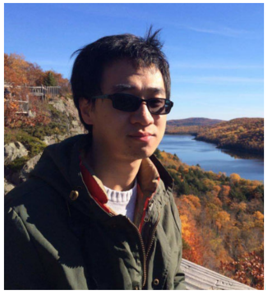
# Strong correlations in 2D semiconductor moiré superlattices

**Jie Shan**
**KITP Reunion Conference**
**"Return of the Intertwined: New Developments in Correlated Materials**
**(July 30, 2020)**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Zui Tao


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**Theory:** Allan MacDonald (UT Austin), Veit Elser (Cornell), Liang Fu (MIT)

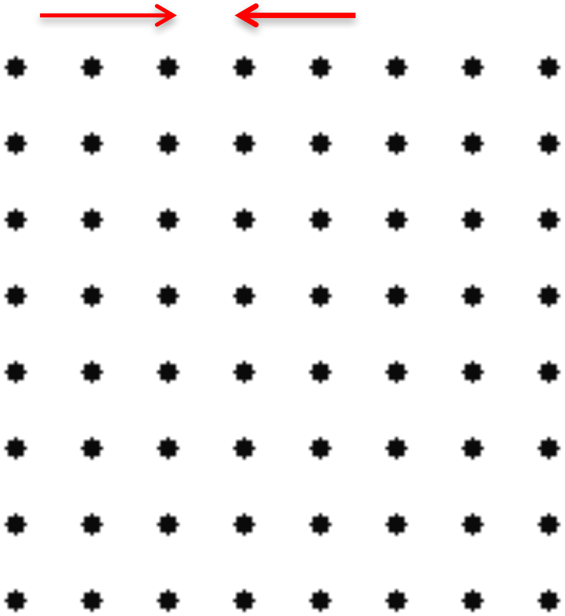
**$WSe_2$, $WS_2$ bulk crystals:** Columbia team (Song Liu, Katayun Barmak, Jim Hone)

**Boron nitride crystals:** Kenji Watanabe, Takashi Taniguchi (NIMS)

# Moiré superlattices, new length & energy scale: Correlation engineering

# Interacting quantum particles on a lattice

moiré length scale *a*



Effect of moiré potential

Flat band

Electron-electron interaction energy

$$U \sim \frac{e^2}{\varepsilon a}$$

Bandwidth of lowest electronic miniband

$$W \sim \frac{\hbar^2 k^2}{2m^*} \sim \frac{\hbar^2 \pi^2}{2m^* a^2}$$

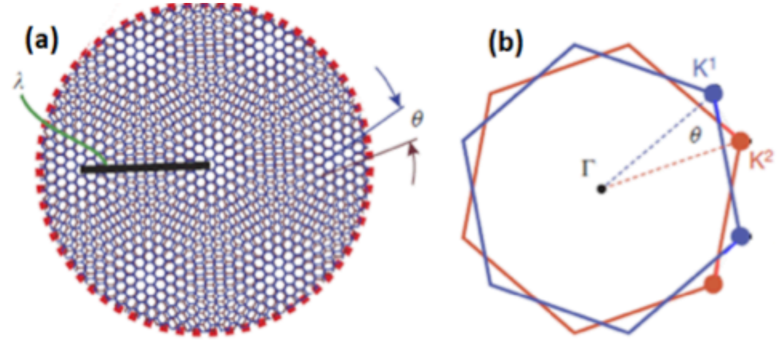
Strong correlation

$$\frac{U}{W} \sim m^* a > 1$$

For TMD monolayers, $m^* \sim 0.5\, m_0$, $\varepsilon \sim 4$, $a \sim 10$ nm

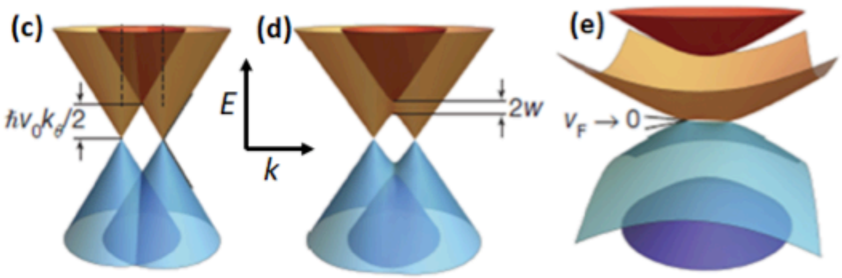
$$\frac{U}{W} \sim 5$$

# MATBG: superconductivity & insulating states



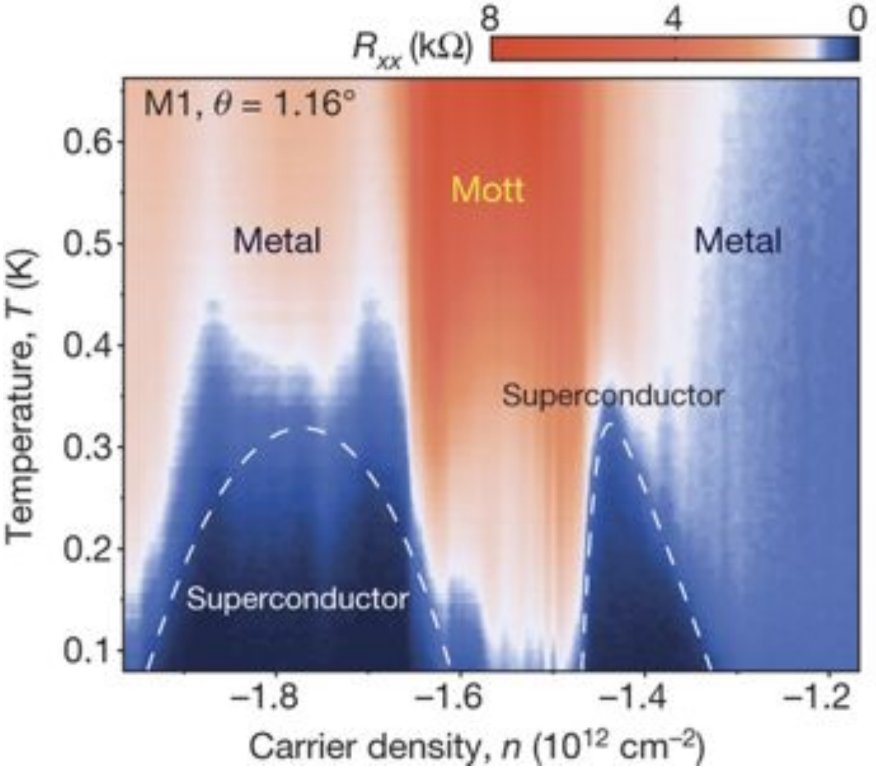
Moiré pattern

Brillouin zones



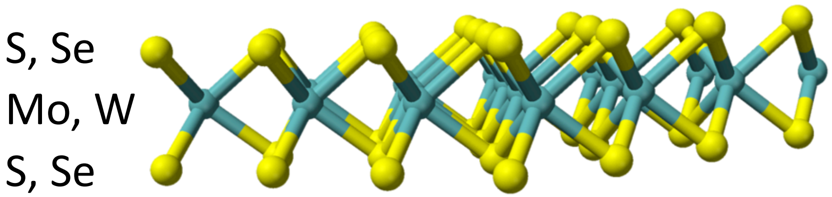
Intersecting Dirac Cones

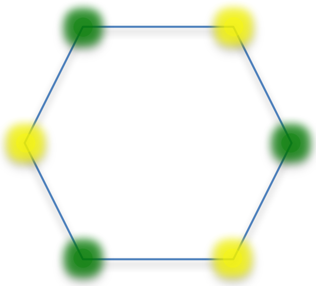
Flat Bands

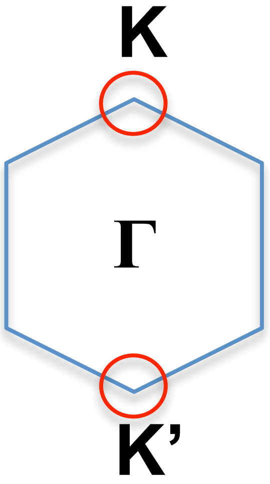


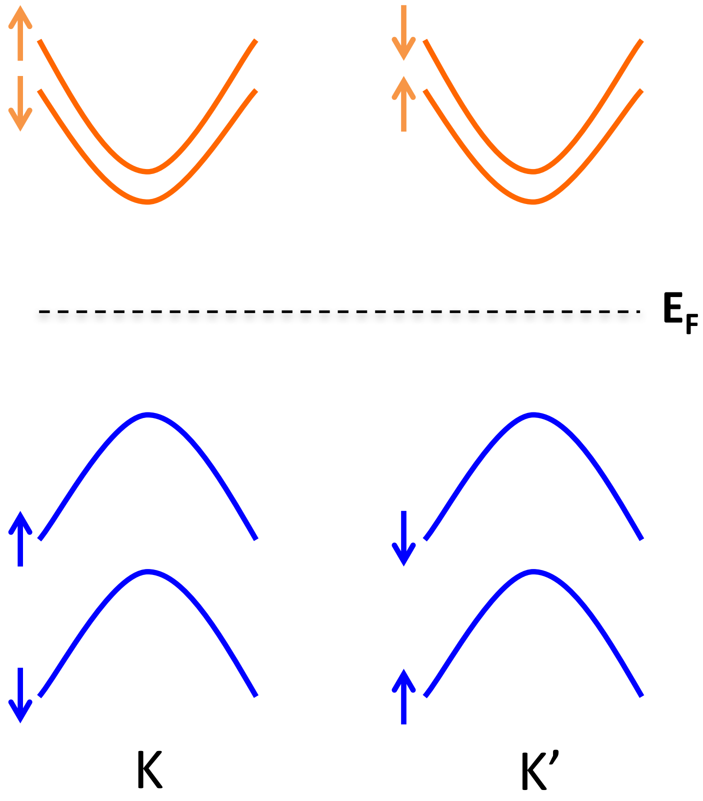
Prediction: Bistritzer & MacDonald, PNAS (2011)
Experiment: Chen, Jarillo-Herrero, Nature (2018)

# Monolayer transition metal dichalcogenides (TMD)







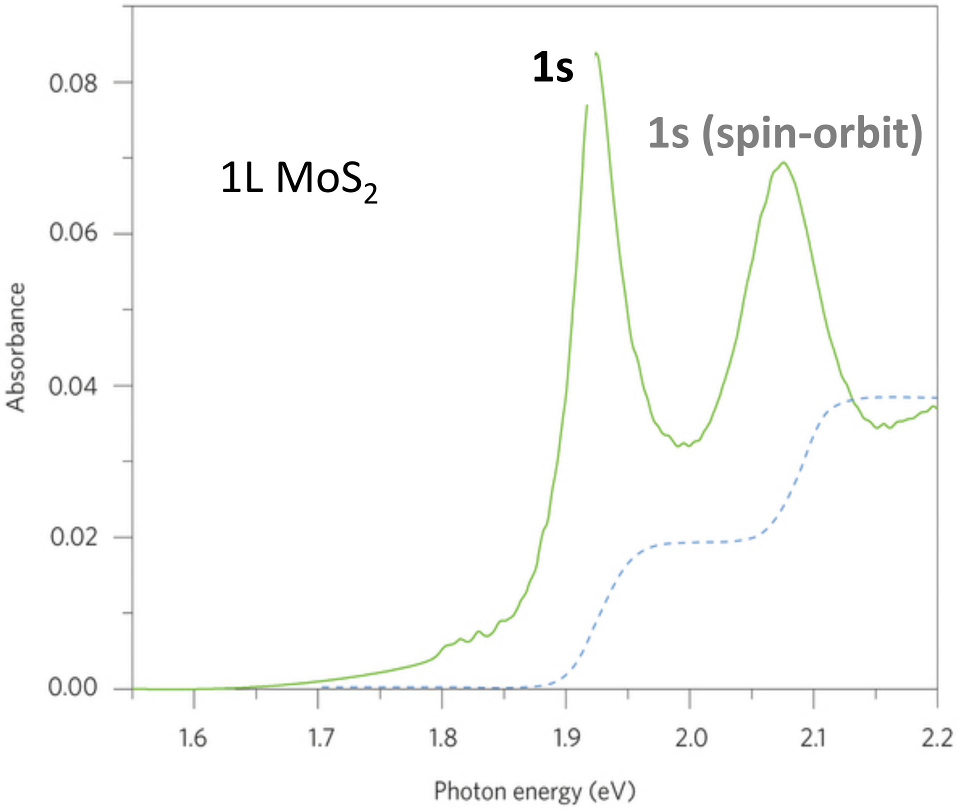


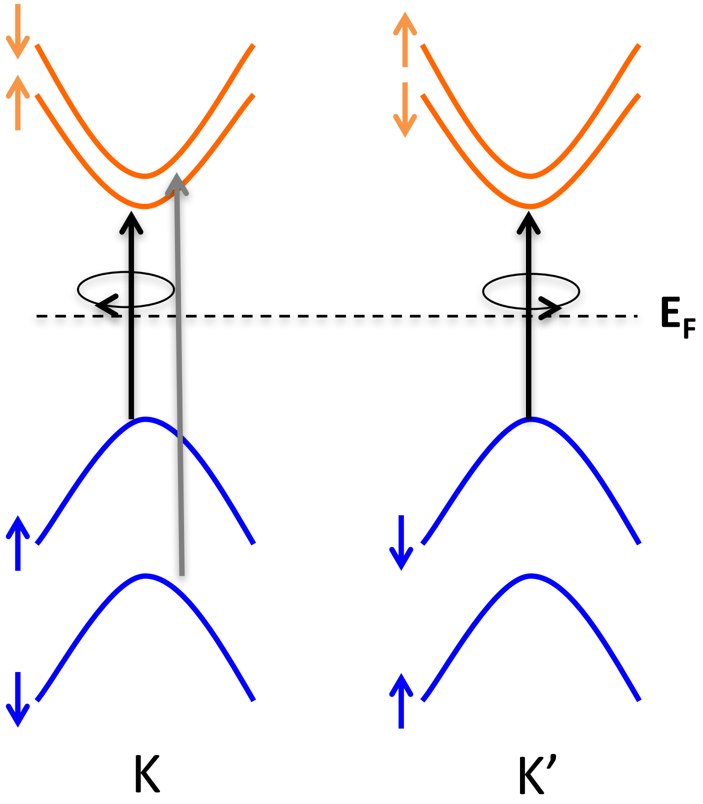
*Broken sublattice symmetry:*

- *Energy gap at K and K’*
- *Mass ~ 0.5* $m_0$
- *Spin splitting at K and K’ from SOC*
- *Spin-valley locking*

Mak, Lee, Hone, Shan, Heinz, PRL (2010)
Splendiani, Wang et al. Nano Lett. (2010)

# Strong light-matter interaction in TMDs



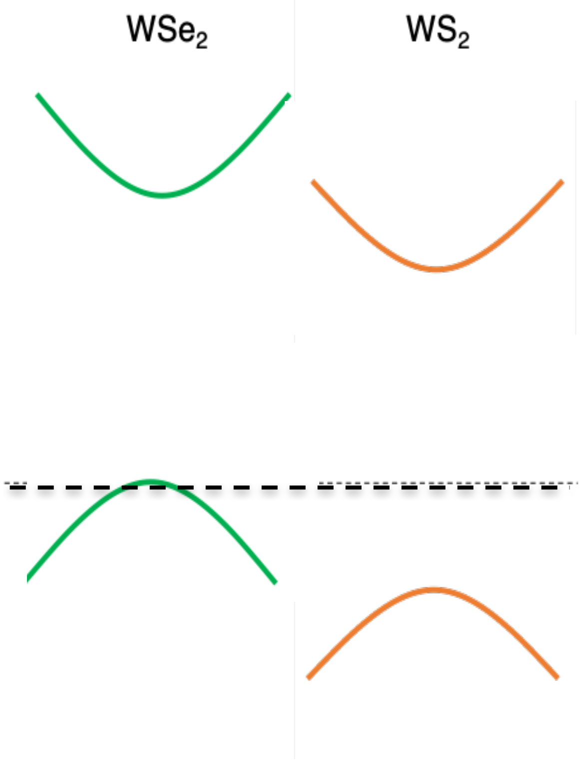


- *Strong exciton effects*
- *Optical selection rules*

# TMD hetero-bilayers

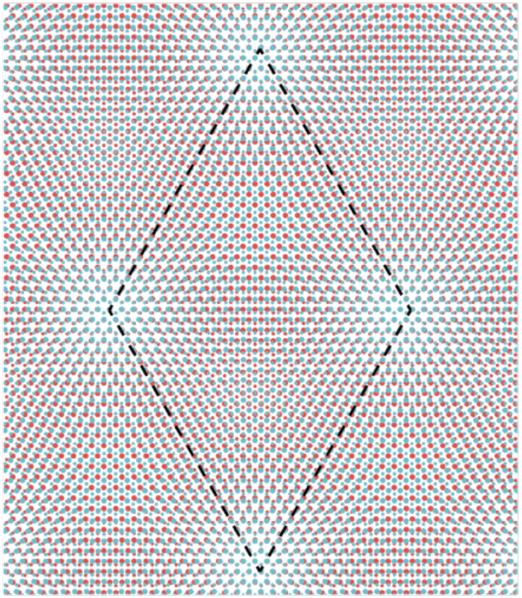
E.g. $WSe_2$-$WS_2$ bilayer

Type-II band alignment



# TMD hetero-bilayers

E.g. $WSe_2$-$WS_2$ bilayer (0-degree, 4% mismatch, 8 nm)



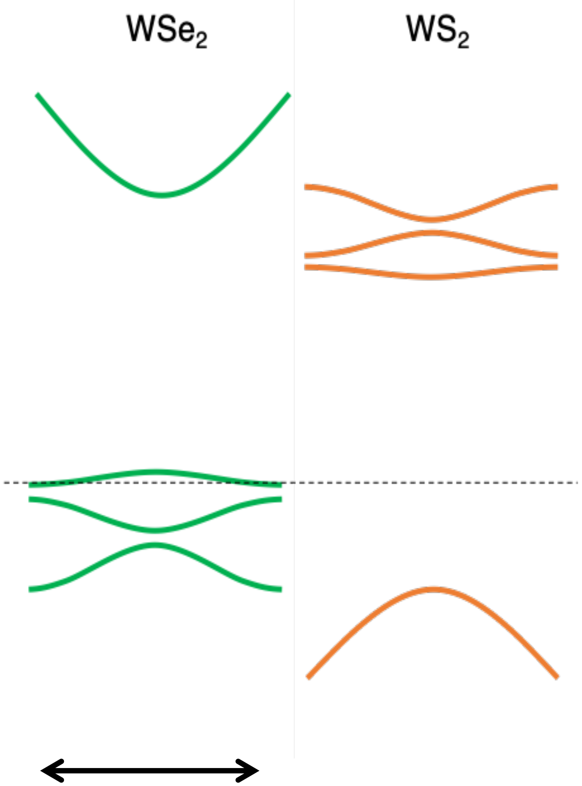
*Lattice mismatch -> moiré superlattice*

$$\lambda \approx \frac{a}{\sqrt{\delta^2 + \theta^2}}$$

*Bragg reflection*

Type-II band alignment

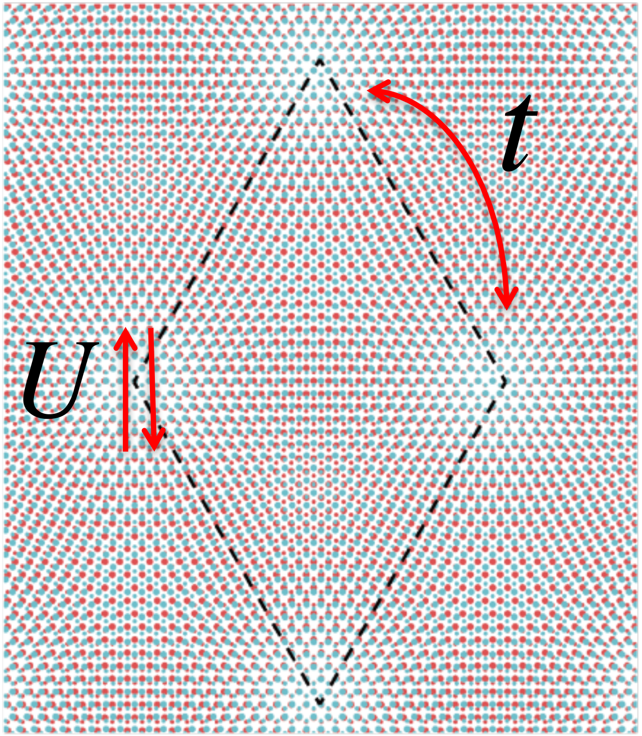
K valley K valley



*Mini-BZ*

# Triangular lattice Hubbard model

$$\mathcal{H} = -t \sum_{\langle ij \rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



Inter-site hopping

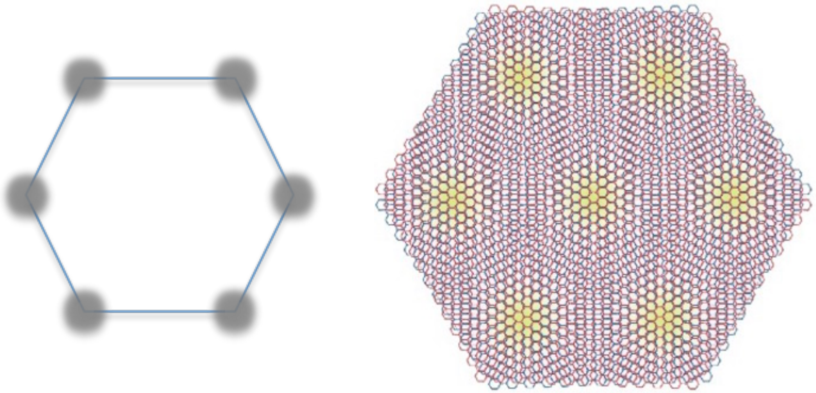
$t \sim$ 1-10 meV

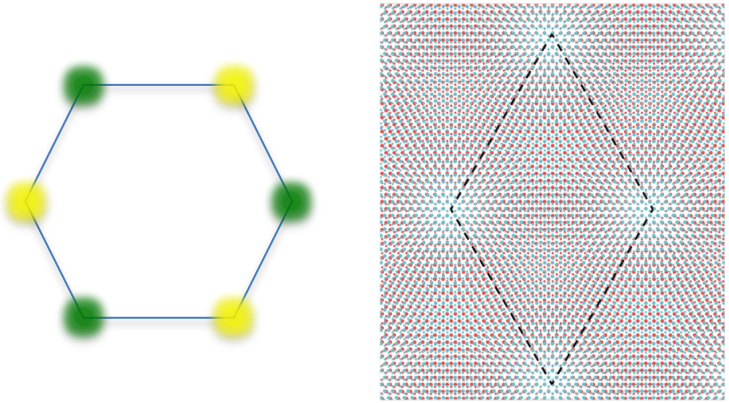
On-site repulsion

$$U \sim \frac{e^2}{\varepsilon a} \sim \text{10's -100 meV}$$

Wu and MacDonald, PRL (2018)

# Twisted bilayer graphene vs TMD hetero-bilayers





*Twisted bilayer graphene (topology)*

- Wannier obstructions

- Total degeneracy: 8-fold

- Magic angle

*TMD hetero-bilayer (correlation)*

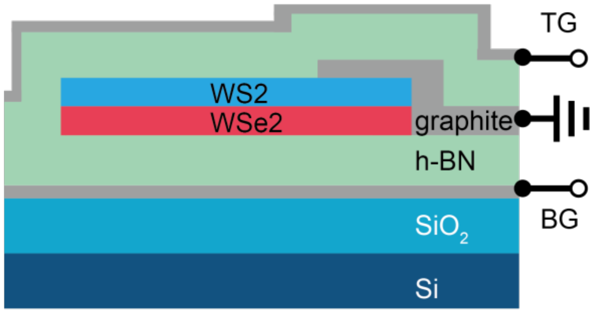
- Localized Wannier orbitals
- Stronger moiré potential (correlation)
- Total degeneracy: 2-fold, spin-valley DOF

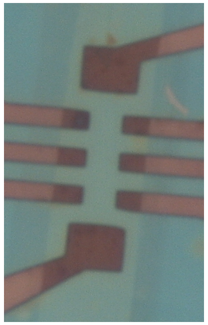
- Wide range of twist angle

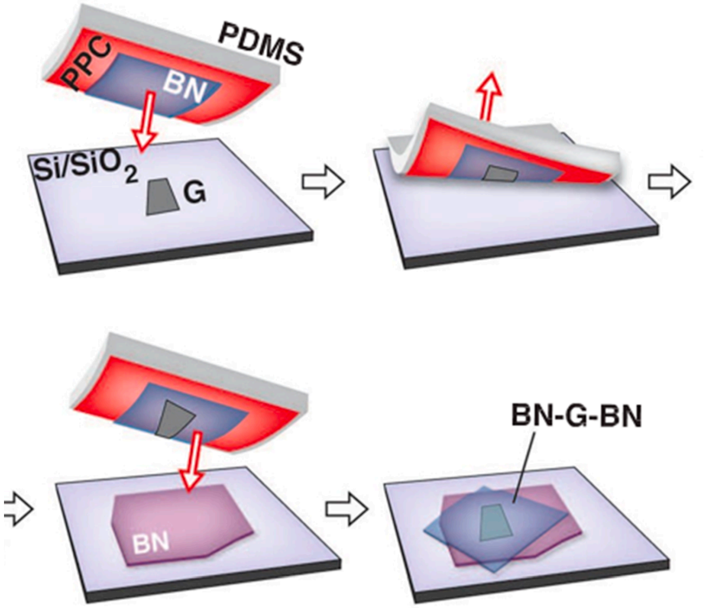
# Sample and device fabrication

Dual-gate device continuous control of fillings

Angle-aligned $WSe_2/WS_2$ (0 and 60 degrees)







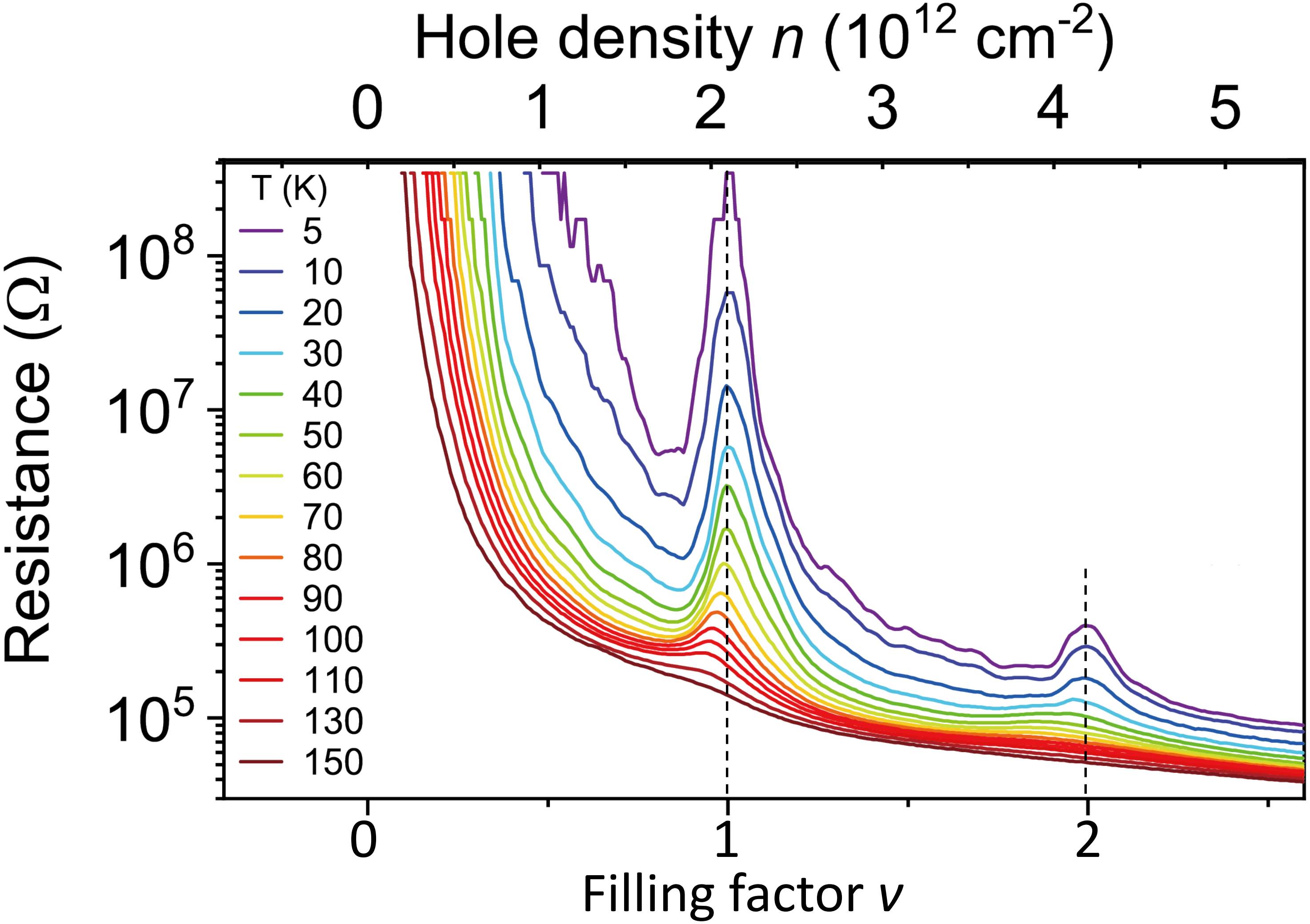
Measurements

- Optical measurements (1 micron)
- In-plane transport
- Capacitance (compressibility)

- Crystal axis orientation determined by nonlinear optical techniques
- Alignment of different materials within 0.5 degree

# TMD moiré superlattices ($\nu = 1$)

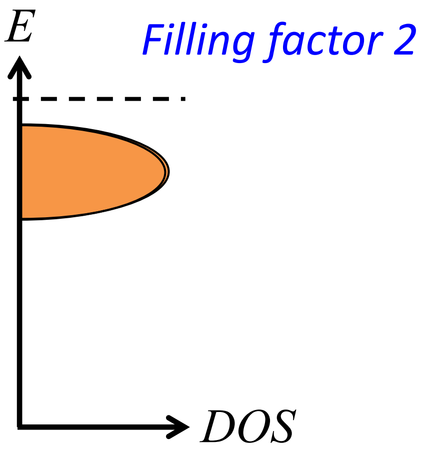
# Insulating state at half filling ($\nu = 1$)

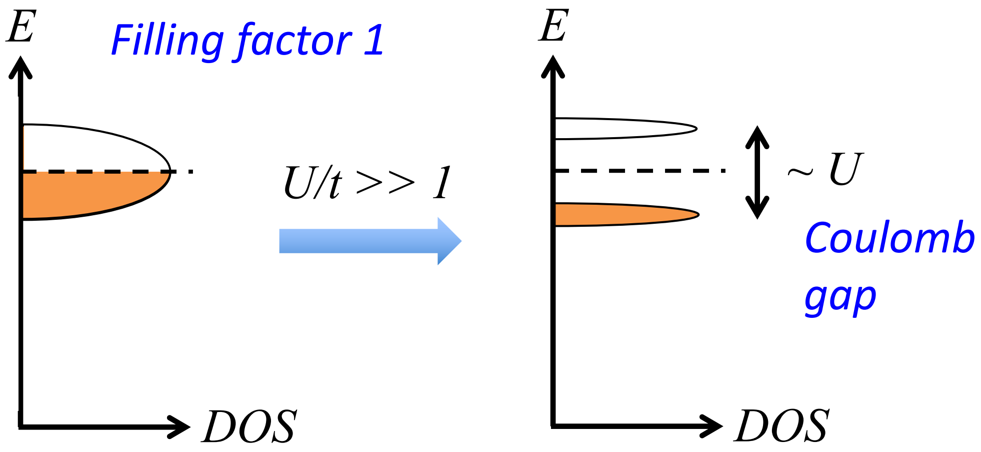


In collaboration with Allan MacDonald

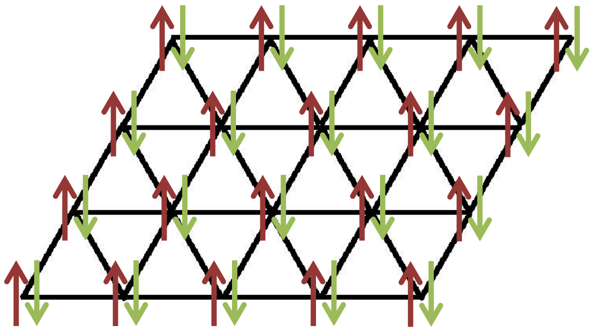
Tang et al. Nature (2020)

# Mott insulating state at half filling ($\nu = 1$)

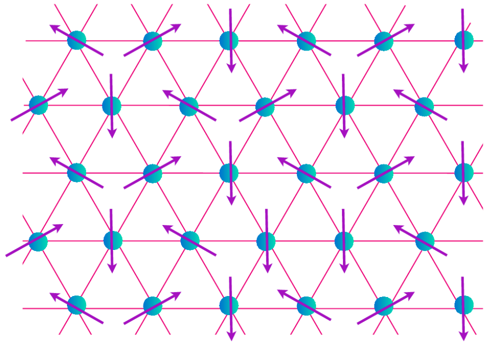




Band insulator



Mott insulator

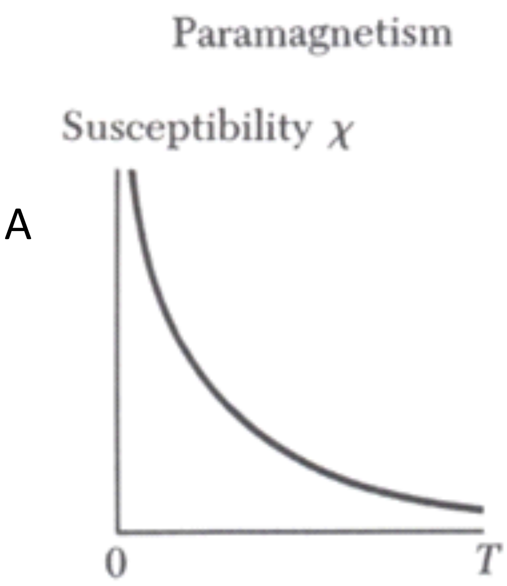


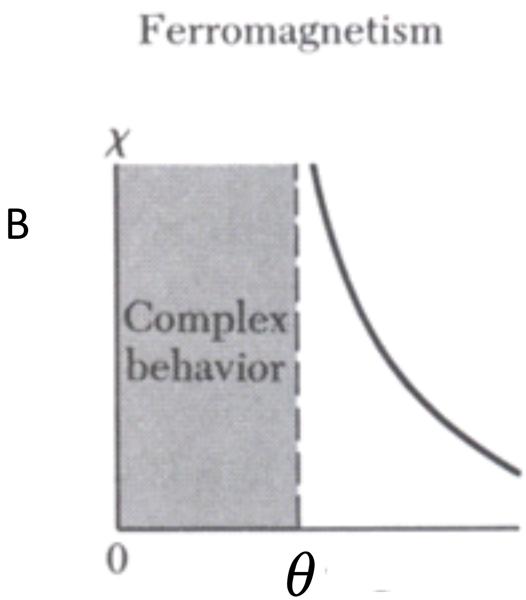
½-filling R peak vanishes at ~ 150-200 K

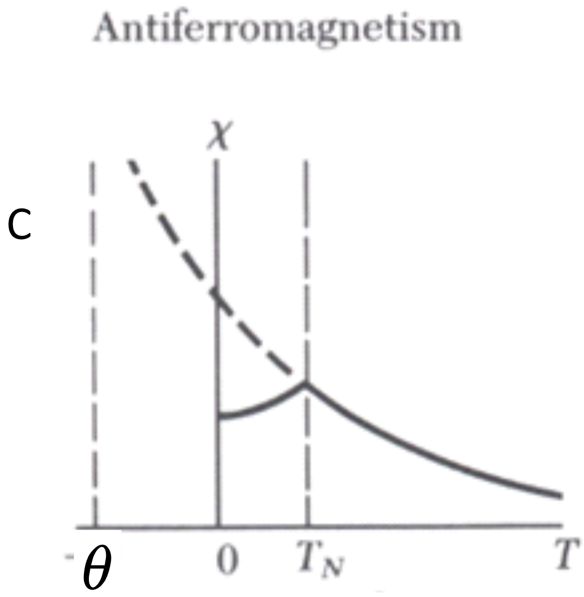
-> $U \sim 20$ meV

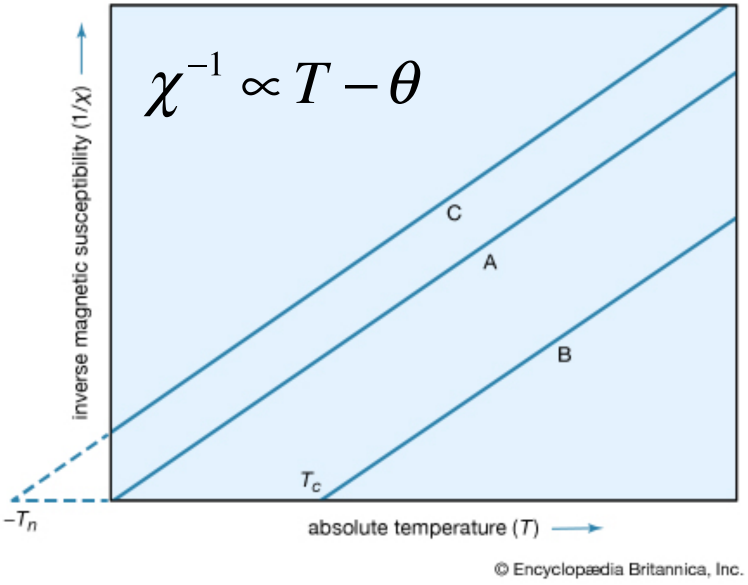
Alternative: Charge-transfer insulator (Liang Fu)
arXiv:1910.14061

# Magnetic susceptibility









$$\chi^{-1} \propto T - \theta$$

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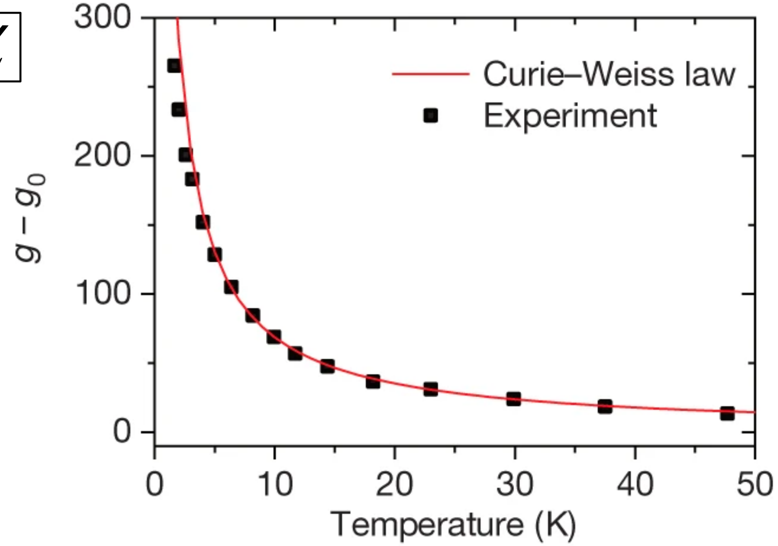
For T >> J $\chi = \dfrac{C}{T-\theta}$ $\theta \sim -J$

Weiss temperature

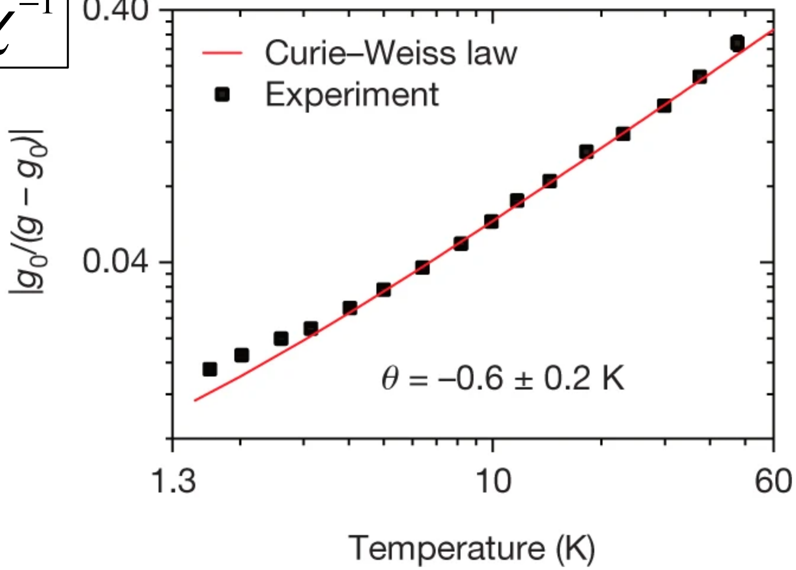
***θ > 0: ferromagnetic***
***θ < 0: antiferromagnetic***

# Magnetic susceptibility measurement

$\boxed{\chi}$



$\boxed{\chi^{-1}}$

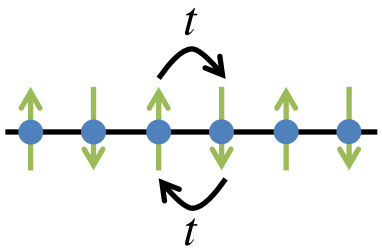


Curie-Weiss law

$$\chi^{-1} \propto T - \theta$$

$$\boxed{\theta \approx -0.6K \sim -0.05meV}$$

$$\theta \sim -J \sim \frac{t^2}{U}$$



Super-exchange

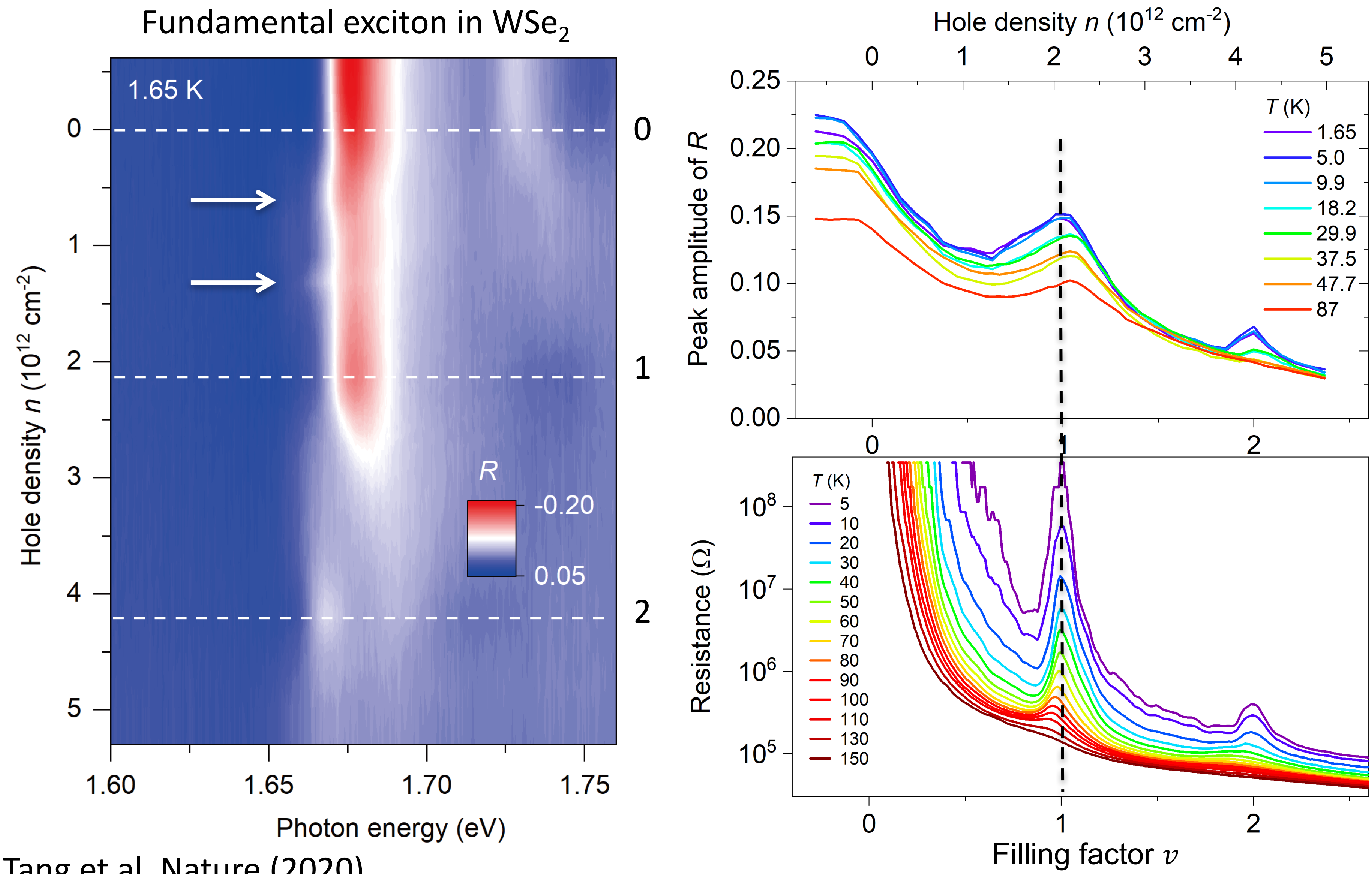
$$\boxed{\begin{array}{l} U \sim 20meV \\ \rightarrow t \sim 1meV \\ \rightarrow \dfrac{U}{t} \sim 20 \end{array}}$$

$$H_S = {\sum_{\boldsymbol{R},\boldsymbol{R}'}}' J(\boldsymbol{R}' - \boldsymbol{R}) \mathbf{S}_{\boldsymbol{R}} \cdot \mathbf{S}_{\boldsymbol{R}'}$$

Heisenberg model

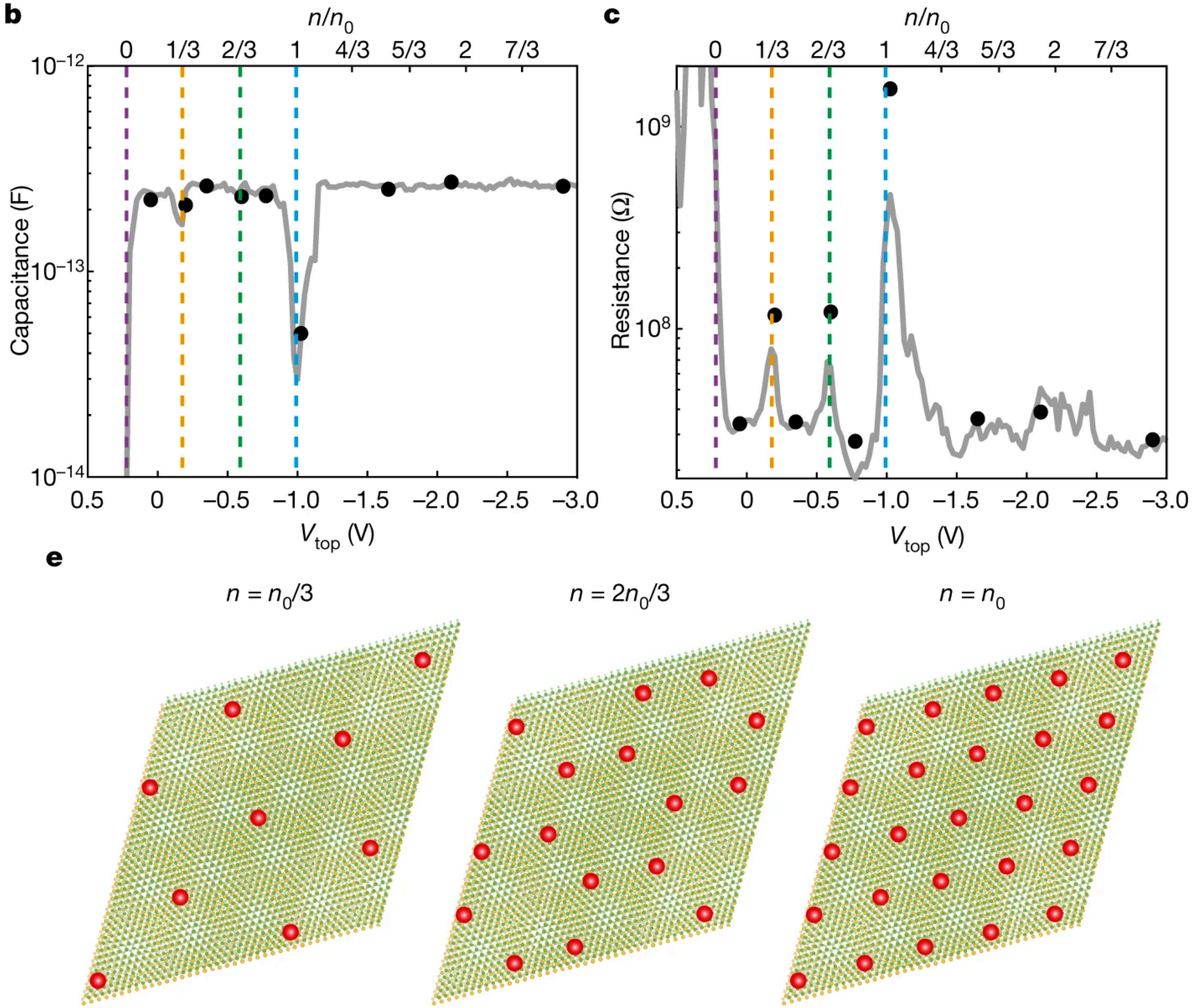
Tang et al. Nature (2020)

# Optical signature of the Mott insulating state



Tang et al. Nature (2020)

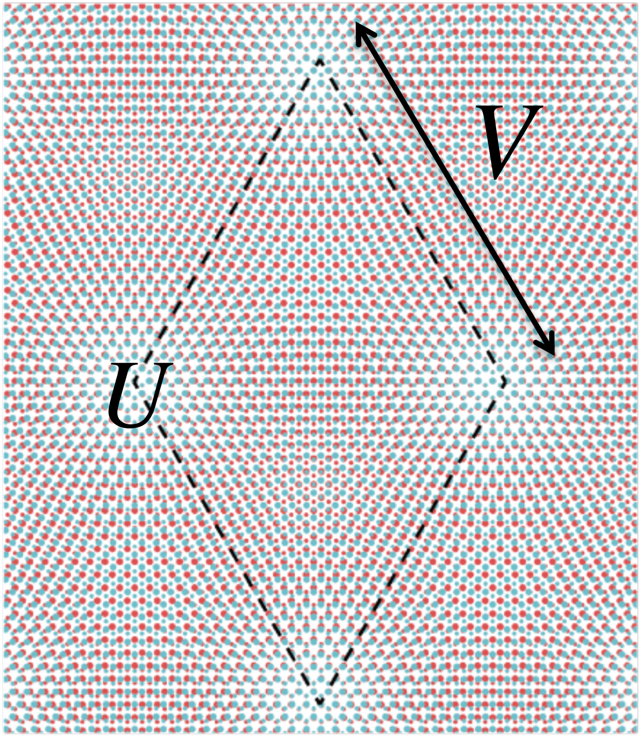
# Charge-ordered states (ν = 1/3, 2/3)



Charge-ordered states
(minimize long-range V)

Regan, Wang, Jin et al. Nature (2020)

# Extended Hubbard model



Gate separation <u>much bigger than</u> moiré period

$$V(r) \approx \frac{e^2}{4\pi\varepsilon\varepsilon_0 r}$$

Long-range Coulomb > *t*

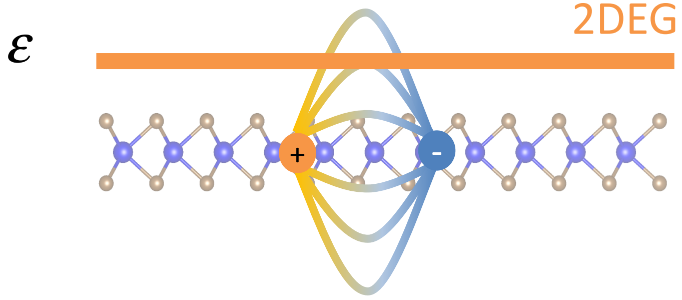
Extended Hubbard model

$$H = H_0 + \frac{1}{2}\sum_i \sum_{j \neq i} V(r_{ij}) n_i n_j$$

$H_0$ Hubbard model Hamiltonian

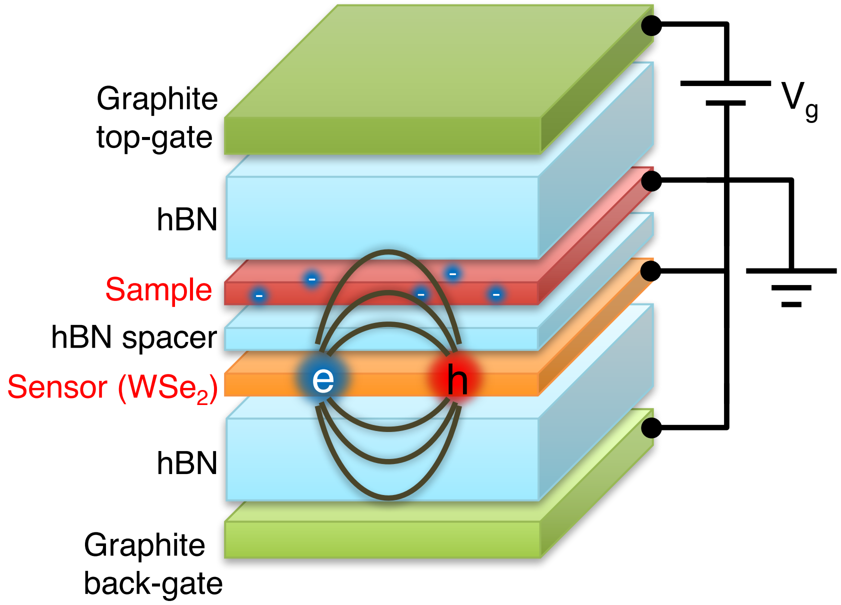
# Charge-ordered states ($\nu < 1$)

# A new exciton sensing technique



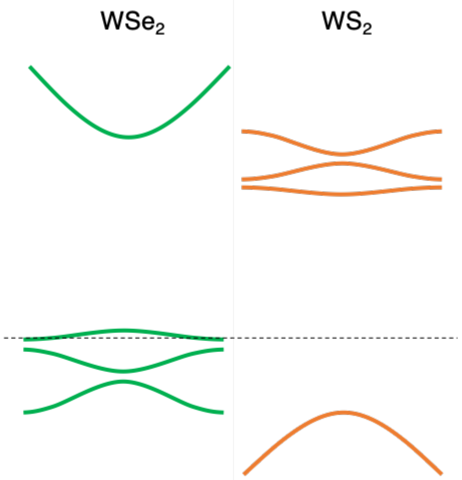
2D H-atom with 1/r potential
1s state ~ 1 nm
2s state ~ 5 nm

$$E_b^{(n)} = \frac{m_r e^4}{2\hbar^2 (4\pi\varepsilon\varepsilon_0)^2 (n-1/2)^2} \propto \frac{1}{(\varepsilon)^2}$$



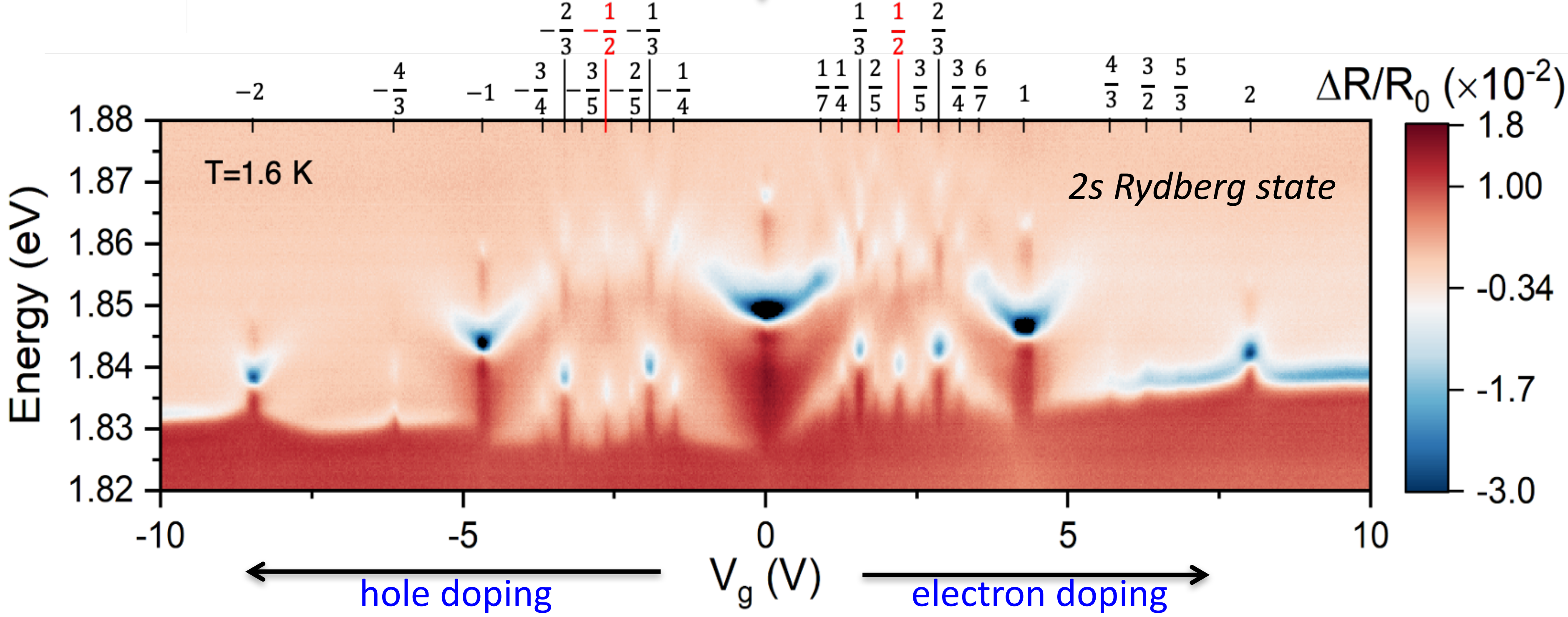
- ***Metallic (compressible): smaller binding energy, lower intensity***
- ***Insulating (incompressible): larger binding energy, higher intensity***

# Abundance of insulating states



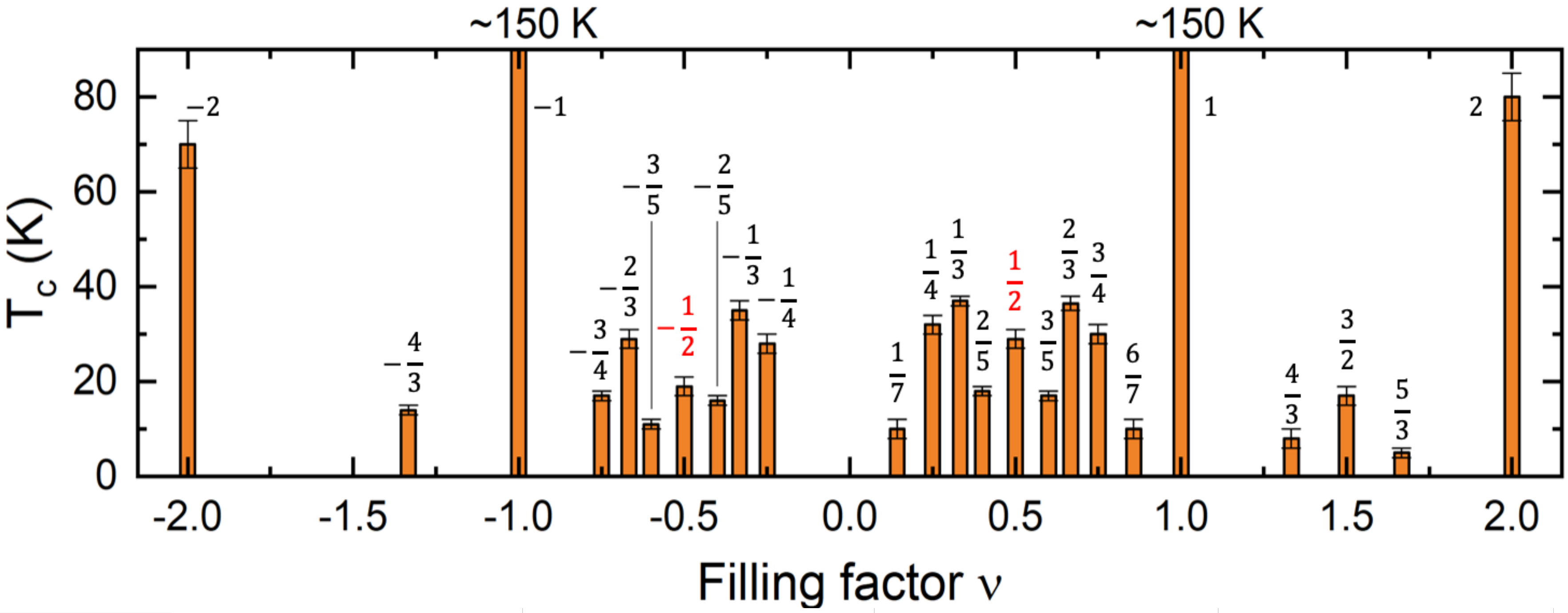
Mott insulator

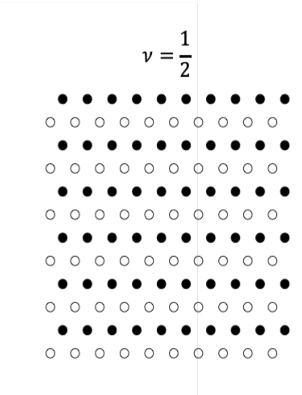
Band insulator

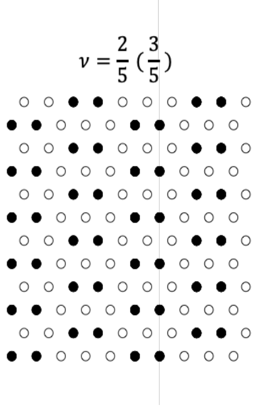


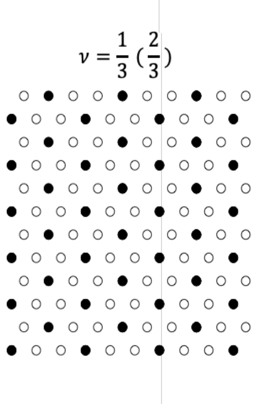
Xu et al. (arXiv:2007.11128)

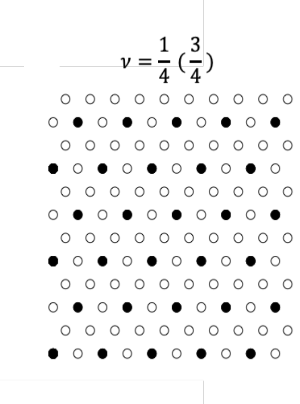
# Ordering temperature

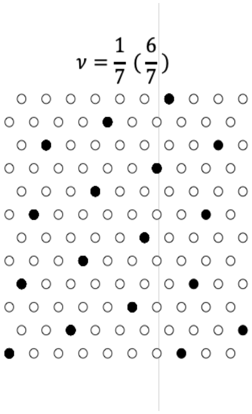










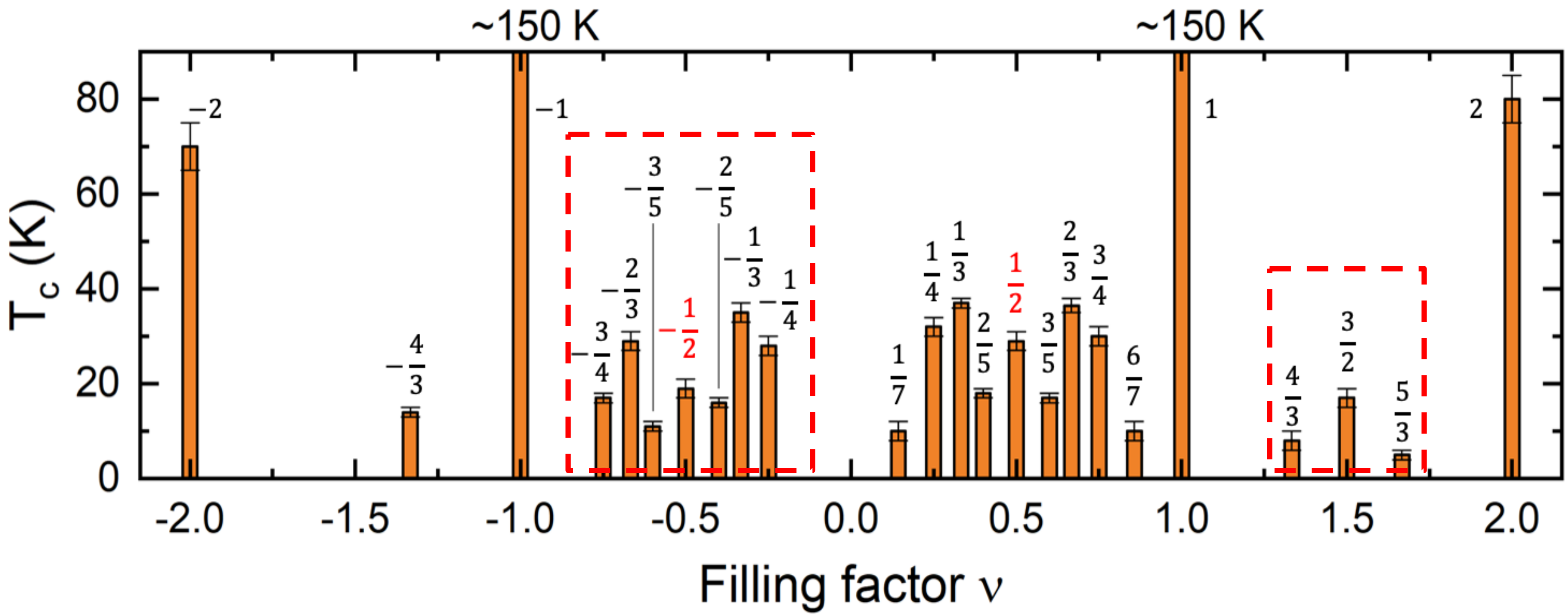


$$H = \frac{1}{2}\sum_i \sum_{j \neq i} V\left(r_{ij}\right) n_i n_j$$

(Monte Carlo, Veit Elser)

Xu et al. (arXiv:2007.11128)

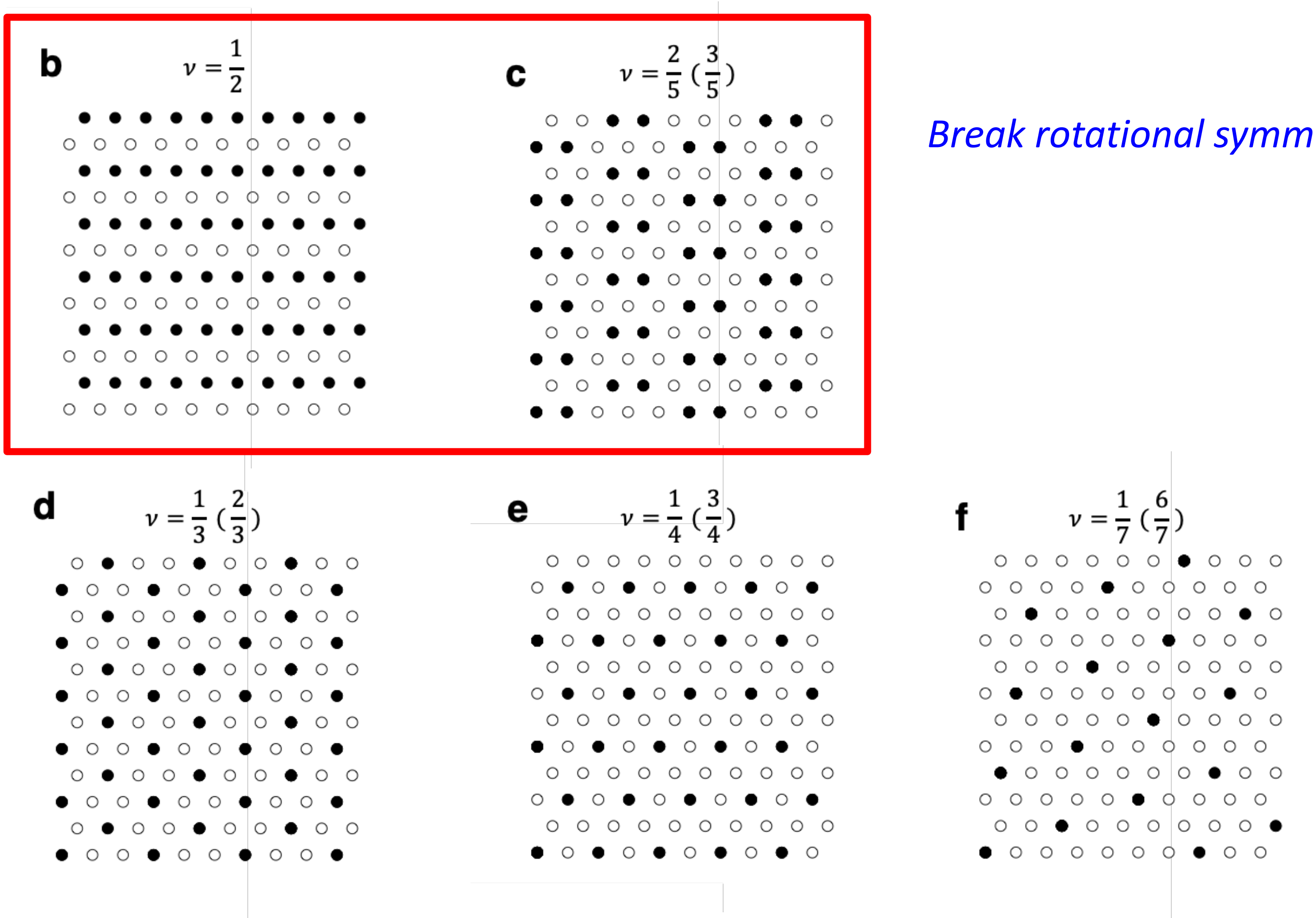
# Quantum effects



- Asymmetry about ½ indicates effects of quantum fluctuations
- Much weaker states for ν>1 -> higher kinetic energy for ν>1
- Stronger insulating states on the electron side

Xu et al. (arXiv:2007.11128)

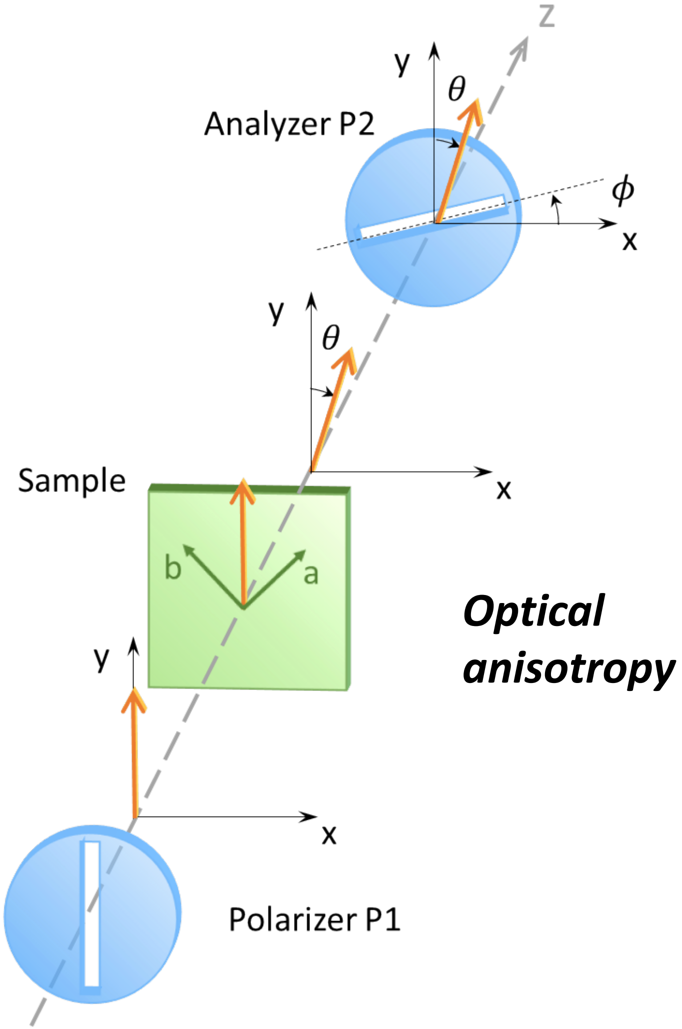
# Stripe phases



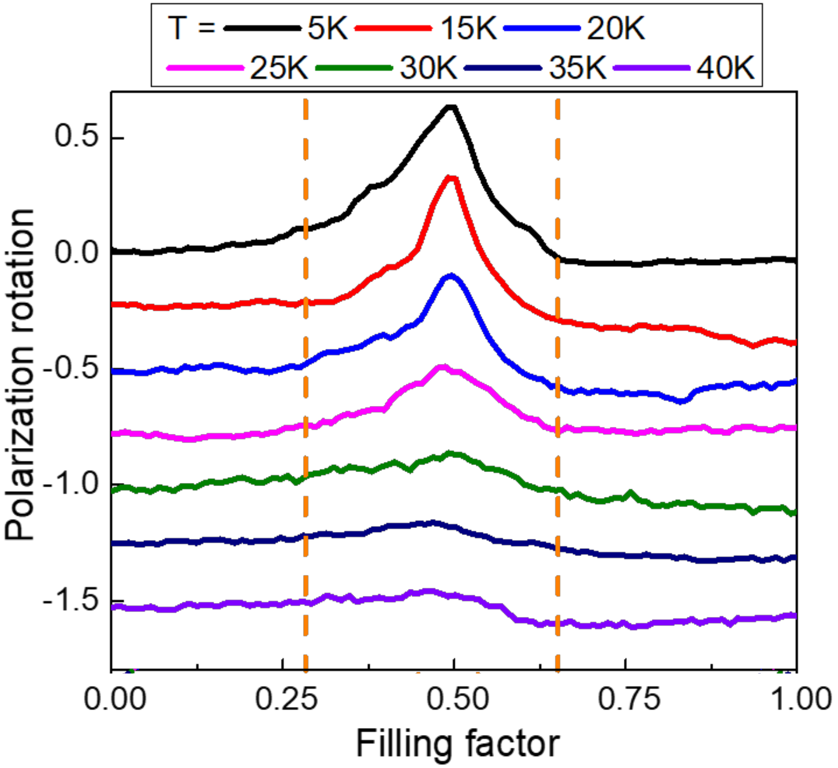
*Break rotational symmetry!*

Xu et al. (arXiv:2007.11128)

# Optical detection of stripe phases



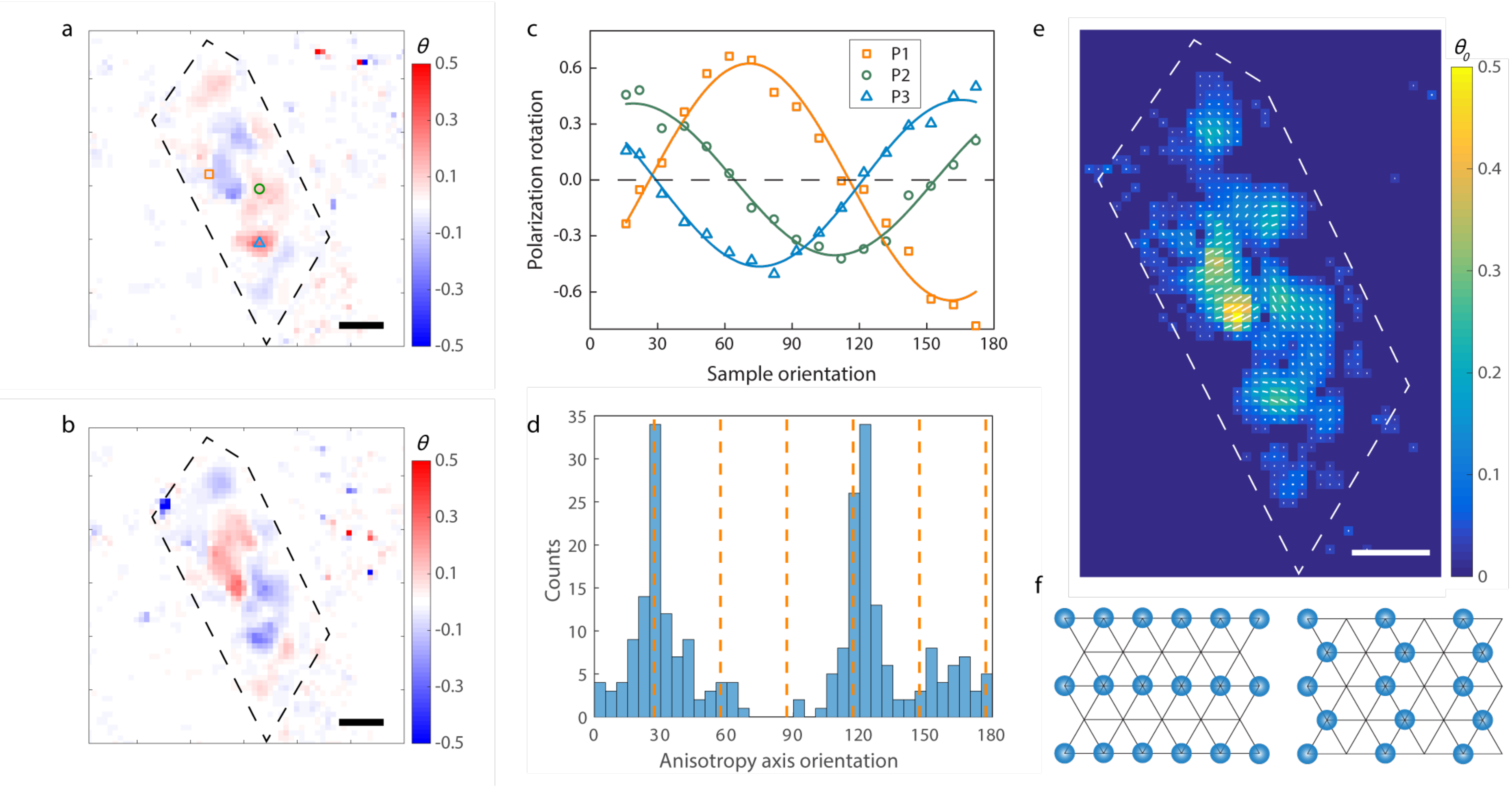
***Optical anisotropy***



In collaboration with Liang Fu
Jin, Tao, Li et al. (arXiv:2007.12068)

- Pronounced electronic anisotropy ν@½
- Disappear linearly with T around 35 K
- Anisotropy @ compressible regions
  -> nematic/smectic phases

# Stripe domain patterns



Jin, Tao, Li et al. (arXiv:2007.12068)

# Summary and outlook

- TMD moiré system provides a unique platform to study strong correlations with highly tunable parameters
- Extended Hubbard model on triangular lattices
- Experimental observation
  - AF Mott insulator at half filling ($\nu = 1$)
  - Abundance of charge-ordered states at fractional fillings
  - Some are stripe crystals, electronic liquid crystals also possible
- The system is very rich. Research is at an early stage.
- Unconventional superconductivity?
- Interplay of topology and correlation?
- Bose-Hubbard model physics (with iexcitons)?
- Ohmic contact?
- new experimental probes that can access the intertwined charge, spin, valley and collective excitations?