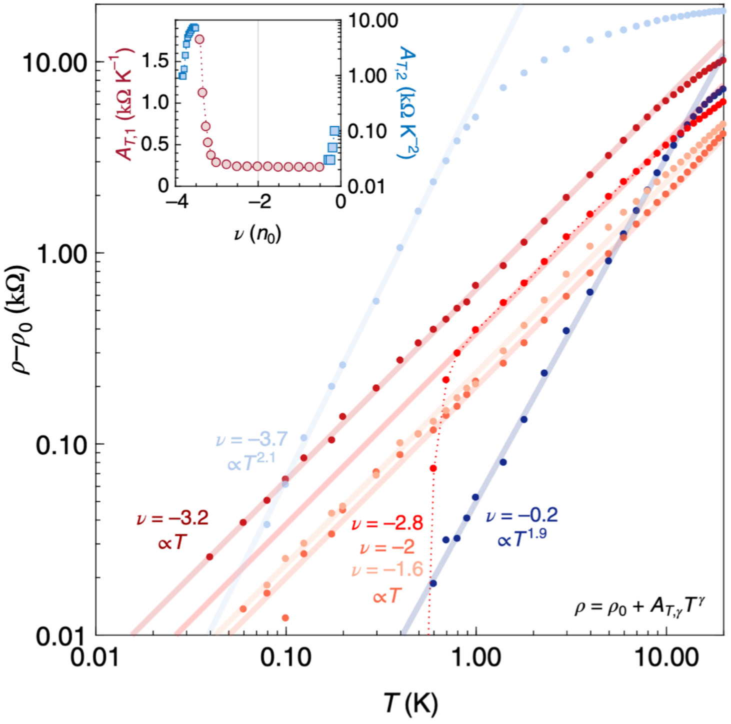
Ref: Cao Nature ’18; Lu Nature ‘19

Quantum Anomalous Hall effect



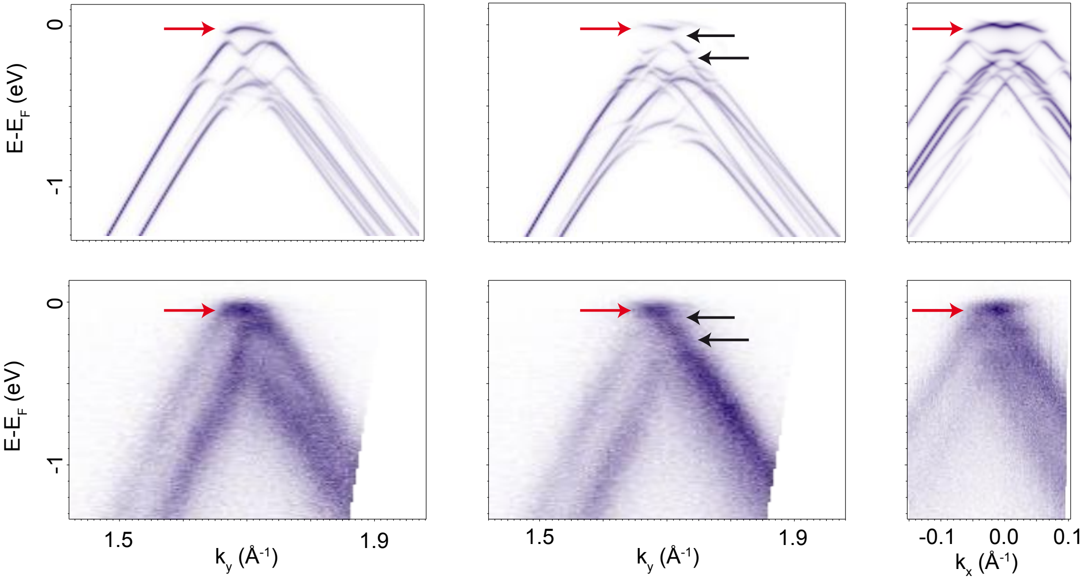


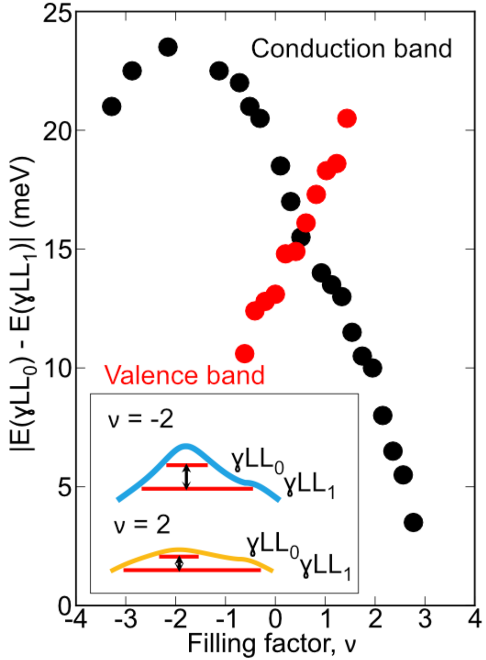
Strange metal



Ref: Serlin Science '20; Jaoui Nat Phys '22

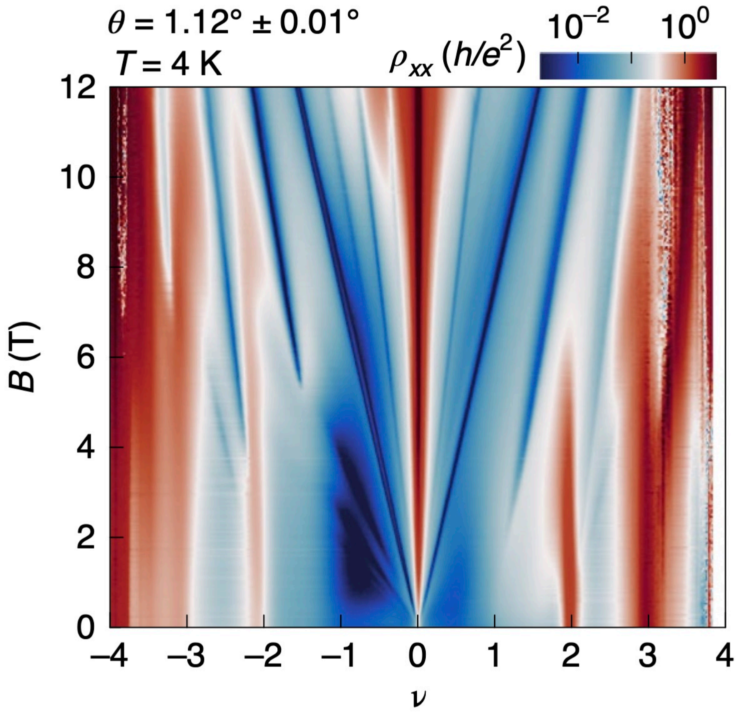
… but bands are not very flat

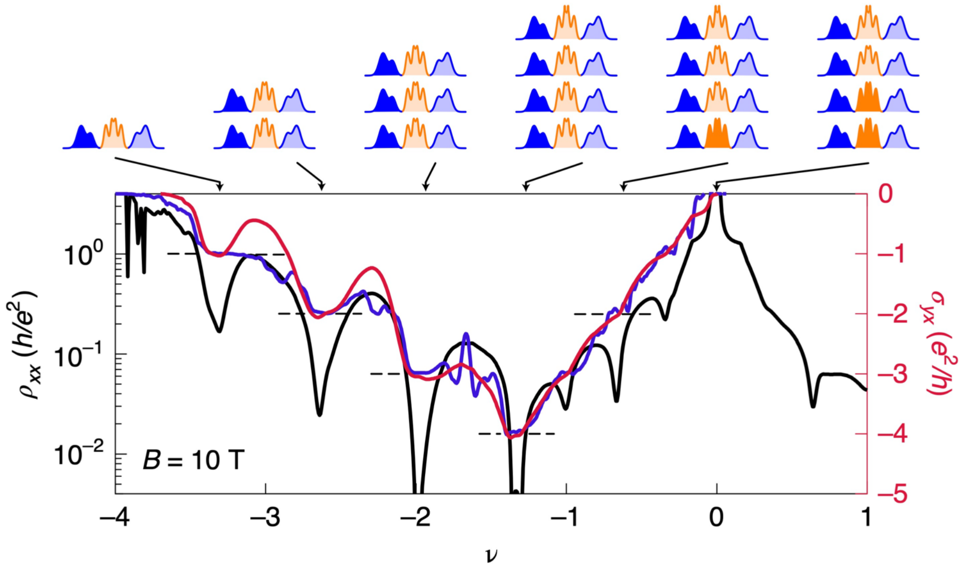




Ref: Rademaker PRB ’18; Rademaker PRB ‘19; Lisi, Rademaker Nat Phys ’20; Choi Nat Phys ‘21

… and correlated insulators are ferromagnets

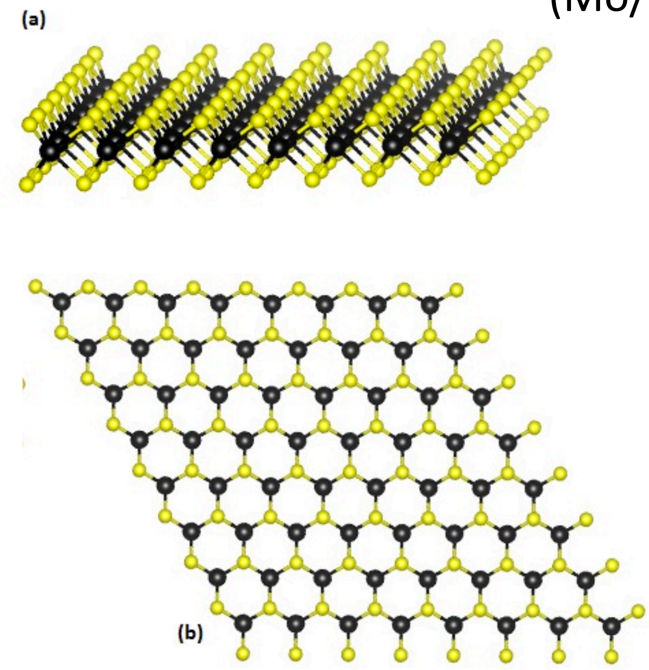


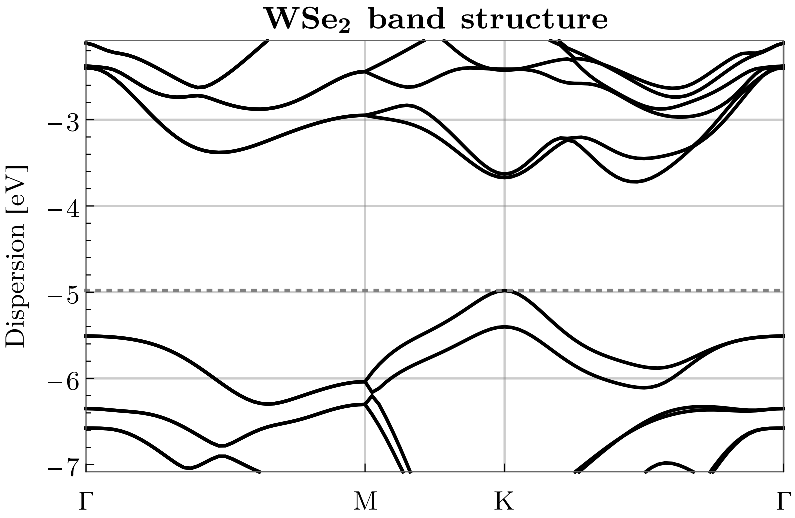


Ref: Saito, Rademaker Nat Phys '21

Monolayer transition metal dichalcogenides (TMDs)

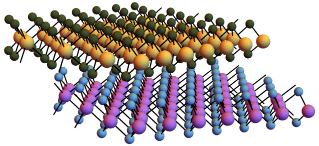
(Mo/W) $(S/Se/Te)_2$



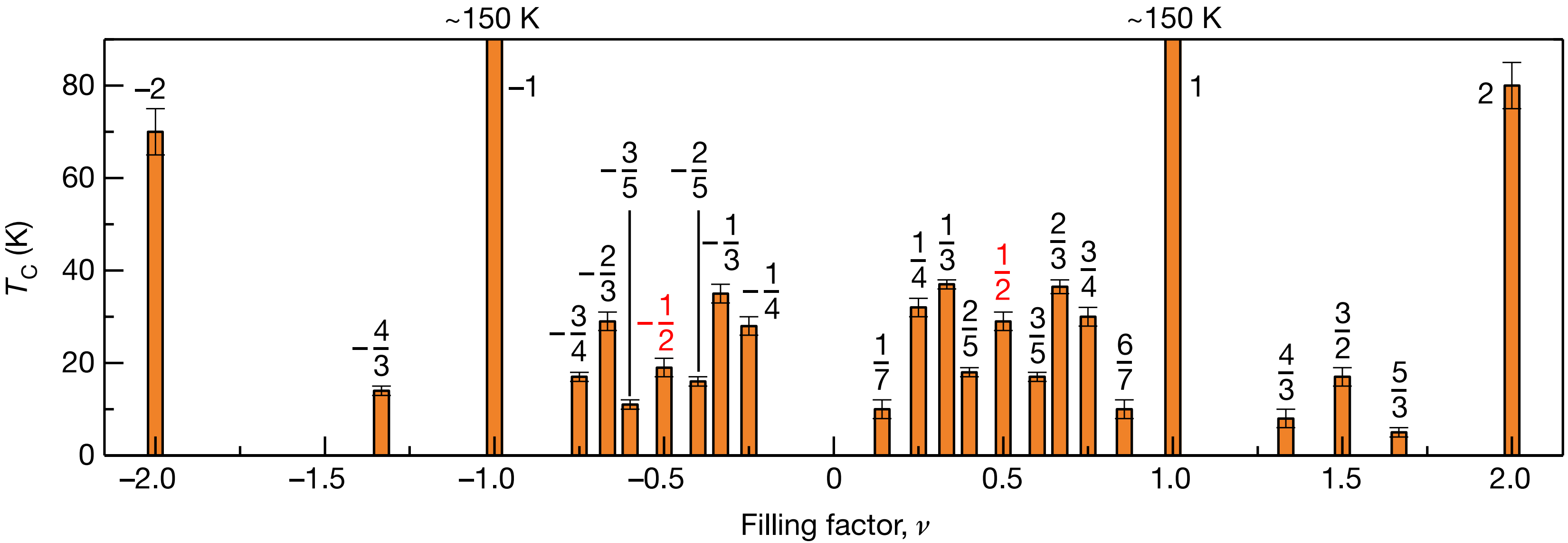


Ref: Rademaker arXiv ‘20

Wigner-Mott insulators

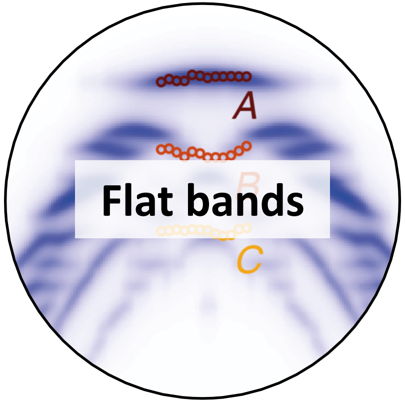


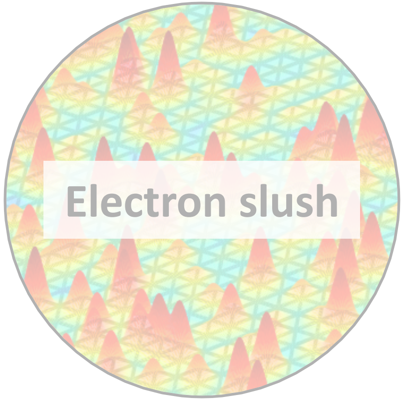
Moiré material from aligned **WS_2/WSe_2** "heterobilayers"

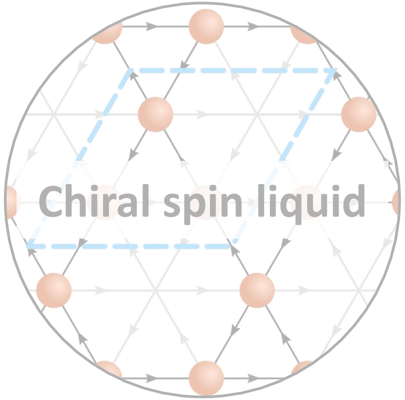


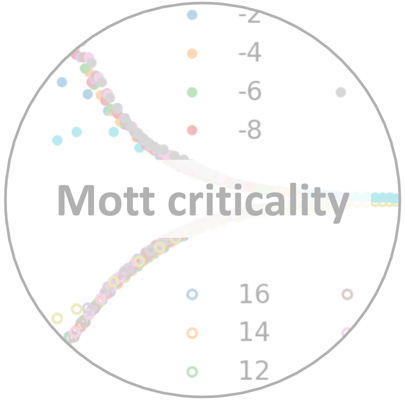
Ref: Xu Nature '20

Overview: exotic moiré physics with TMDs



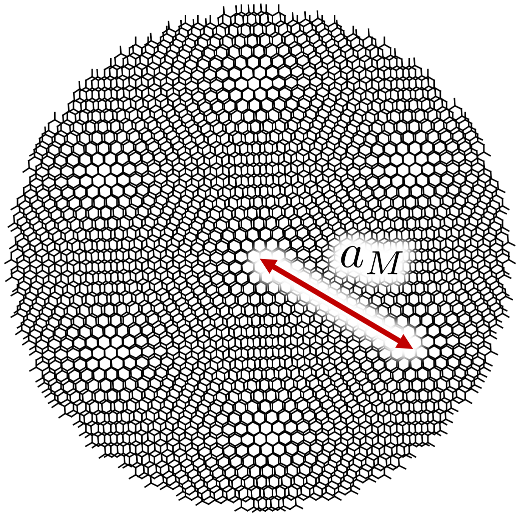




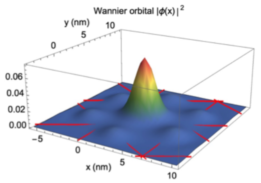


Natural Strong Correlations

Moiré unit cell

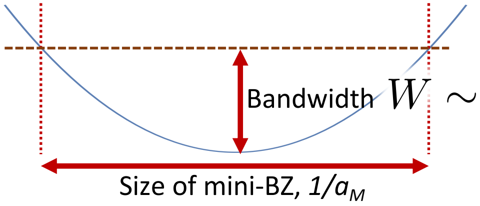


Coulomb Interaction



$U \sim 1/a_M$

Effective bandwidth

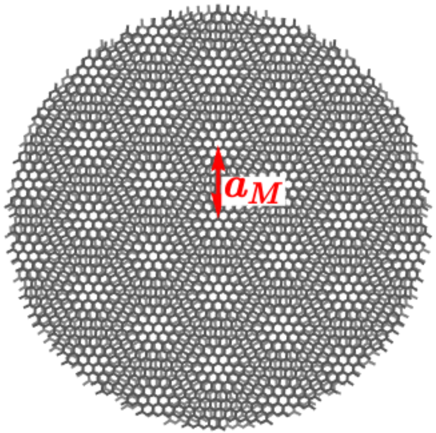


$W \sim 1/a_M^2$

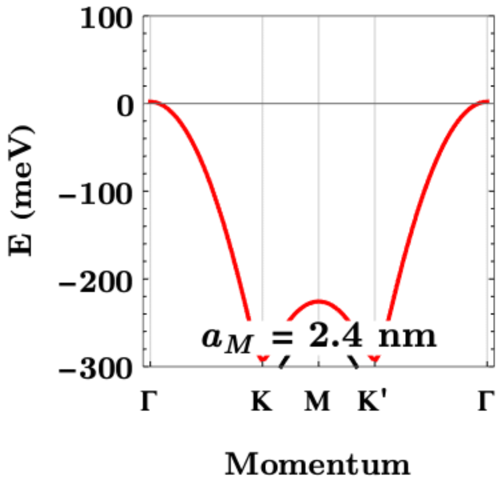
Small twist angle = Large Moiré unit cell = Strong correlations $U/W \sim a_M$

Tuneability

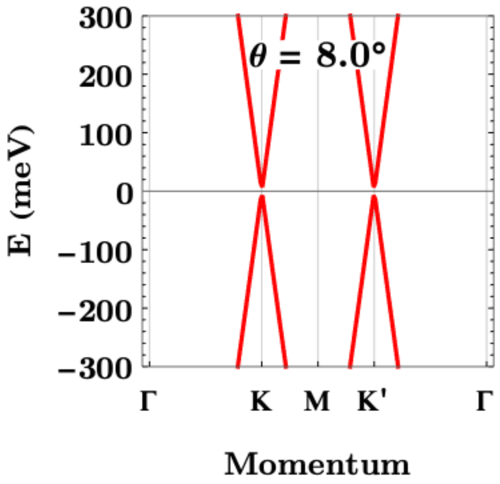
Tuning **twist** angle



Twisted **TMD** bilayer



Twisted Bilayer **Graphene**



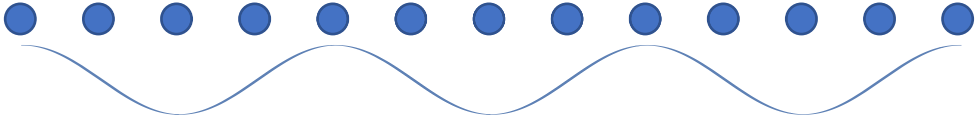
Tuning **chemical potential** = electron density using gates

More knobs: lattice mismatch, **pressure**, **screening**, …

How to observe flat bands?

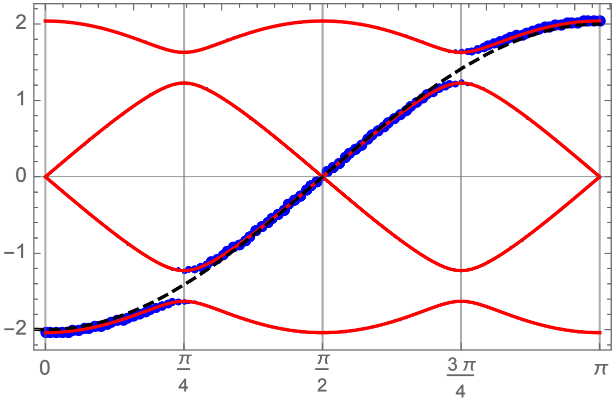
Idea: use Angle-Resolved Photo-Emission Spectroscopy (**ARPES**)

How to measure in a 'mini-Brillouin zone'? **Example:**



1d chain

Superlattice potential



Arpes intensity is given by

$$w_{fi} = \frac{2\pi}{\hbar}\sum_{\boldsymbol{k}} \left|M_{\boldsymbol{k}_f\boldsymbol{k}}\right|^2 \underbrace{\left|\langle \Psi_f^{N-1}|\hat{c}_{\boldsymbol{k}}|\Psi_i^N\rangle\right|^2 \delta(E_f^{N-1}+E_{kin}-E_i^N-h\nu).}_{\sum_f \Rightarrow A^-(\boldsymbol{k},\omega)}$$

$\sum_f \Rightarrow A^-(\boldsymbol{k},\omega)$ (bandstructure)

$\left|M_{\boldsymbol{k}_f\boldsymbol{k}}\right|^2$ → Overlap between Bloch states and plane waves

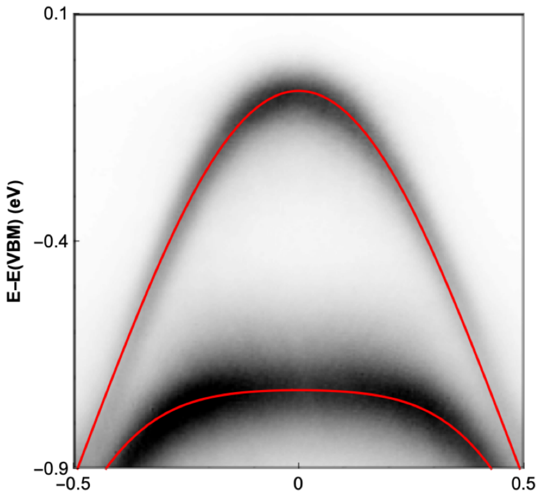
Ref: Moser JESRP '17

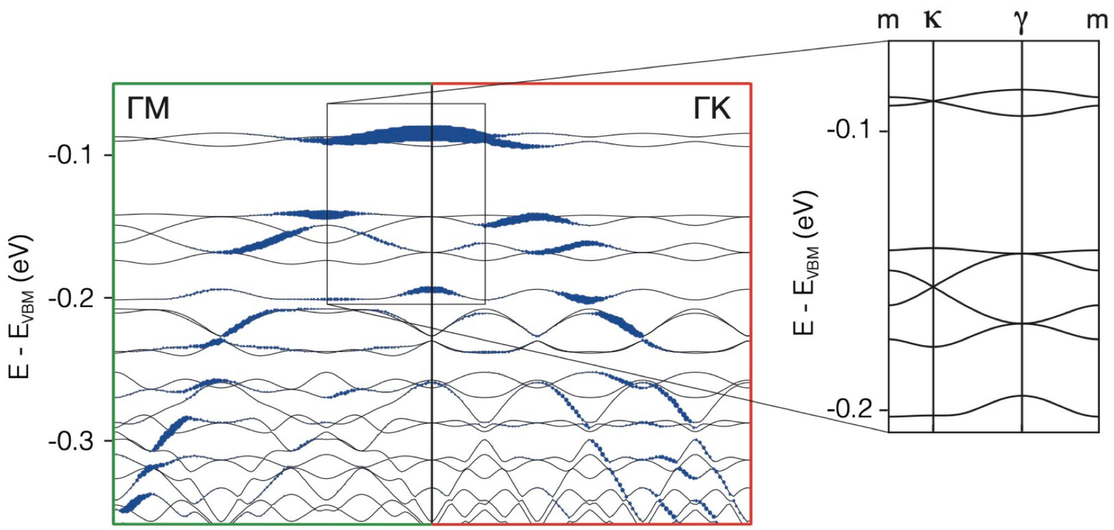
Continuum flat band model

$$H = -\frac{\hbar^2 \mathbf{k}^2}{2m^*}\mathbb{1}_2 + t_\perp(\mathbf{k})\sigma^1 + \sum_{j=1}^{6} V_0 e^{\pm i\phi} e^{i\mathbf{G}_j^M \cdot \mathbf{r}}$$

WSe2 bilayer

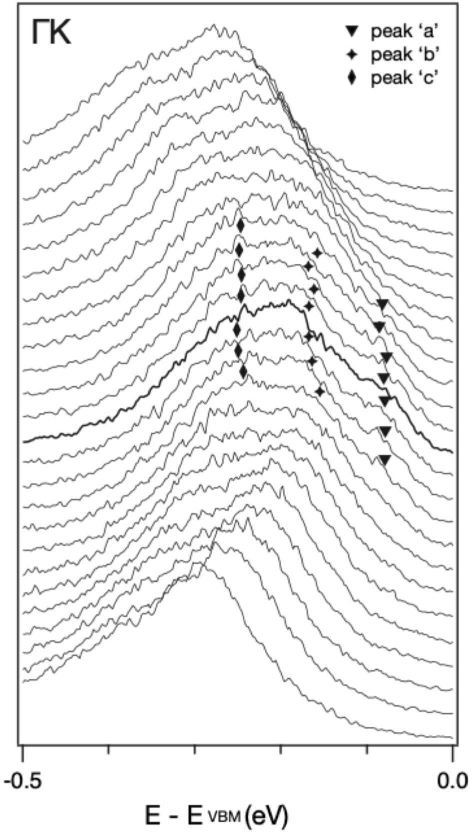
Moiré

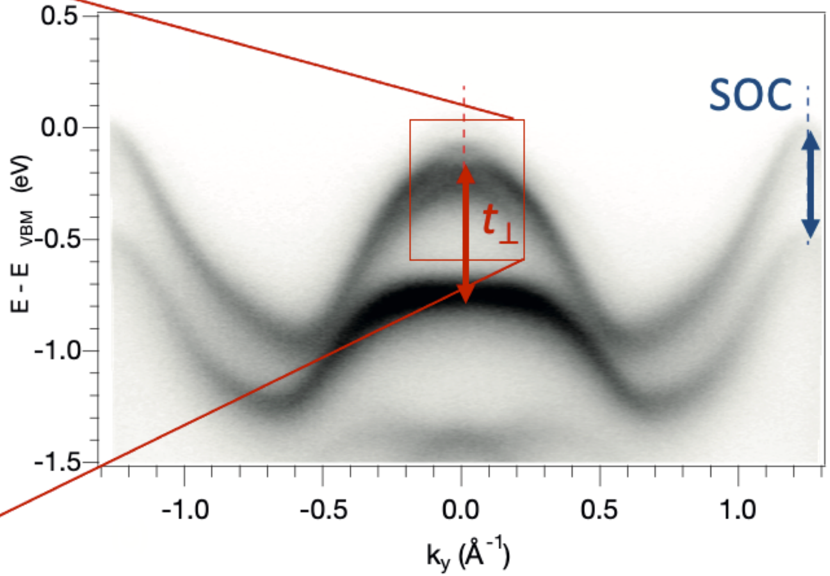




Ref: Gatti, Rademaker tbp ‘22

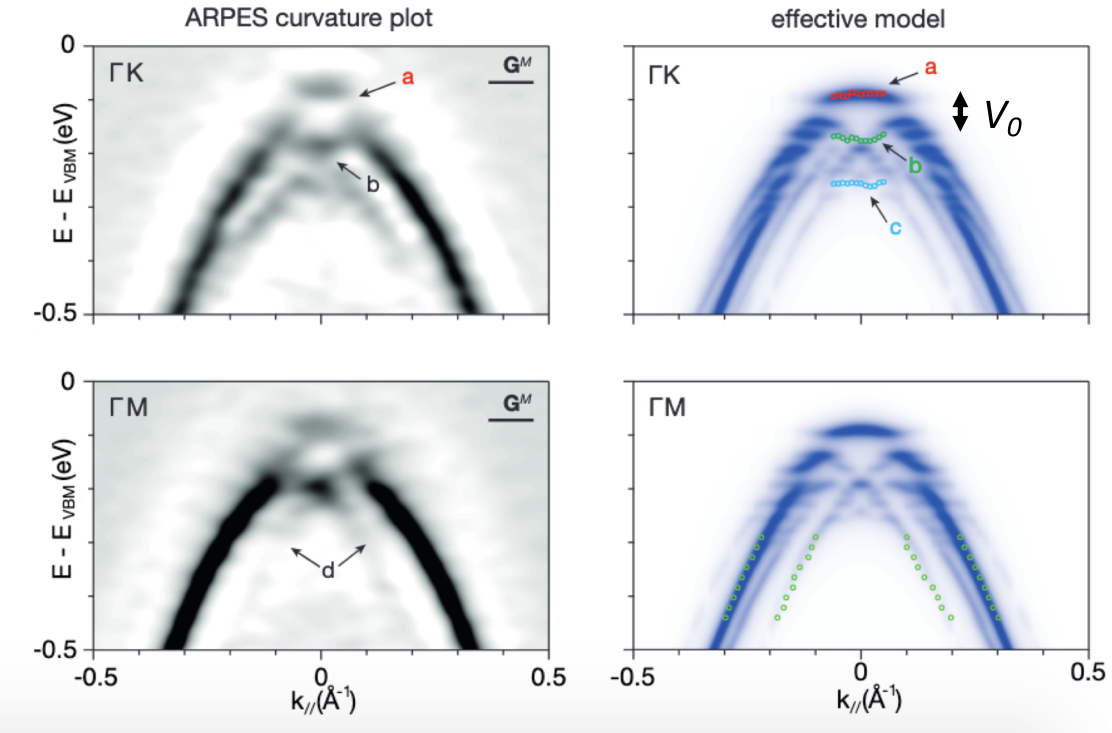
ARPES results on 57.4° tWSe2





Ref: Gatti, Rademaker tbp '22

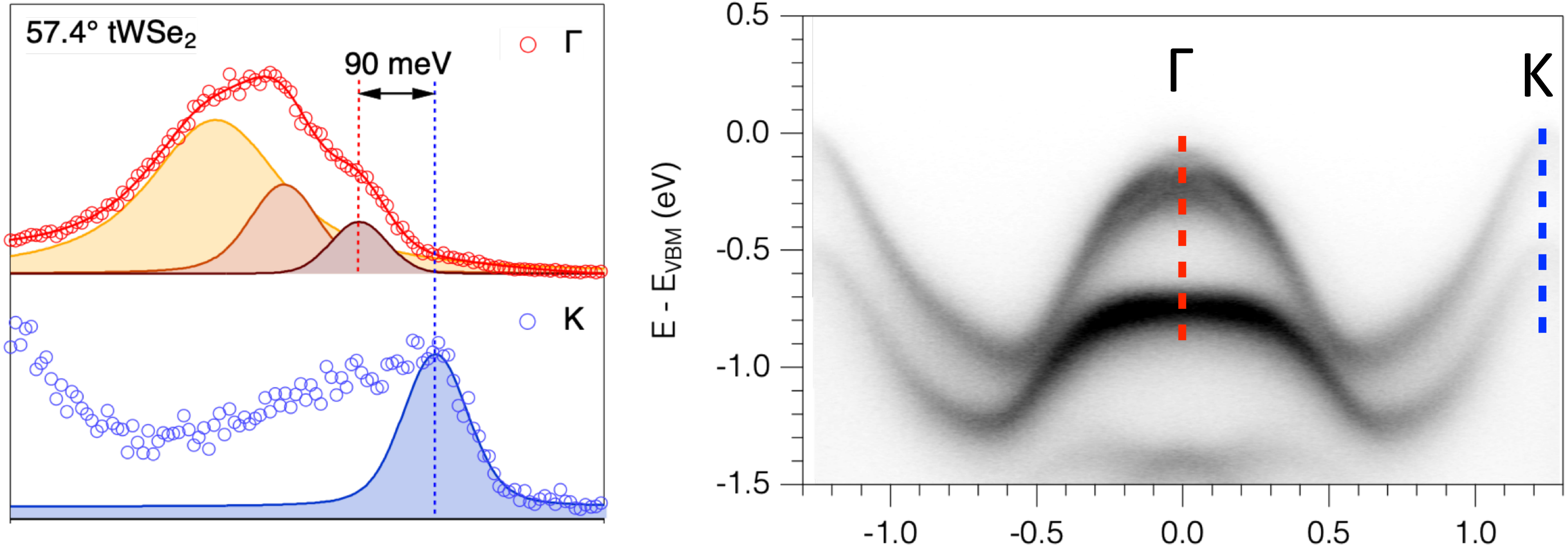
Fitting the data



θ = 57.4° (aka 2.6°)
V_0 = 40 – 60 meV
ϕ = 120°

Ref: Gatti, Rademaker tbp '22

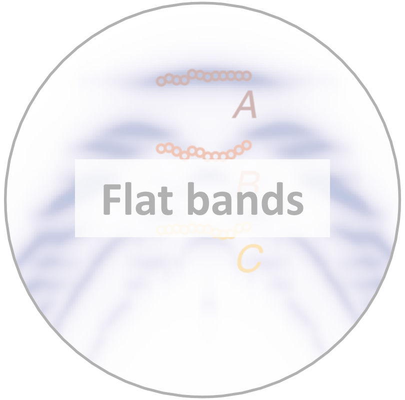
Gamma vs K

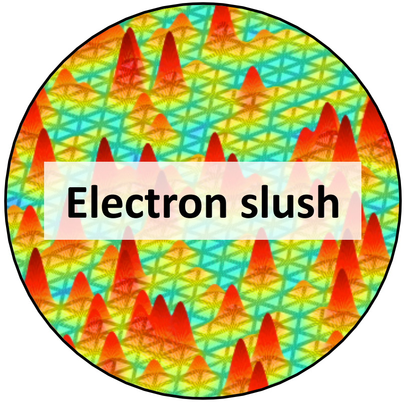


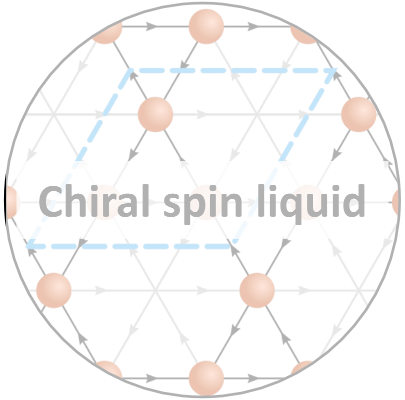
K states **higher in energy** but have **no moiré flat bands**?

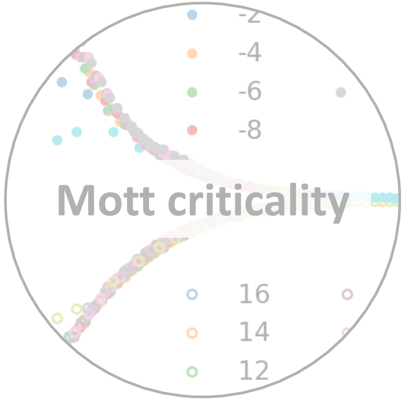
Ref: Gatti, Rademaker tbp ‘22

More exotic moiré physics with TMDs

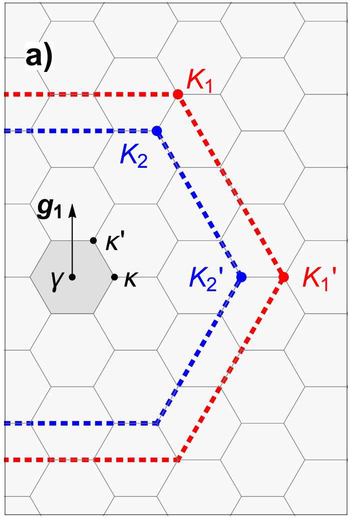








Heterobilayers

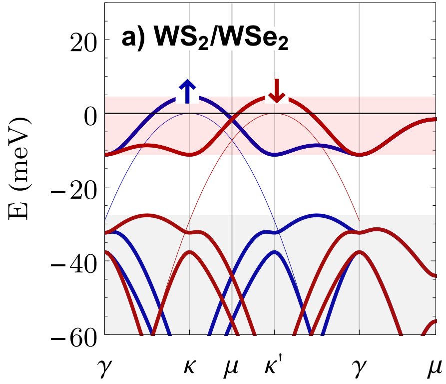


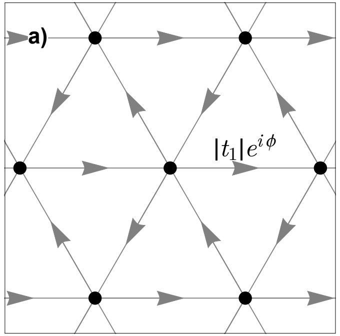
Moiré pattern **without a twist**:

$$\frac{1}{a_M} = \sqrt{\frac{1}{a_1^2} + \frac{1}{a_2^2} - \frac{2\cos\theta}{a_1 a_2}}$$

Hopping model on **triangular lattice** with **spin-orbit coupling**

$$H = t_1 \sum_{\langle ij \rangle \sigma} e^{i\phi\sigma^z \nu_{\langle ij \rangle}} c_{i\sigma}^\dagger c_{j\sigma}$$

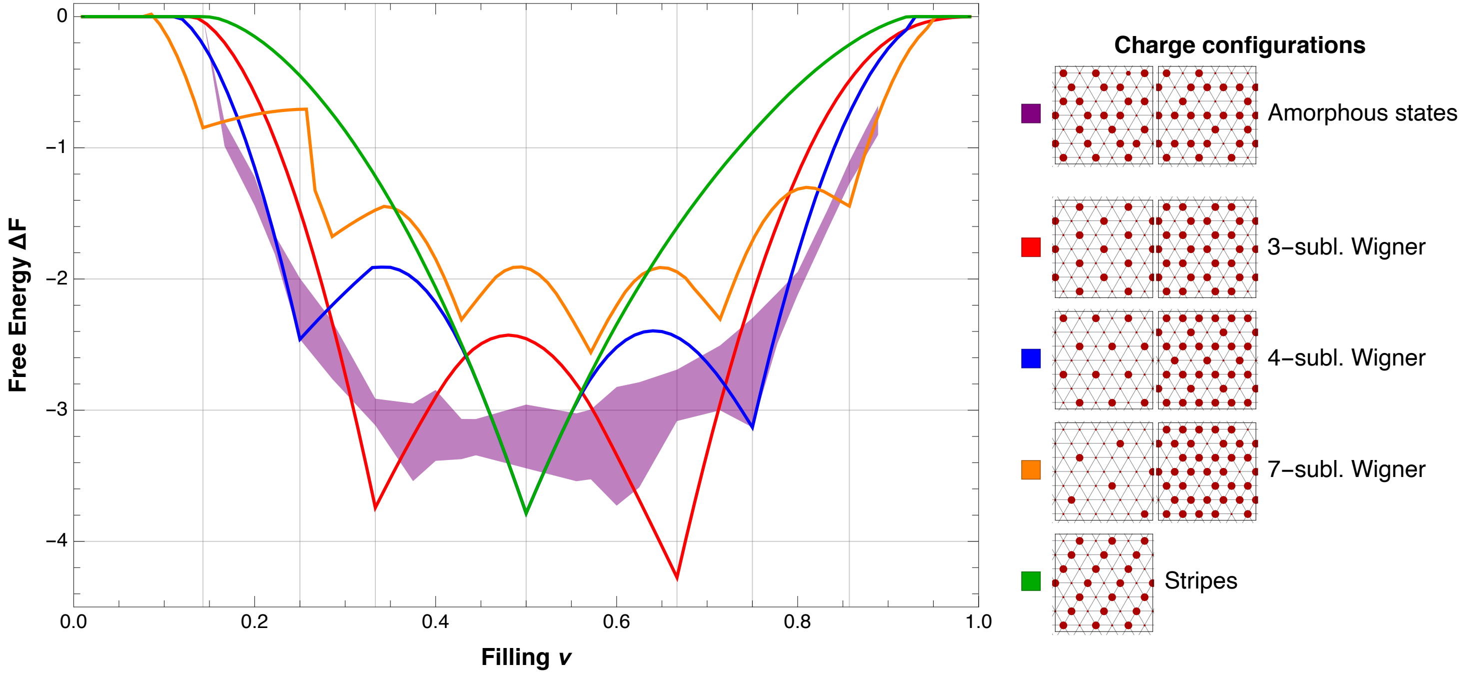




Ref: Rademaker PRB '21

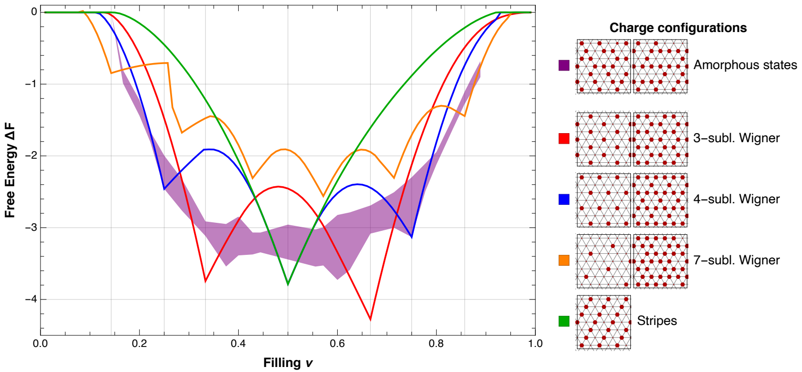
Long-range interactions: Wigner-Mott states

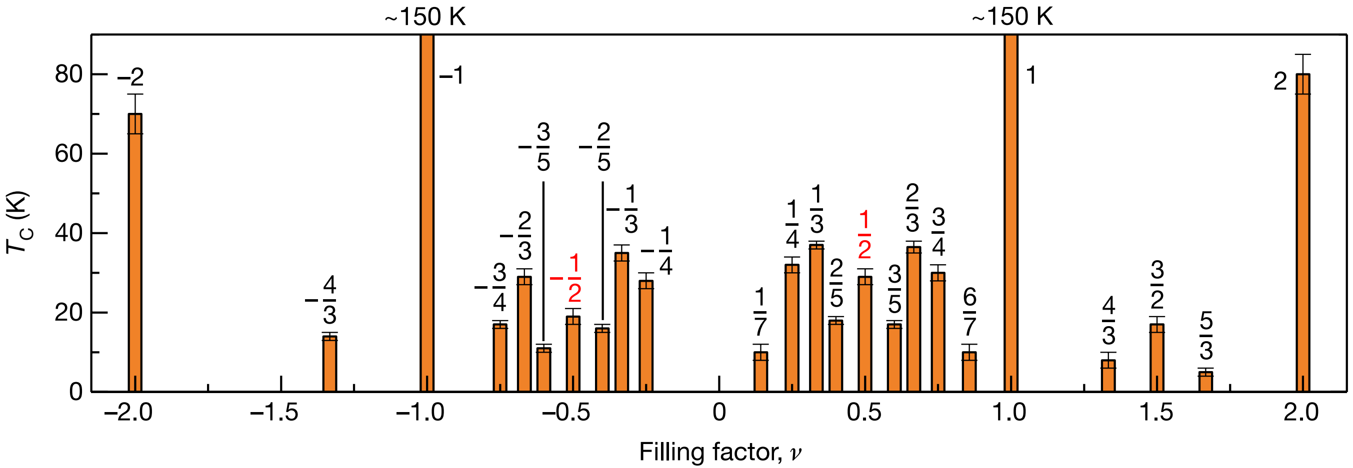
$$V_{\rm sc}(r) = \frac{e^2}{4\pi\epsilon}\left(\frac{1}{r} - \frac{1}{\sqrt{r^2+d^2}}\right)$$ Strong long-range repulsion: $V/t \approx 13$



Ref: Tsang, …, Rademaker tpb '22

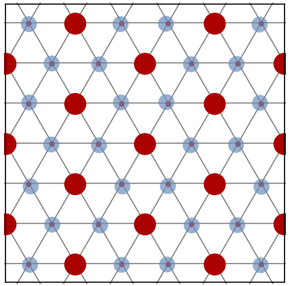
Long-range interactions: Wigner-Mott states

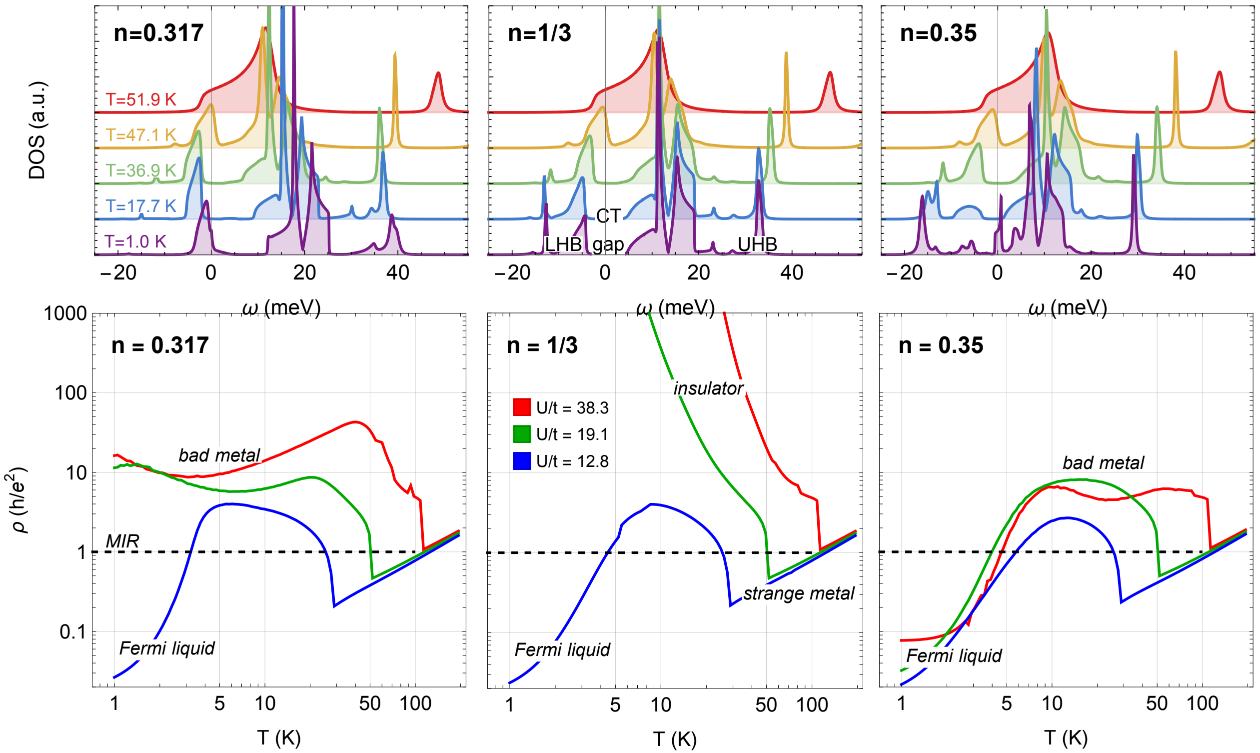




Ref: Tsang, …, Rademaker tpb '22; Xu Nature '20

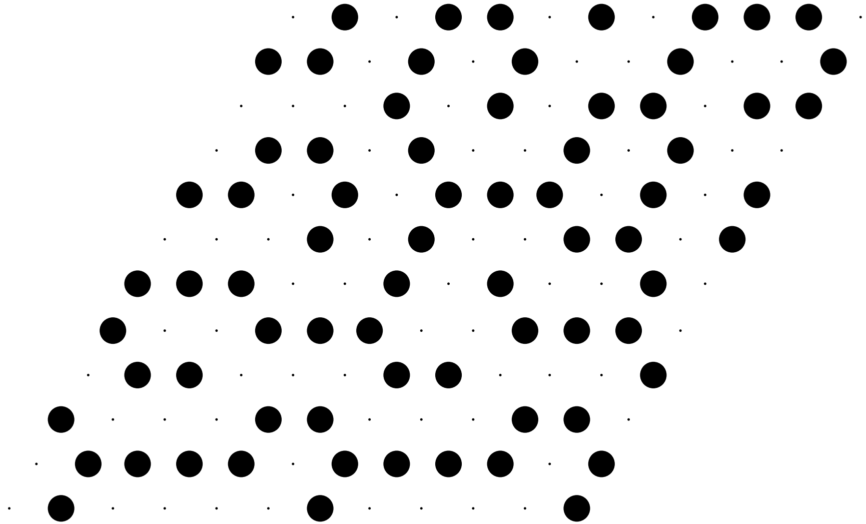
Doping the Wigner-Mott insulator

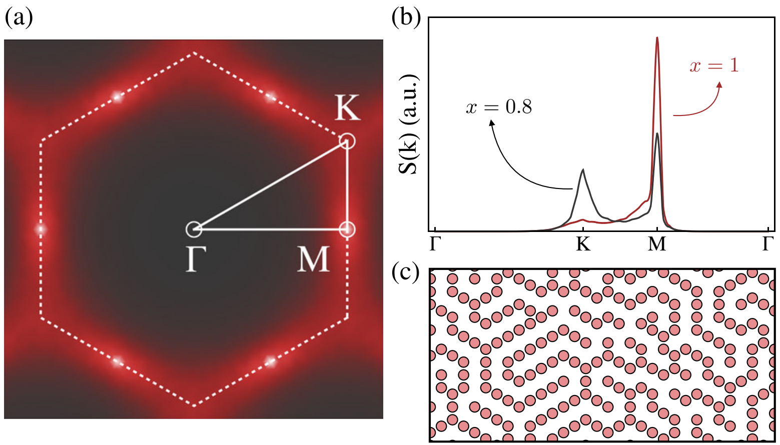




Ref: Tsang, …, Rademaker tpb ‘22

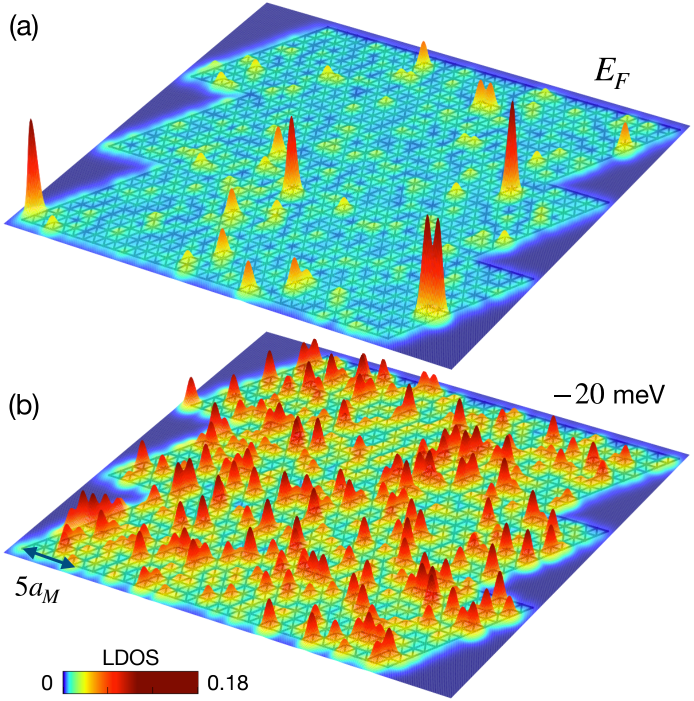
Amorphous configurations

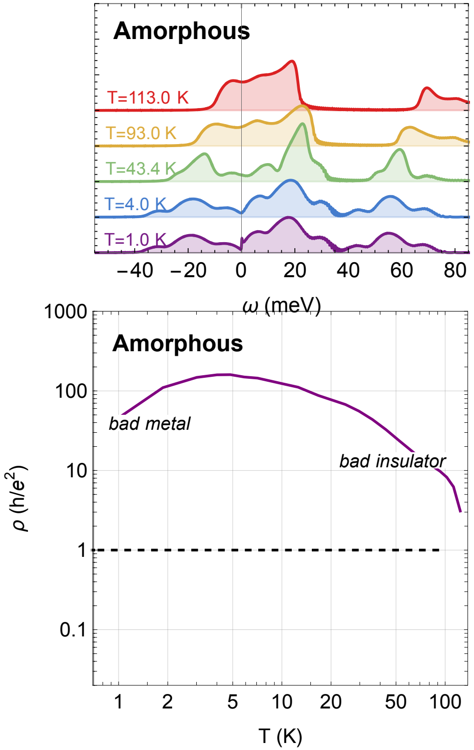




Ref: Tsang, …, Rademaker tpb ’22; Mahmoudian, Rademaker PRL ‘16

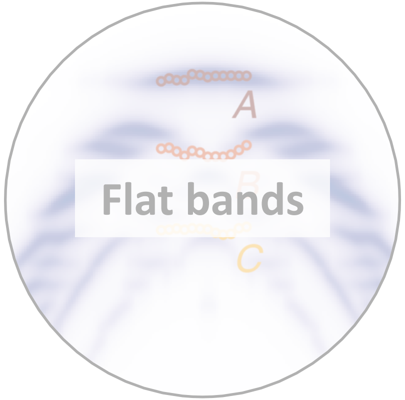
Conducting amorphous state: Electron slush

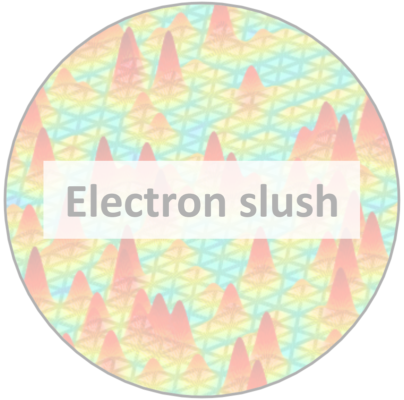


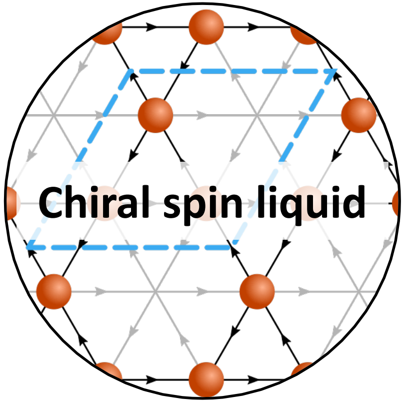


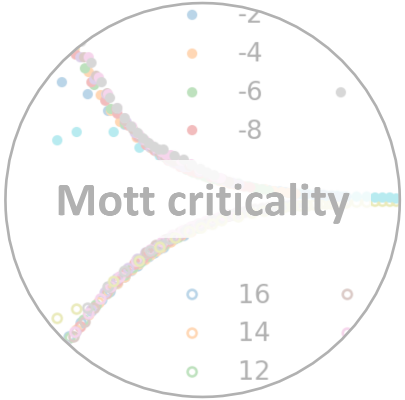
Ref: Tsang, …, Rademaker tpb '22

Overview: exotic Moiré physics with TMDs

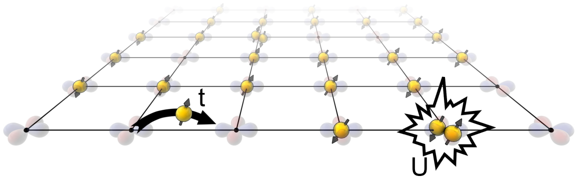




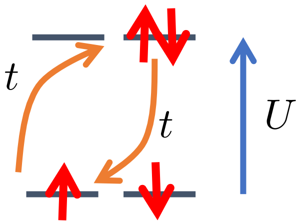




Spin degrees of freedom



Hubbard model with strong U

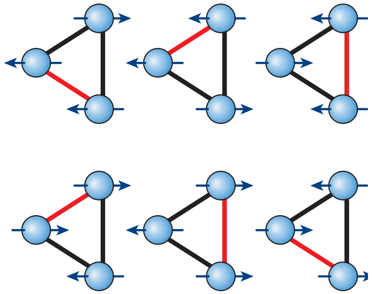


Virtual **exchange**

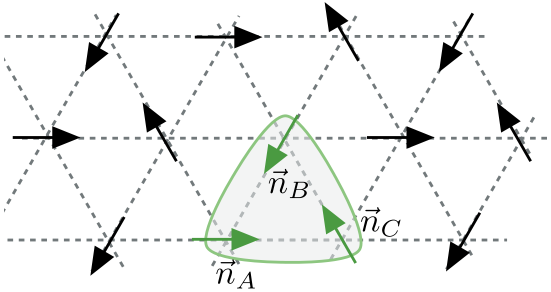
$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$J = \frac{2t^2}{U}$$

Antiferromagnetic Heisenberg



Frustration on **triangular** lattice

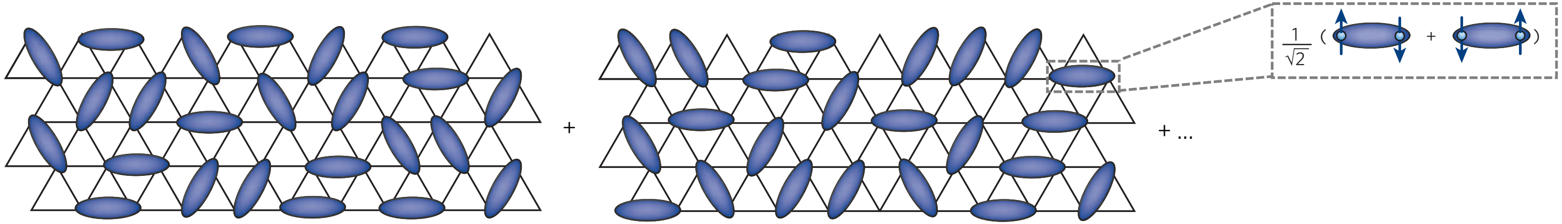


Classical **120º** Néel coplanar antiferromagnet

Ref: Balents Nature '10; Rademaker PRB '15

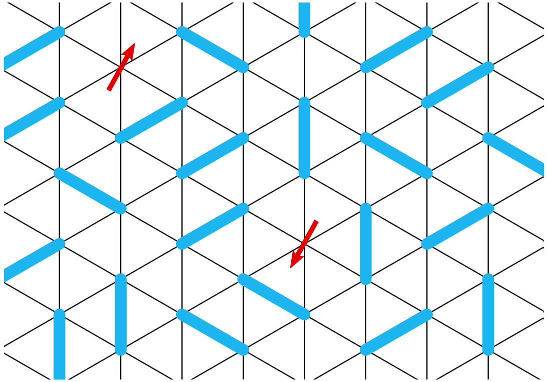
Spin liquids

Resonating valence bond (RVB)



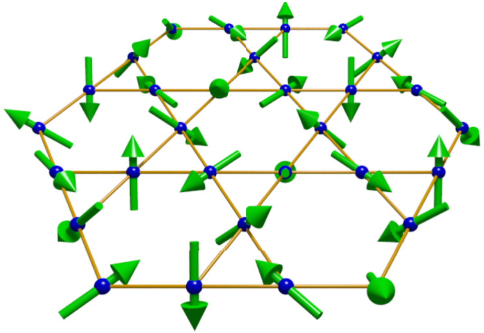
In general, **spin liquids**:

- **No magnetic** order
- High degree of **entanglement**
- **Fractionalization** of excitations
- Require **frustration**

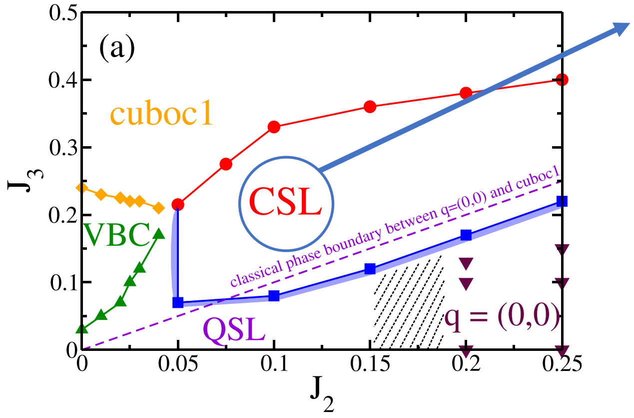


Ref: Balents Nature '10

Kagome lattice



Most frustrated spin model



Candidate for **spin liquid**

Chiral spin liquid

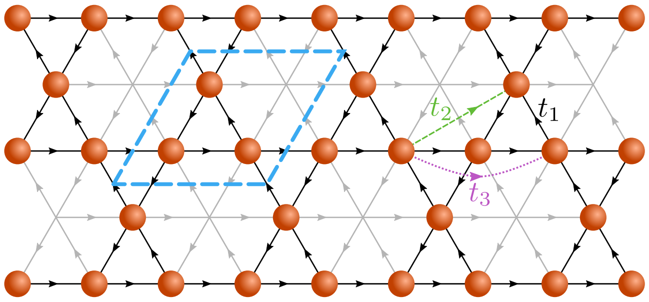
- Spin analog of **FQHE**
- ‘**Semion**’ fractional excitations
- Spontaneous **chiral** order

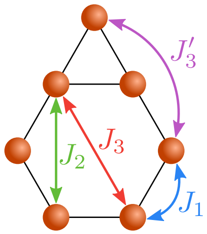
$$\sum_{\triangle} \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$$

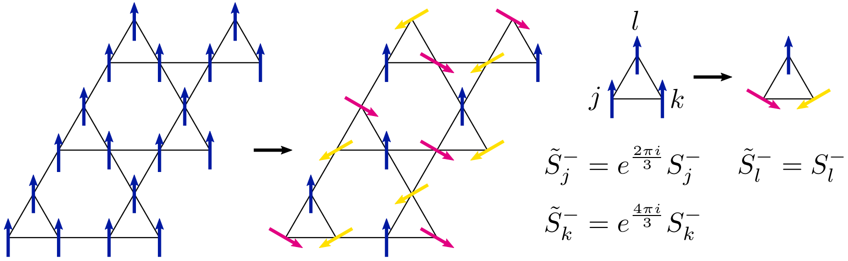
Ref: Gong PRB ’15; Savary Rep Prog Phys ‘16

Kagome physics in TMD heterobilayers

Charge order at **n=3/4 filling** forms kagome lattice!







$$\tilde{S}_j^- = e^{\frac{2\pi i}{3}} S_j^- \qquad \tilde{S}_l^- = S_l^-$$

$$\tilde{S}_k^- = e^{\frac{4\pi i}{3}} S_k^-$$

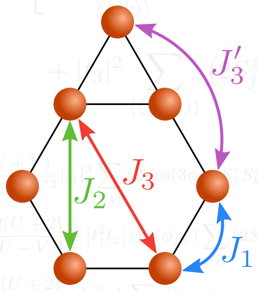
$$H_{\text{spin}} = \sum_{ij} J_{ij} \left[S_i^z S_j^z + \cos\left(\tilde{\phi}_{ij}\right) \left(S_i^x S_j^x + S_i^y S_j^y\right) + \sin\left(\tilde{\phi}_{ij}\right) \left(\mathbf{S}_i \times \mathbf{S}_j\right) \cdot \hat{\mathbf{z}} \right]$$

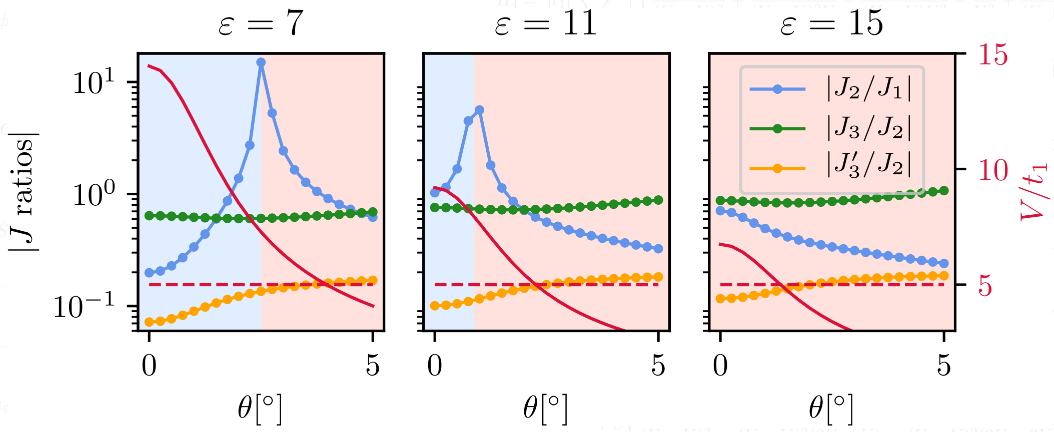
XXZ **DM**

Ref: Motruk, …, Rademaker tpb ‘22

Effective spin model

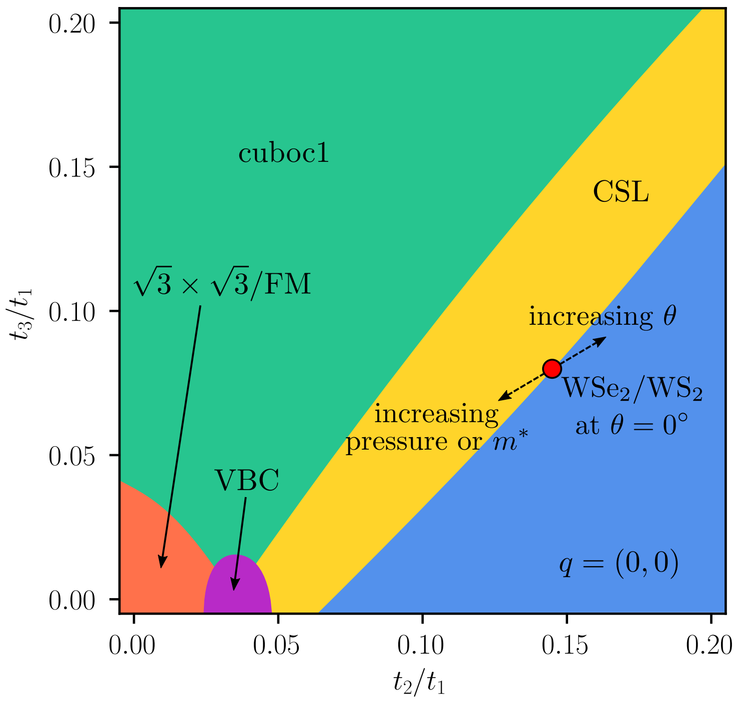
Virtual exchange to get **spin model** from **tight-binding** model

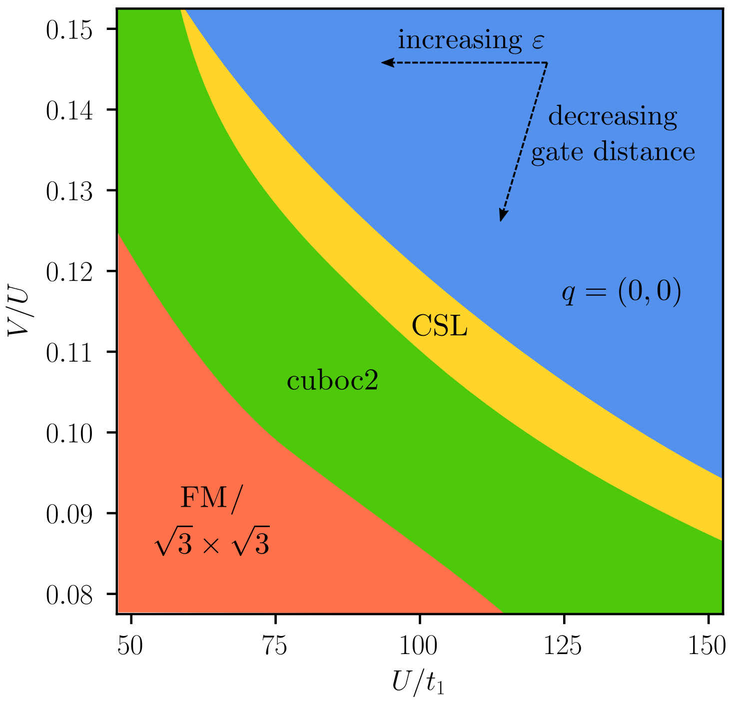




Ref: Motruk, …, Rademaker tpb '22

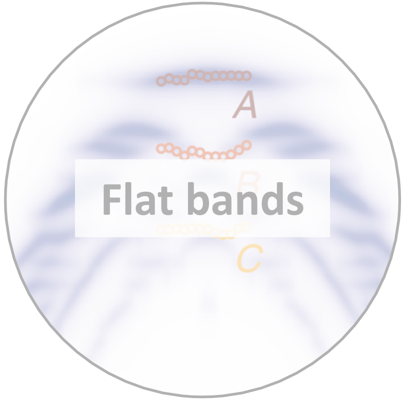
DMRG phase diagram

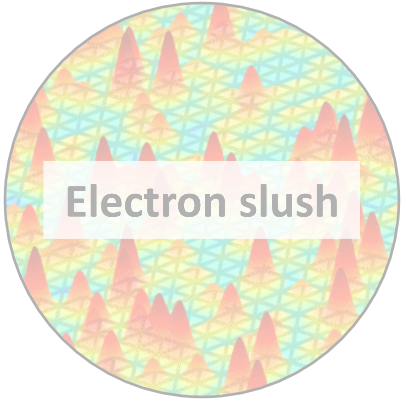


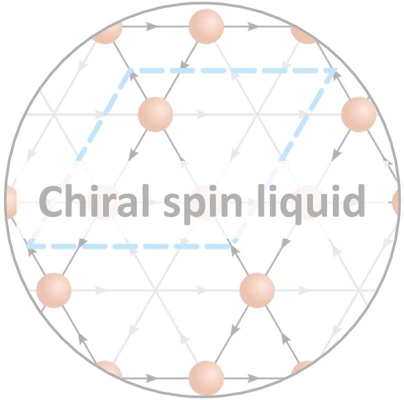


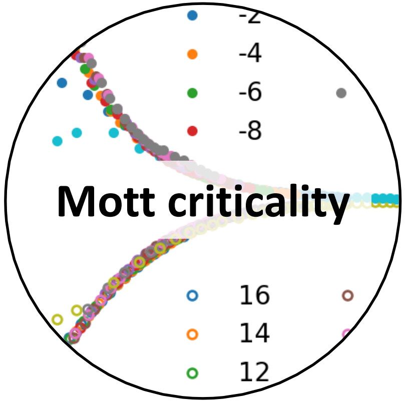
Ref: Motruk, …, Rademaker tpb ‘22

Overview: exotic Moiré physics with TMDs



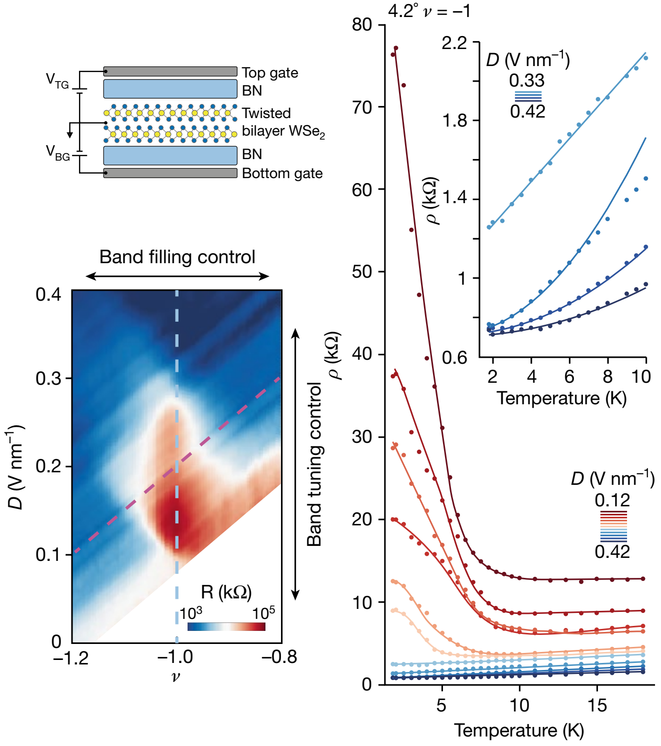




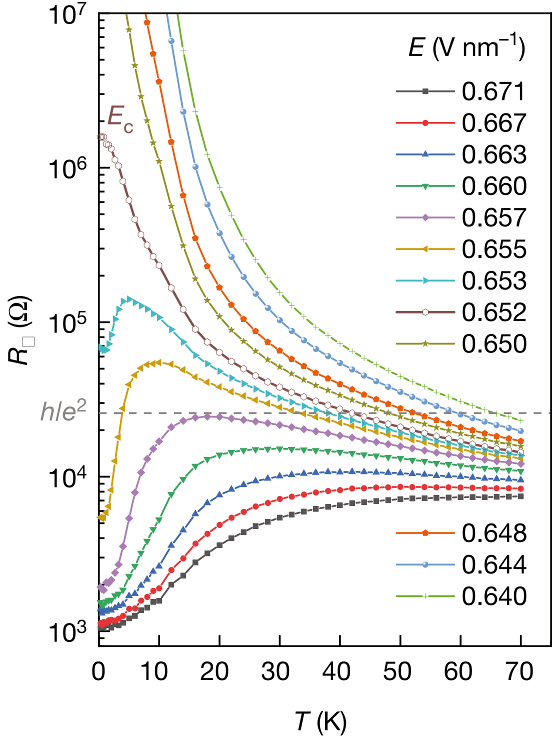


Observed Mott criticality

Twisted bilayer WSe_2



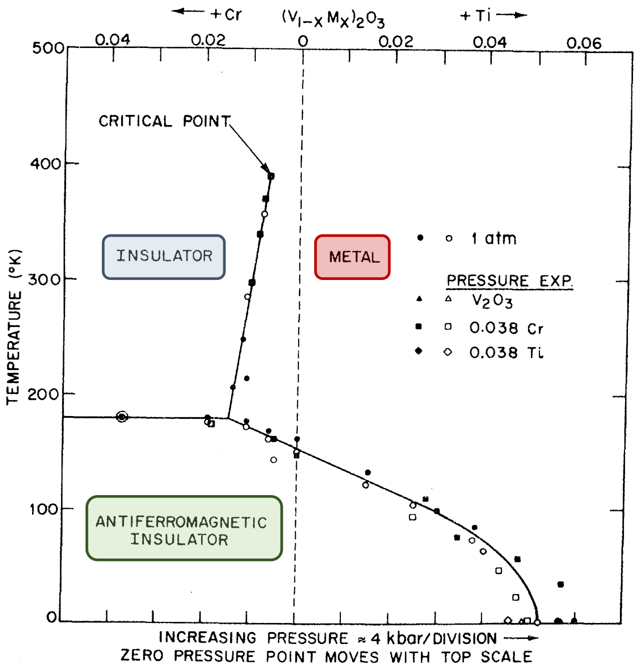
Aligned $MoTe_2/WSe_2$



Ref: Ghiotto Nature ‘21; Li Nature ‘21

Problem with Mott criticality

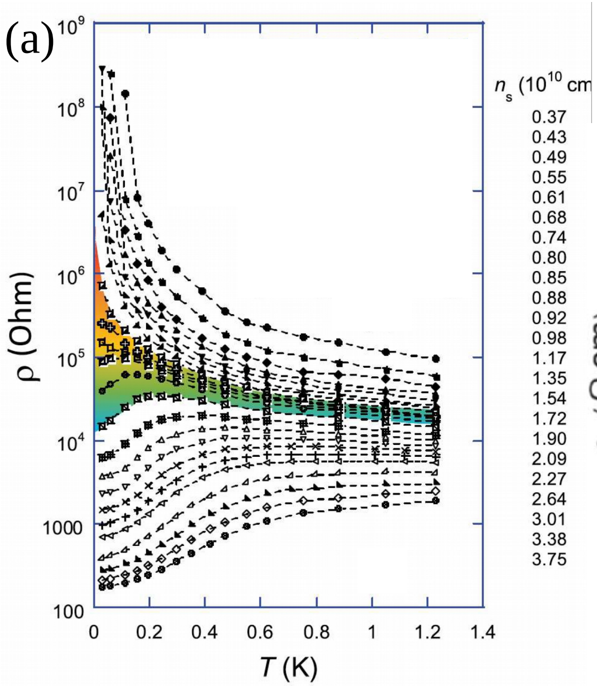
Doped V_2O_3



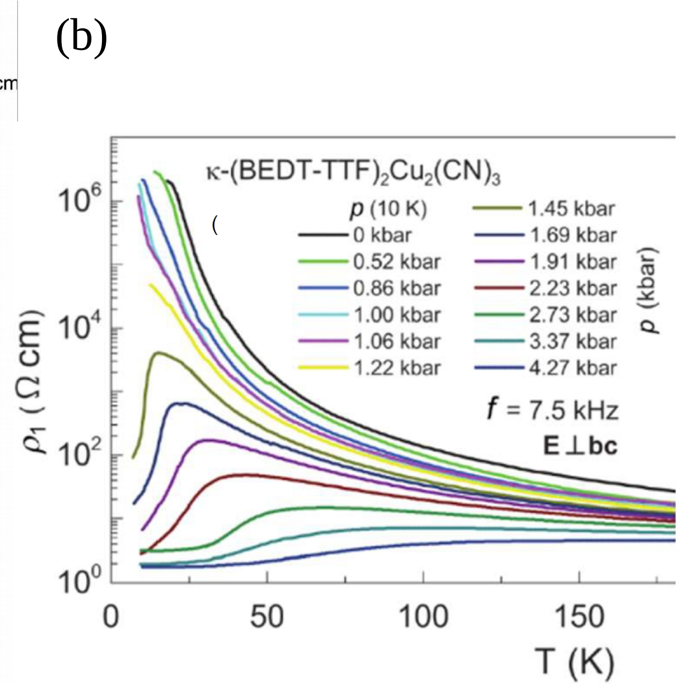
Ref: McWhan PRB '83; Mott '90

Other material realizations

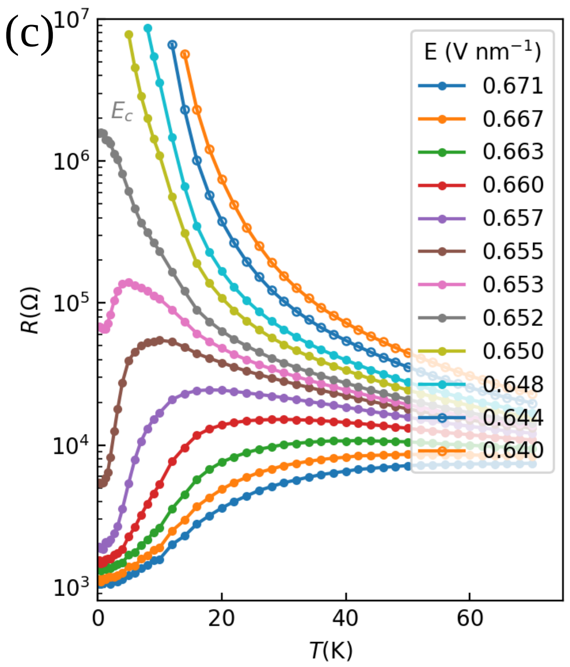
Si 2DEGs



Mott organics



$MoTe_2/WSe_2$



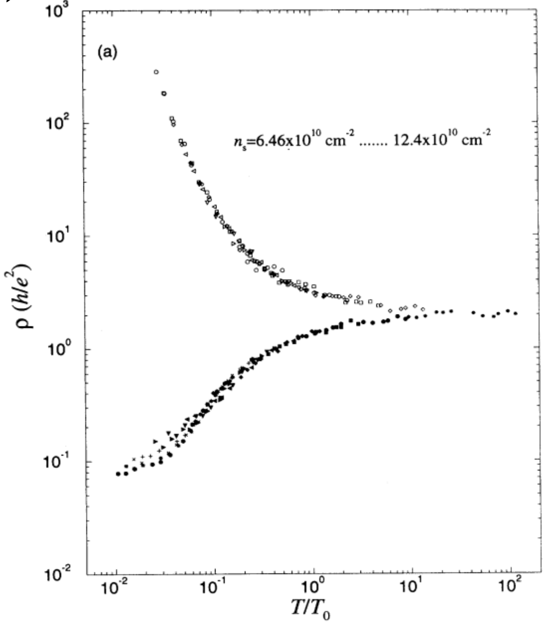
Ref: Tan, ..., Rademaker Crystals '22

Critical scaling

$$R(\delta, T)/R_c(T) = f_\pm(T/T_0(\delta))$$

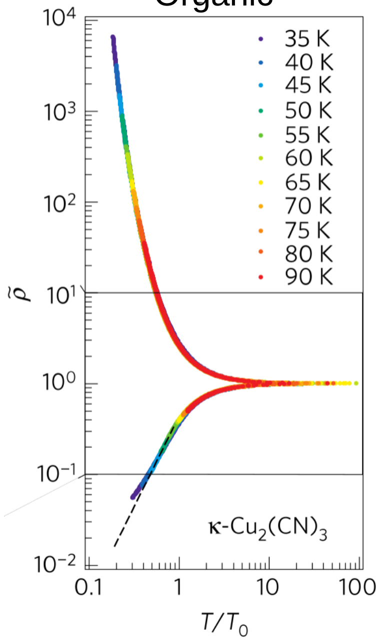
$$T_0(\delta) \sim |\delta|^{\nu z}$$

(a) Dilute 2DEG

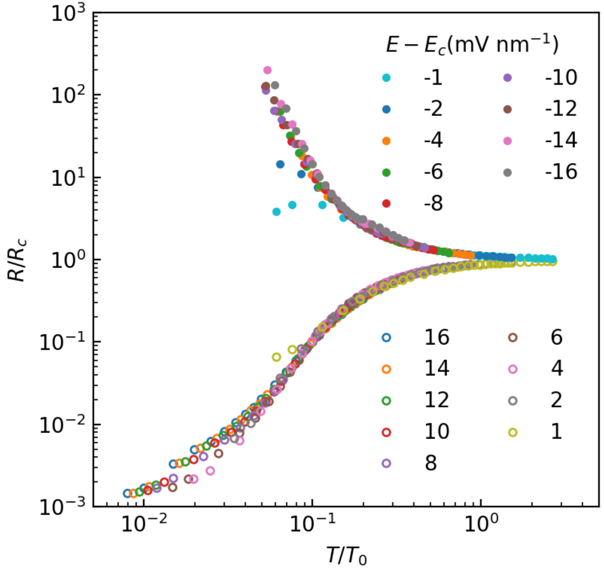


Ref: Tan, ..., Rademaker Crystals ‘22

(b) Organic



(c) TMD Moiré



Exponents

System	Dilute 2DEG	Mott Organics	TMD Moiré Bilayers
Transition Type	continuous?	weakly first order (at $T < T_c \sim 0.01 T_F$)	continuous?
Δ	$\lvert n - n_c \rvert$	$\lvert P - P_c \rvert^{\nu z}$, $\nu z \approx 0.7 - 1$	$\lvert E - E_c \rvert^{\nu z}$, $\nu z \approx 0.6$
$\frac{1}{m^*}$	$\lvert n - n_c \rvert$	?	?
T_o	$\lvert n - n_c \rvert^{\nu z}$, $\nu z \approx 1.6$	$\lvert P - P_c(T) \rvert^{\nu z}$, $\nu z \approx 0.5 - 0.7$	$\lvert E - E_c \rvert^{\nu z}$, $\nu z \approx 0.7$
T_{FL}	?	$\lvert P - P_c \rvert$	$\lvert E - E_c \rvert^{\nu z}$, $\nu z \approx 0.7$
T_{max}	$\lvert n - n_c \rvert$	$\lvert P - P_c \rvert$	$\lvert E - E_c \rvert^{\nu z}$, $\nu z \approx 0.7$

Ref: Tan, ..., Rademaker Crystals ‘22

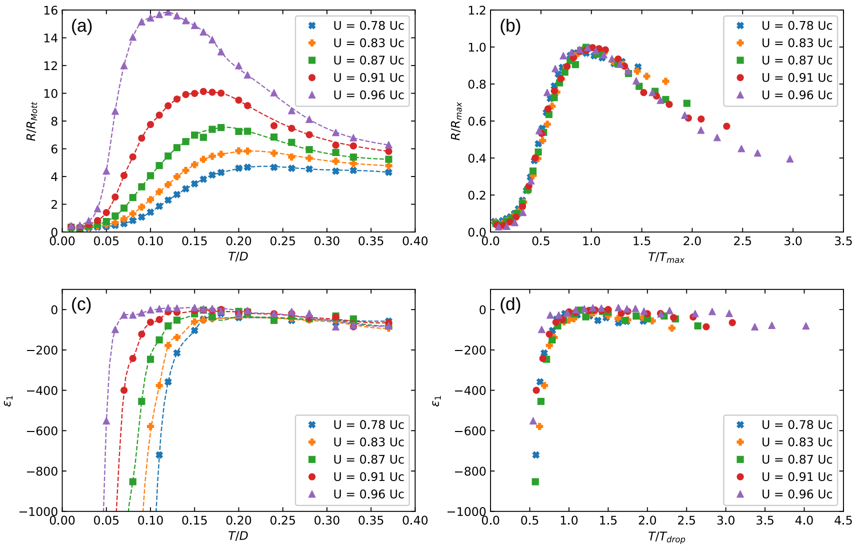
Theories of Mott criticality

Theory Predictions	2D Spinon Theory	DMFT	Percolation Theory
Transition Type	continuous	weakly first order (at $T < T_c \sim 0.01 T_F$)	first order
Δ	$\|g - g_c\|S^{\nu z}$, $\nu z = 0.67$	$\|U - U_{c1}\|^{\nu z}$, $\nu z \approx 0.8$	remains finite
m^*	weak: $\ln \frac{1}{\|g-g_c\|}$	strong: $\|U - U_{c2}\|^{-1}$	no divergence
$A/(m^*)^2$	?	constant (KW law obeyed)	diverges: $(x_o - x_c)^{-t}$; $t = s/m$
T_{FL}	$\|g - g_c\|^{2\nu}$	$\|U - U_{c2}\|$	$T^* \sim \|x_o - x_c\|$
T_{max}	$T_{max} = \infty$	$\|U - U_{c2}\|$	$T^* \sim \|x_o - x_c\|$

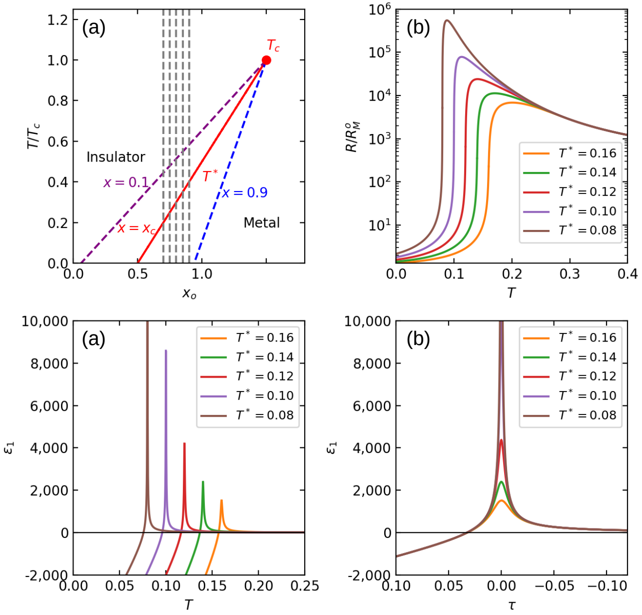
Ref: Tan, ..., Rademaker Crystals ‘22

Optical response

DMFT: large **negative** dielectric response



Percolation: large **positive** dielectric response



Ref: Tan, ..., Rademaker Crystals '22

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Exotic moiré physics with TMDs