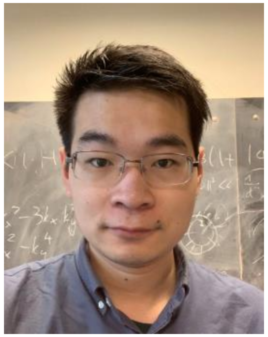
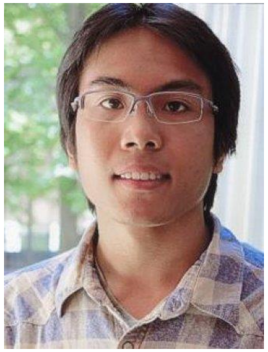
Topological Mott Insulator in Semiconductor Moire Heterostructure

Liang Fu

SIMONS FOUNDATION



Yang Zhang

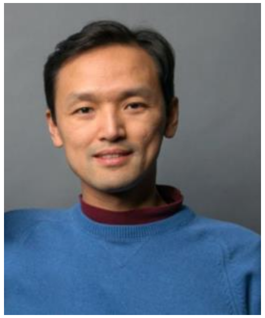


Trithep Devakul

Margarita Davydova

Cornell:

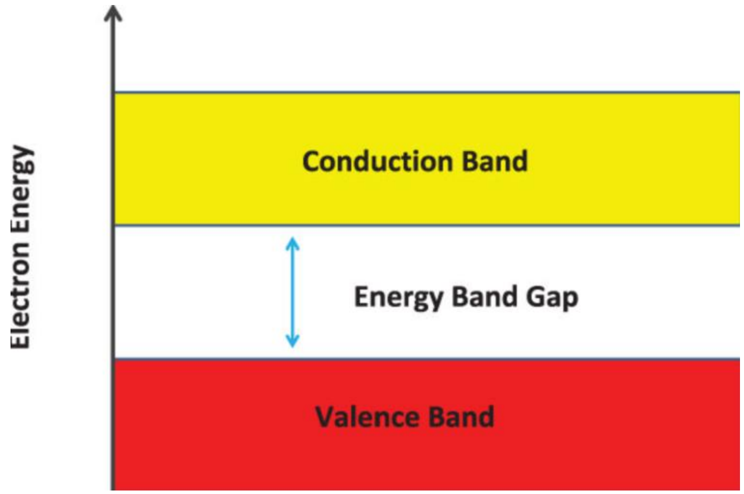
Jie Shan



Kin Fai Mak

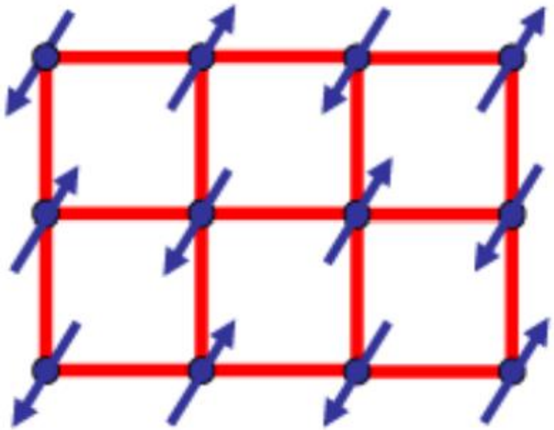
Two Types of Insulators

Band insulators



- even integer fillings
- energy gap due to Pauli exclusion

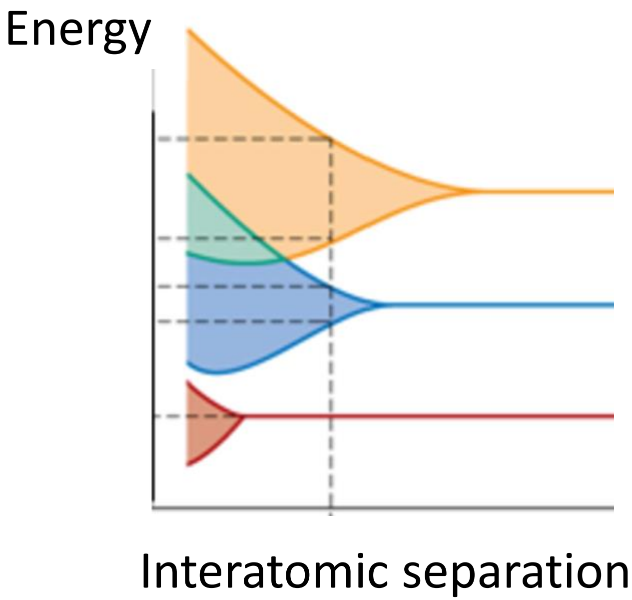
Mott insulators

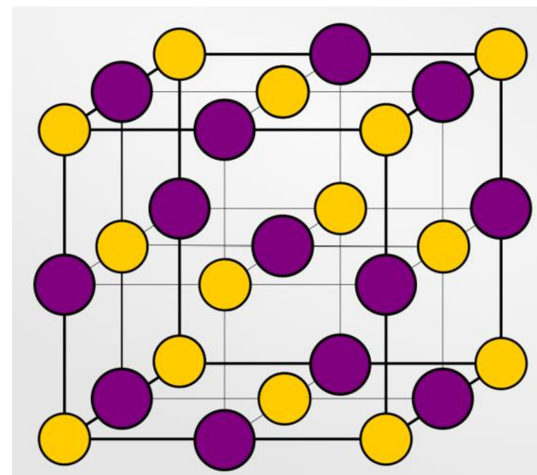


- odd integer fillings
- interaction induced gap

Normal Band Insulators

- energy gap remains finite as the crystal is taken apart
- topologically equivalent to atomic limit

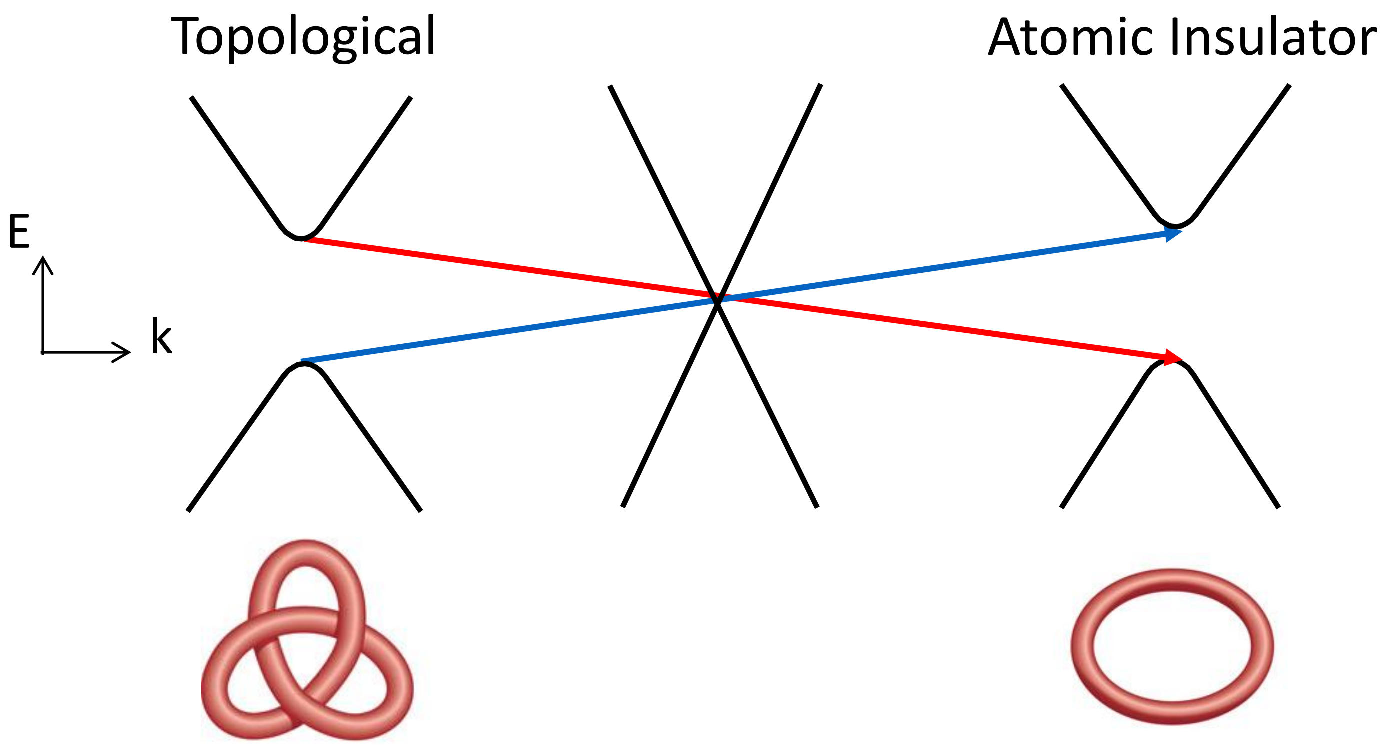




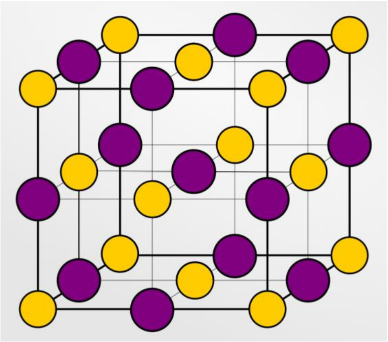
Band insulator: NaCl = Na^{1+} & Cl^{1-}

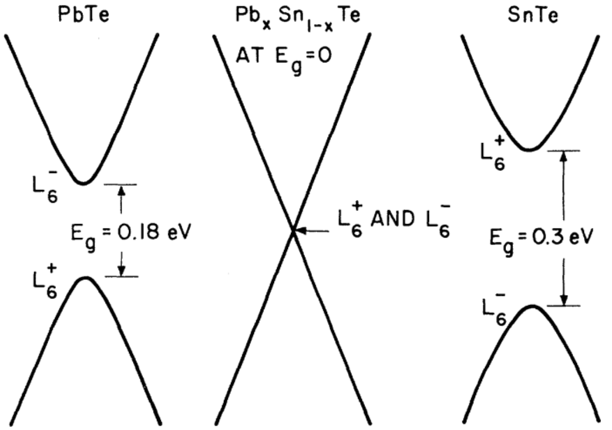
Topological Insulators

- cannot be taken apart smoothly
- rely on the wave nature of electron



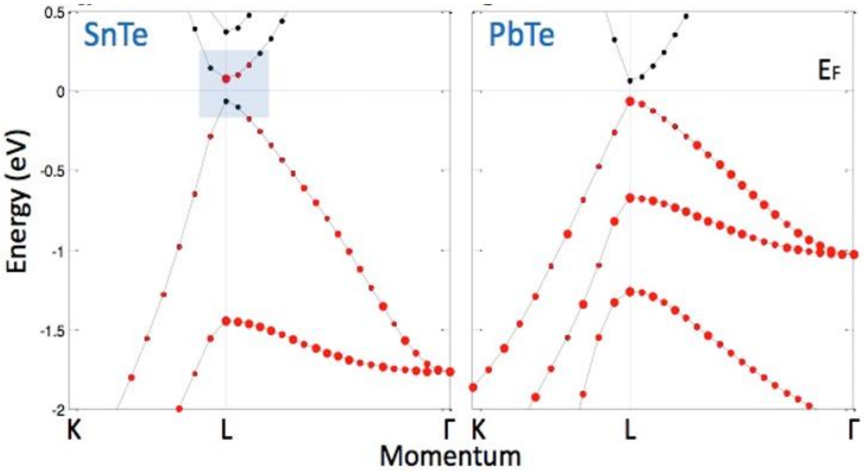
Atomic versus Topological Insulators





Dimmock et al (1966)

- PbTe = Pb^{2+} & Te^{2-}
- SnTe ≠ Sn^{2+} & Te^{2-}

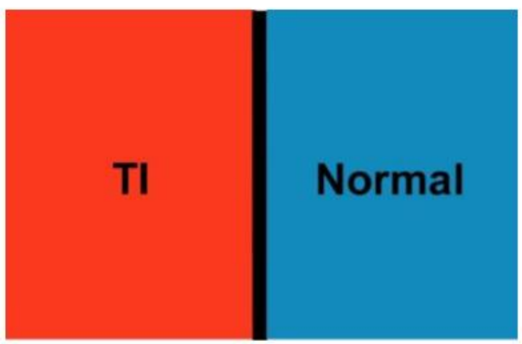


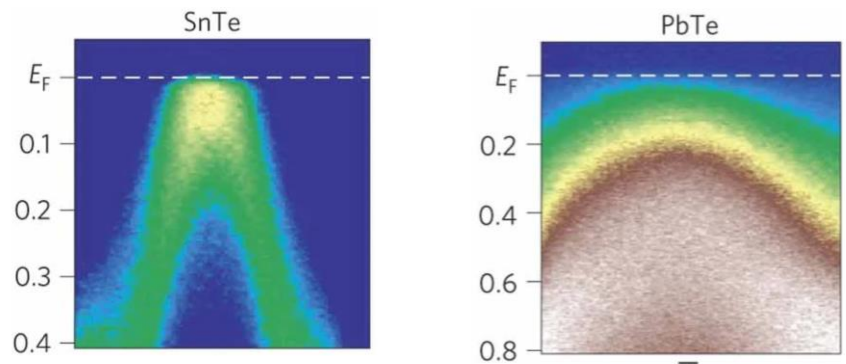
Hsieh et al (2012)

Continuous Phase Transition

between normal and topological band insulators

Dirac field theory: $H = -i\,\nabla \cdot \Gamma + m\Gamma_0$



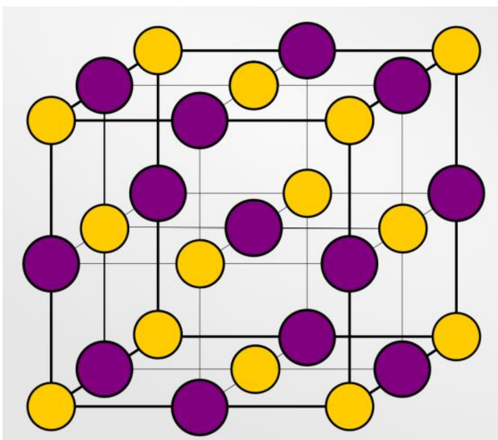


Ando et al (2012)

- change of topology = sign change of Dirac mass
- boundary (= domain wall) hosts massless Weyl fermion
- interaction is irrelevant at critical point

Mott Insulators

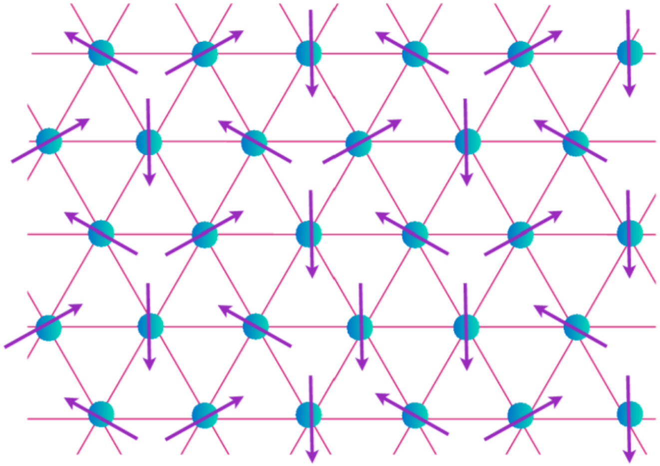
NiO = Ni^{2+} & O^{2-}



- electrons bound to individual atoms
- electron motion prohibited by local repulsion $U n_{i\uparrow} n_{i\downarrow}$


Mott
Topology

Part 1: Inverting Mott Insulators



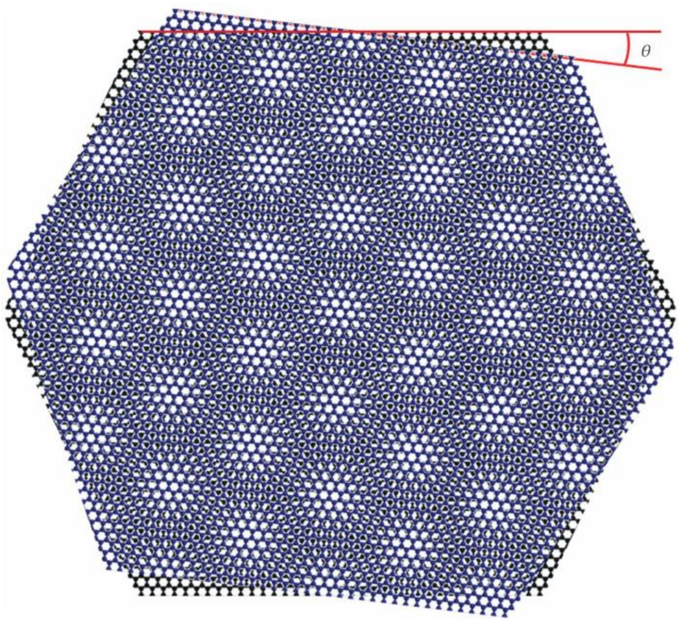
Continuous phase transition from 120° AFM Mott insulator to Chern insulator with spin chirality

Zhang, Devakul & LF, PNAS (2021)

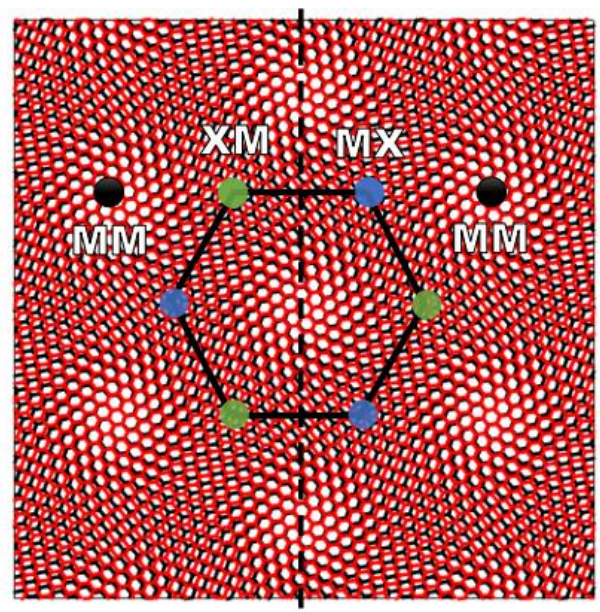
Devakul & LF, PRX (2022)

Moire Superlattices

Twisted bilayer graphene

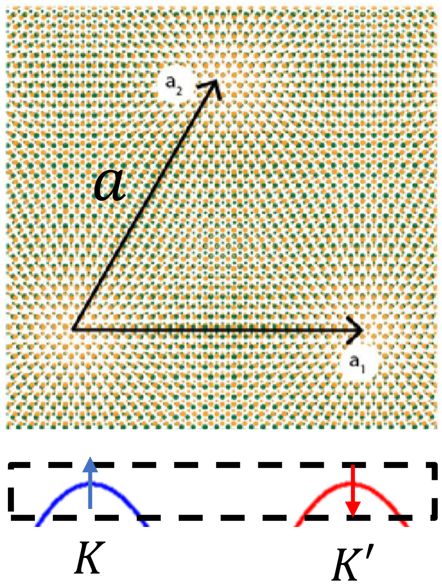


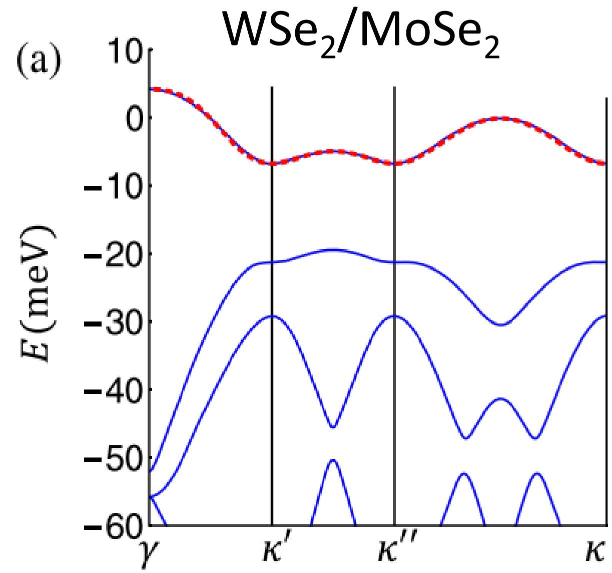
Semiconductor heterostructure



Hubbard Model Physics in Transition Metal Dichalcogenide Moiré Bands

Fengcheng Wu,[1] Timothy Lovorn,[2] Emanuel Tutuc,[3] and A. H. MacDonald[2]





$$H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})$$

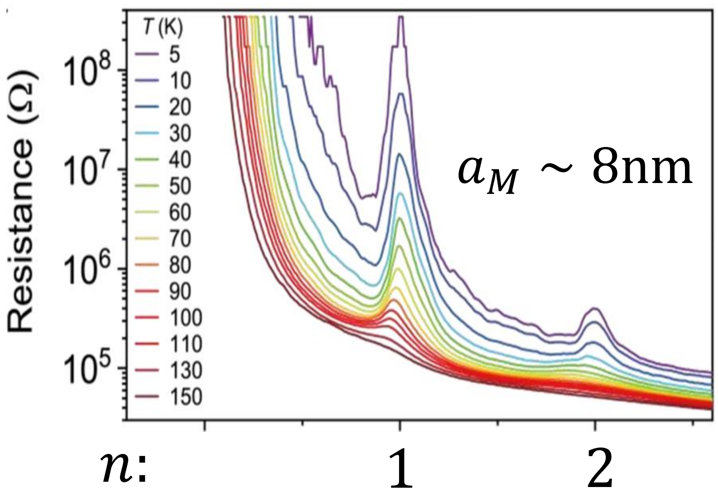
$V(\boldsymbol{r})$: superlattice potential

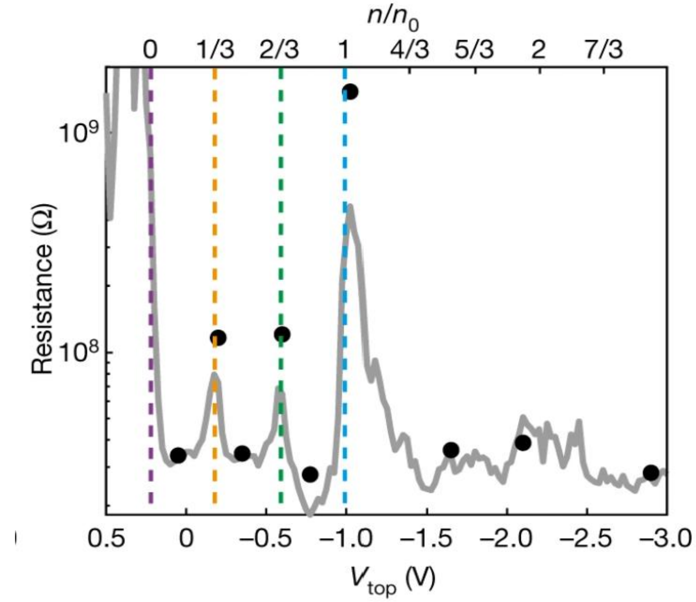
Tight-binding regime at large moire period: $\hbar^2/ma^2 \ll V$

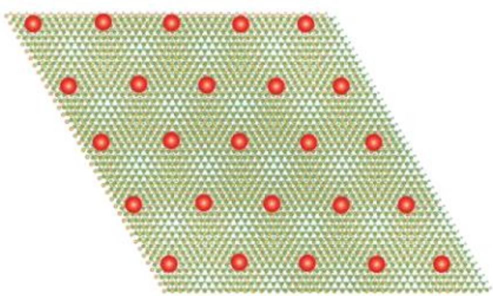
=> triangular lattice of "quantum dots" & Hubbard model

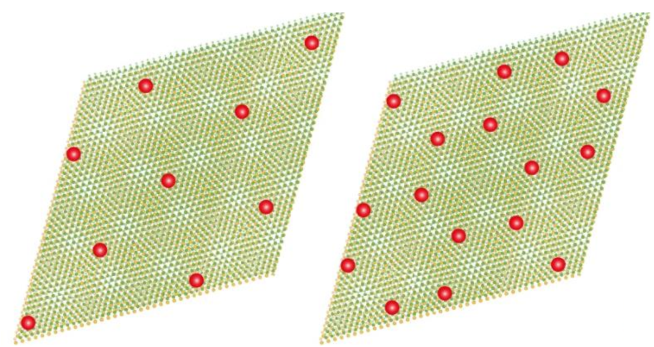
Simulation of Hubbard model physics in WSe_2/WS_2 moiré superlattices

Mott and generalized Wigner crystal states in WSe_2/WS_2 moiré superlattices







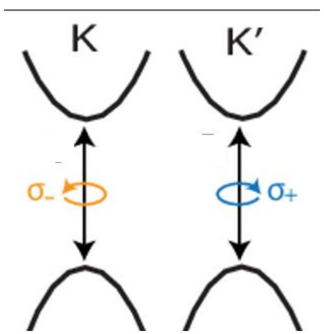


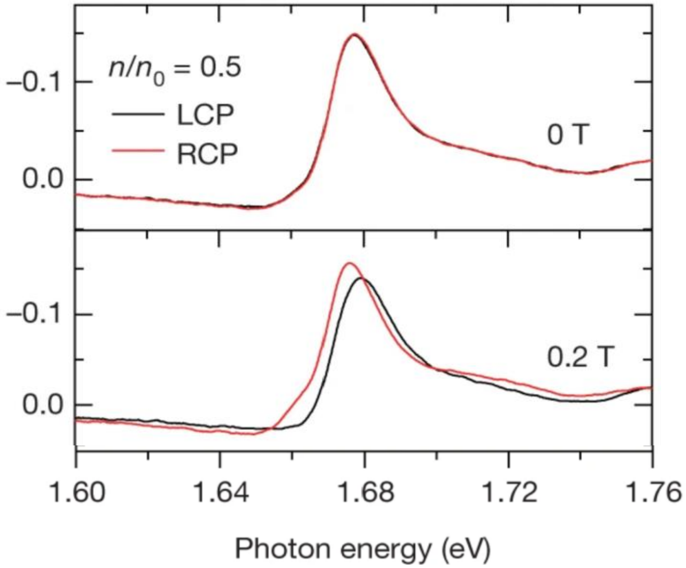
Mott insulator at $n = 1$ (half band filling)

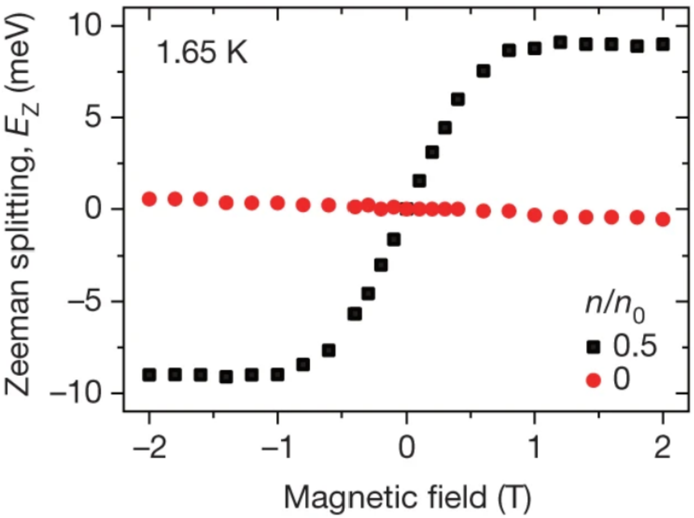
Wigner crystals at $n = \frac{1}{3}, \frac{2}{3}$ ...

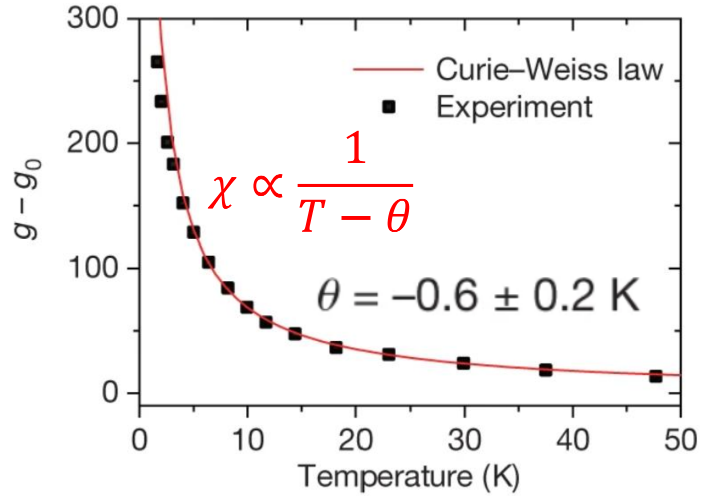
WC & MIT: Chenhao Jin, Cenke Xu, Senthil, Kim, Das Sarma, Philips, MacDonald ...

Local Moment and AFM Interaction





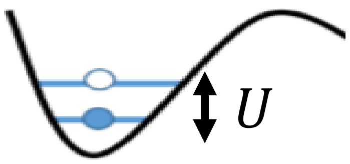


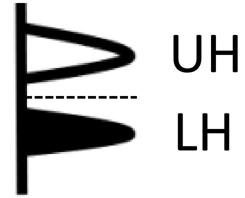


Tang et al, Nature (2020)

Charge-Transfer Mott Insulator

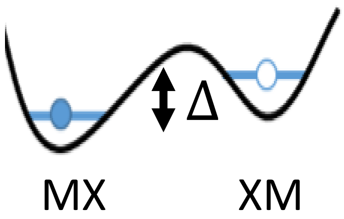
Mott-Hubbard insulator

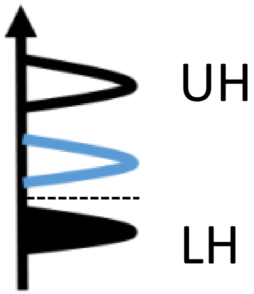




$U > \Delta$:
Charge transfer insulator

(similar to CuO_2)





- moire potential may have two minima in a unit cell
- doped charges at n>1 occupy secondary minima to avoid U.
- insulating gap at n=1 set by Δ

Zhang, Yuan & LF, PRB (2020)

Moiré quantum chemistry: Charge transfer in transition metal dichalcogenide superlattices

Yang Zhang,* Noah F. Q. Yuan,* and Liang Fu

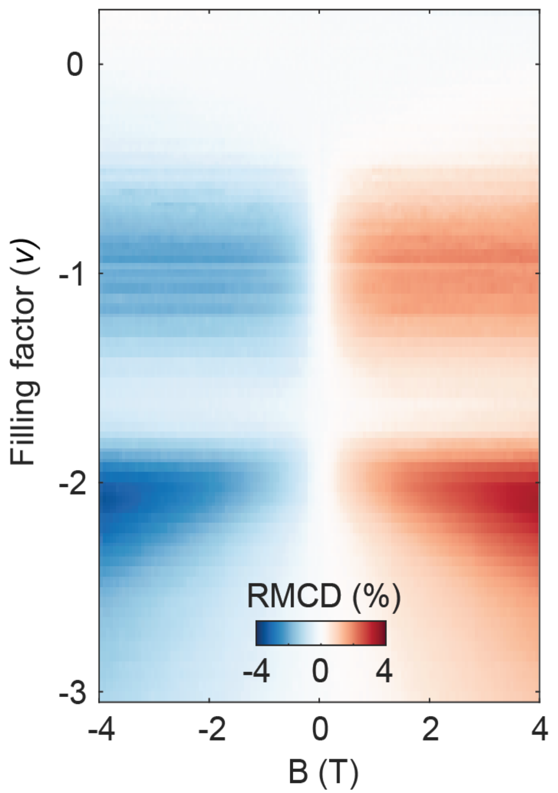
Charge transfer excitations, pair density waves, and superconductivity in moiré materials

Kevin Slagle[1,2] and Liang Fu[3]

Electronic structures, charge transfer, and charge order in twisted transition metal dichalcogenide bilayers

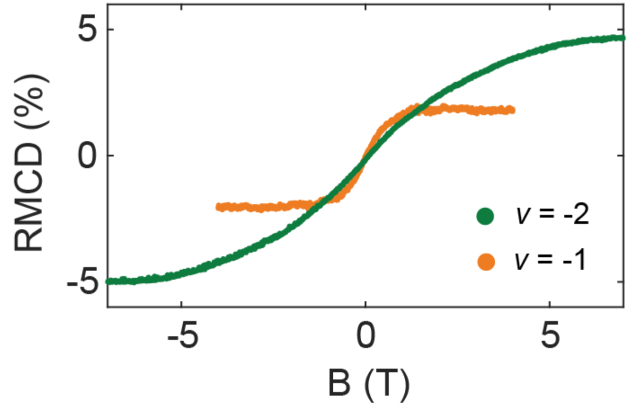
Yang Zhang,* Tongtong Liu, and Liang Fu

Intralayer Charge Transfer in WSe_2/WS_2

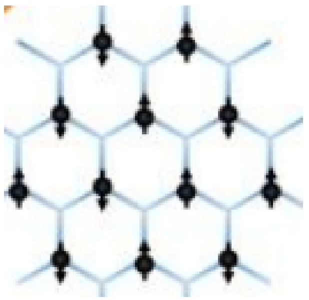


Xiaodong Xu's group (submitted)

See also Xu et al, arXiv:2202.02055

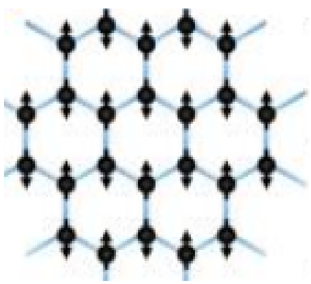


$n = 1$



charge-transfer Mott insulator

$n = 2$



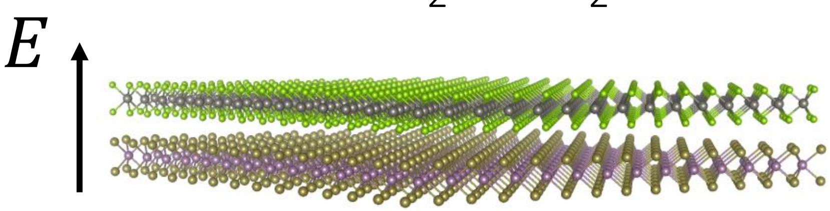
honeycomb lattice Mott-Hubbard

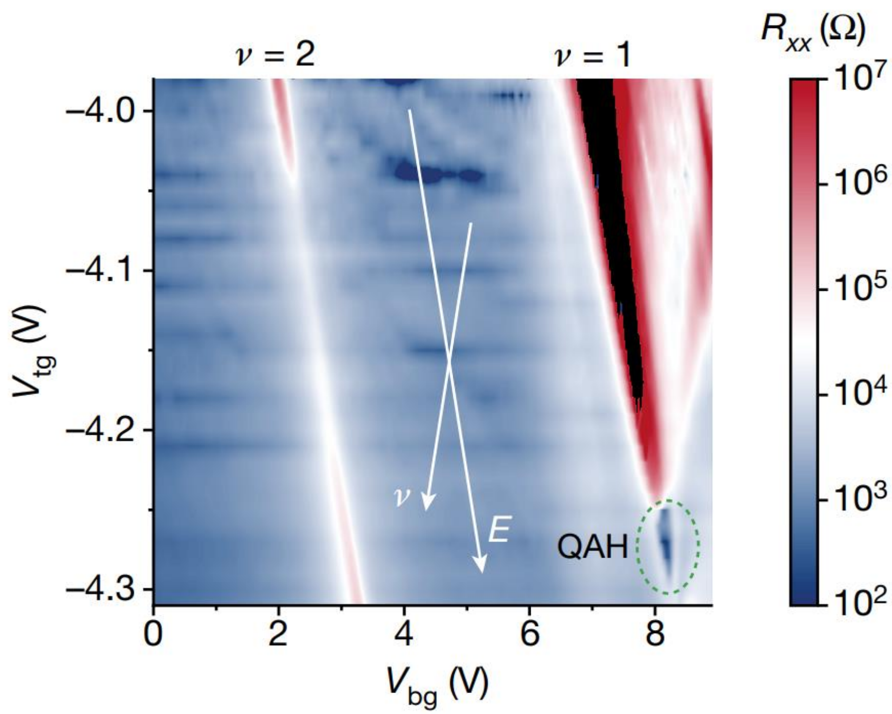
Article | Published: 22 December 2021

Quantum anomalous Hall effect from intertwined moiré bands

Tingxin Li, Shengwei Jiang, Bowen Shen, Yang Zhang, Lizhong Li, Zui Tao, Trithep Devakul, Kenji Watanabe, Takashi Taniguchi, Liang Fu, Jie Shan & Kin Fai Mak

$MoTe_2/WSe_2$

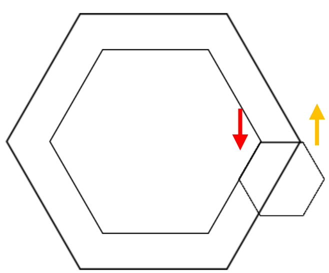


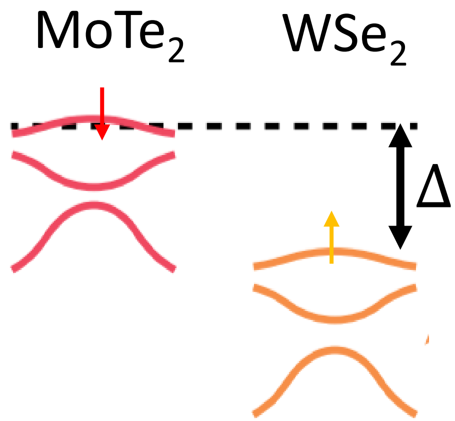


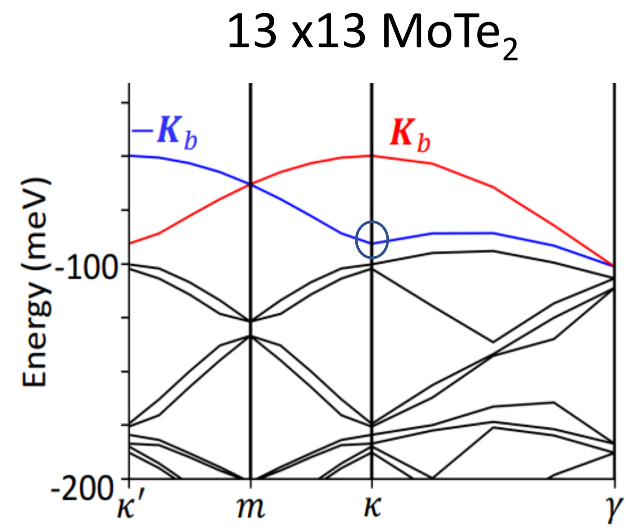
- Electric field tunes interlayer charge transfer

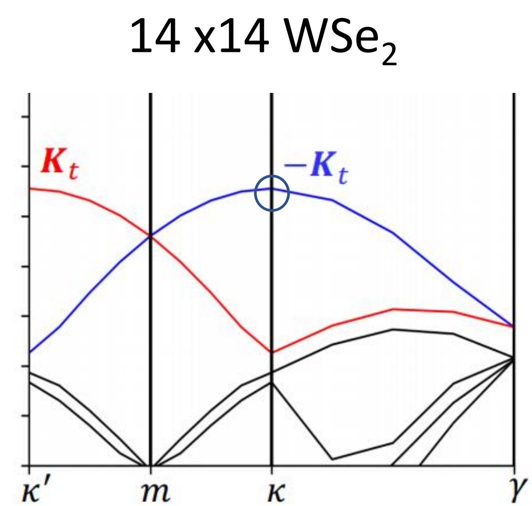
Moire Bands in $MoTe_2/WSe_2$

$a_M = 4.6\text{nm}$



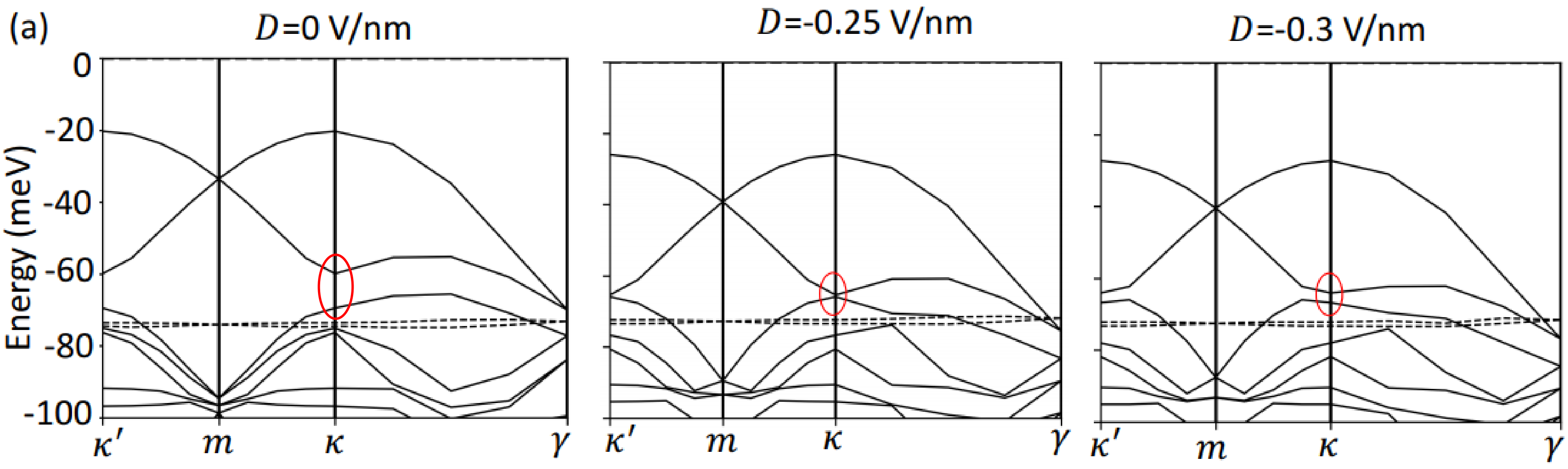






- $\Delta = 0.13\text{eV}$ at zero E field
- majority layer: $MoTe_2$
  minority layer: WSe_2
- moire band due to lattice corrugation with bandwidth ~ 50 meV

E Field Tunes Band Inversion

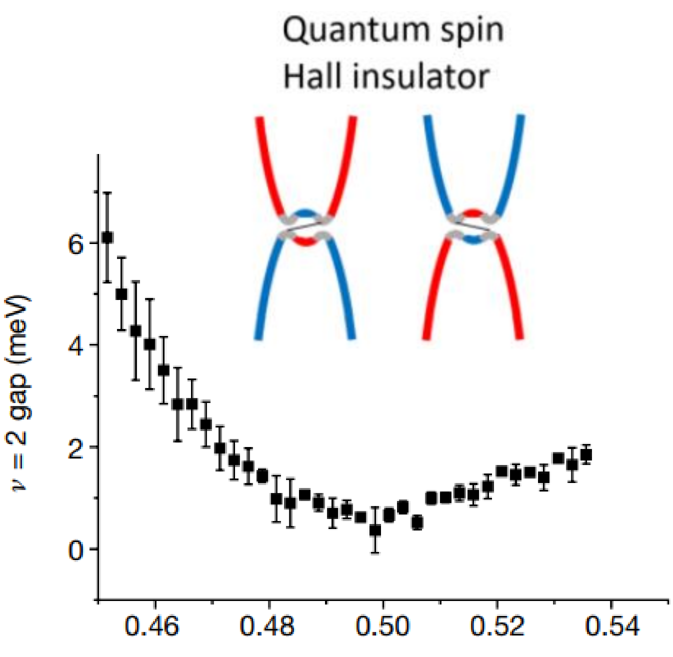


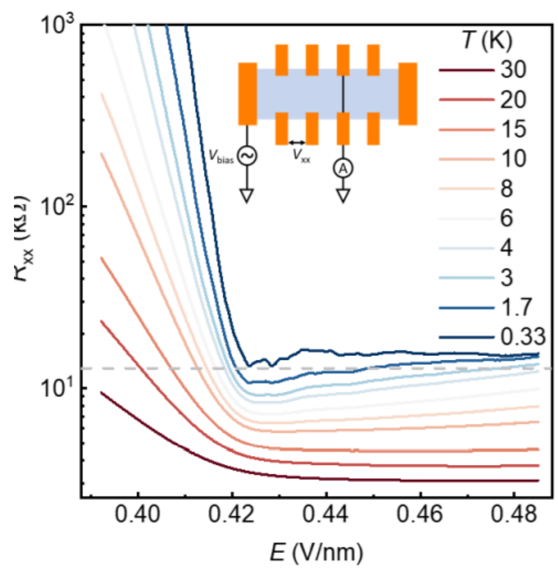
- electric field inverts minibands on two layers
- band inversion + p-wave interlayer tunneling => valley Chern number

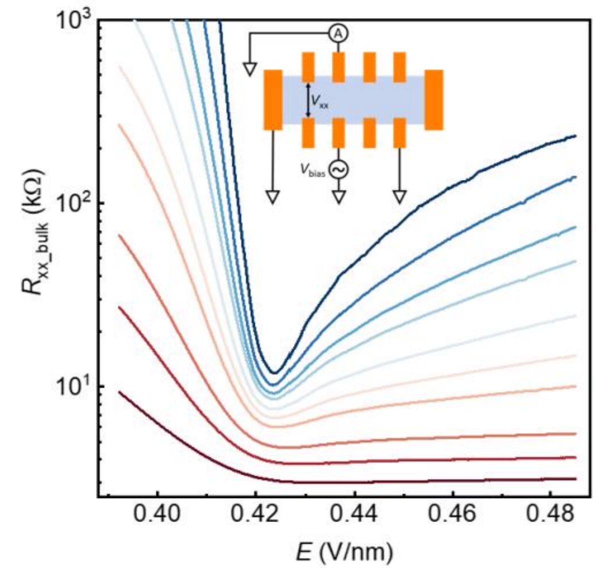
Prediction: E field induced quantum spin Hall insulator at n=2

Zhang, Devakul & LF, PNAS (2021)

Edge Transport in $MoTe_2/WSe_2$

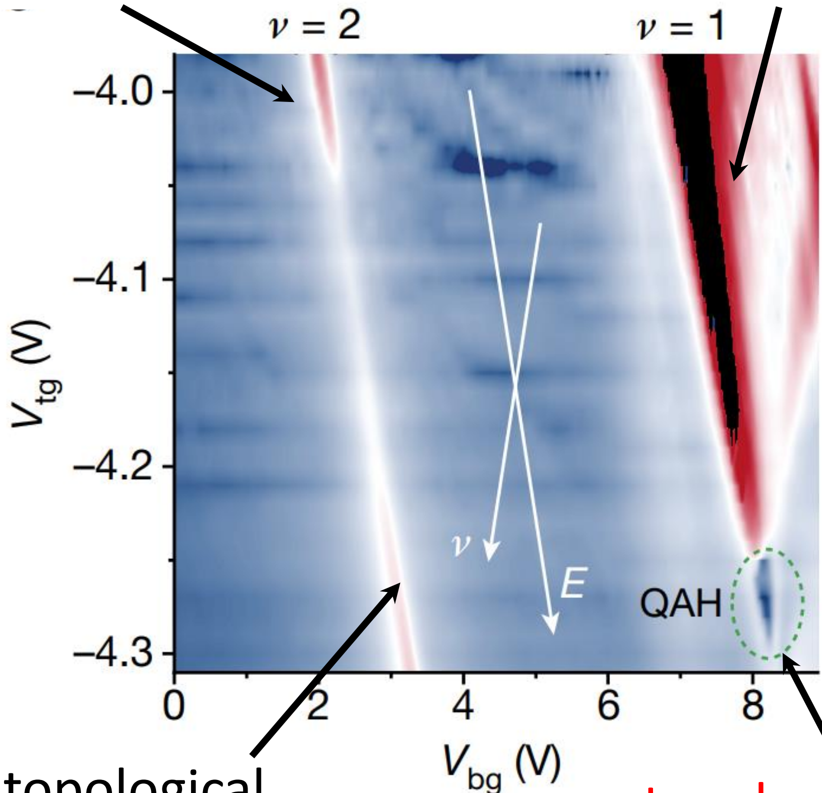


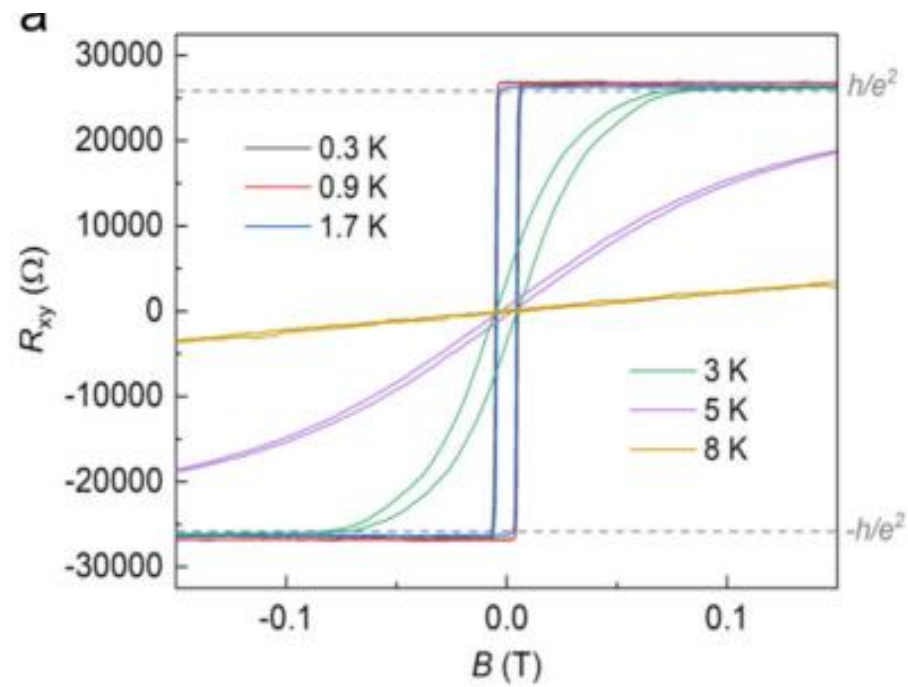




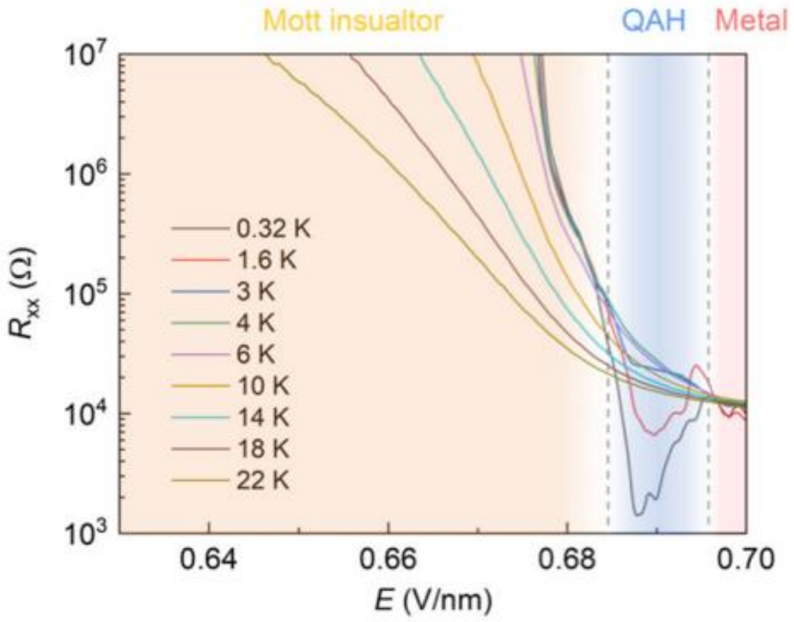
Zhao et al, arXiv:2207.02312

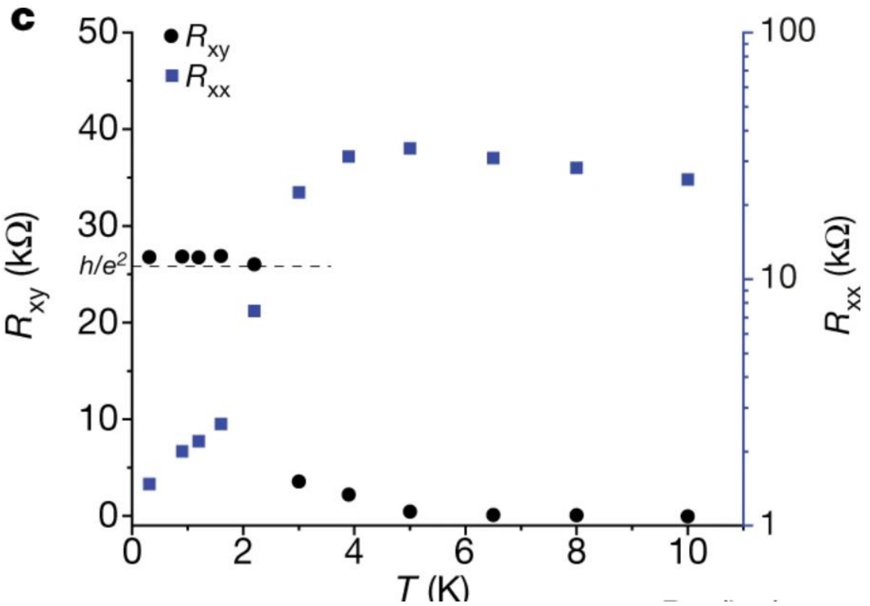
Quantum Anomalous Hall Effect at Half Filling





E Field Induced Mott-QAH Transition

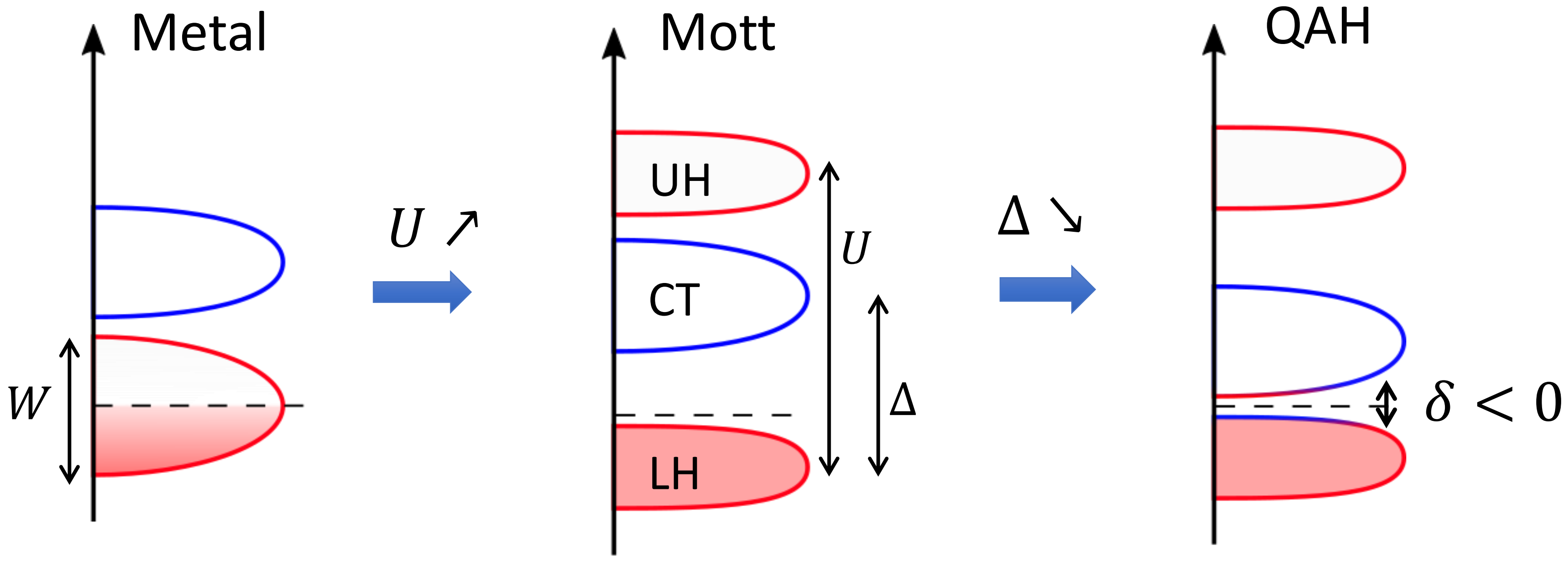




- absence of E field hysteresis
- robust and reproducible

Mott to QAH Insulators

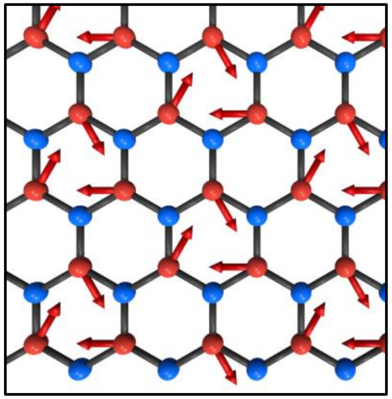
Mott-QAH transition by inverting charge transfer gap

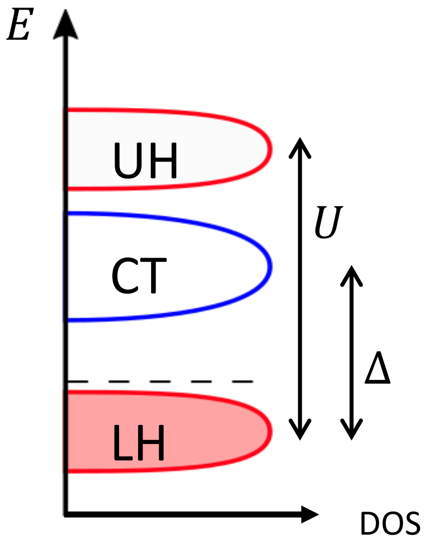


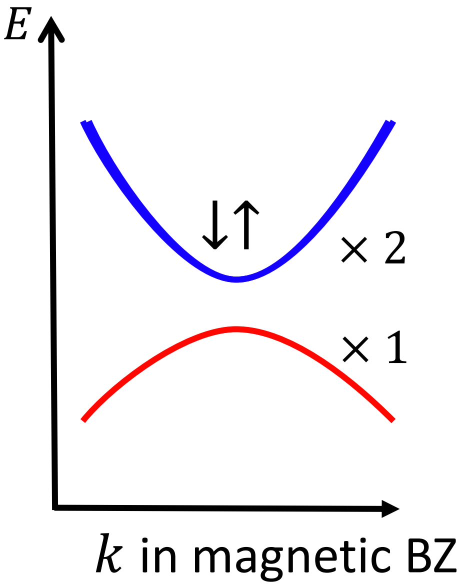
Devakul & LF, PRX (2022)

$\delta \sim \Delta - W$

120°-AFM Mott Insulator



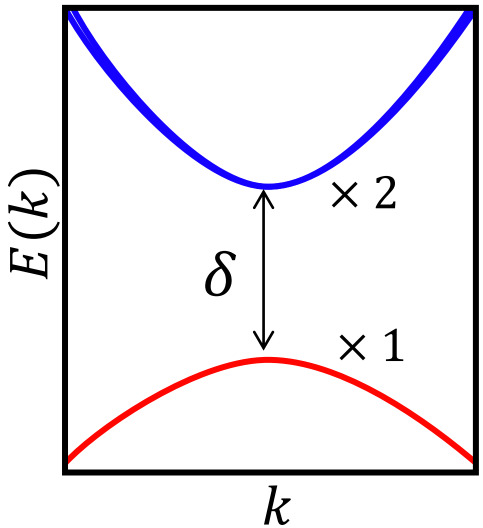




- Quasiparticle bands in magnetically ordered insulator are different from noninteracting bands.
- Low-energy states: spin-polarized holes on majority layer & spin-degenerate electrons on minority layer

Interacting Field Theory

$$\mathcal{H}_{\text{eff}} = \int \psi^{\dagger} H_{\text{eff}}\, \psi\, d\boldsymbol{k} + g \int n_{B\uparrow}(r) n_{B\downarrow}(r) d\boldsymbol{r} \qquad \psi = (\psi_A, \psi_{B\uparrow}, \psi_{B\downarrow})$$

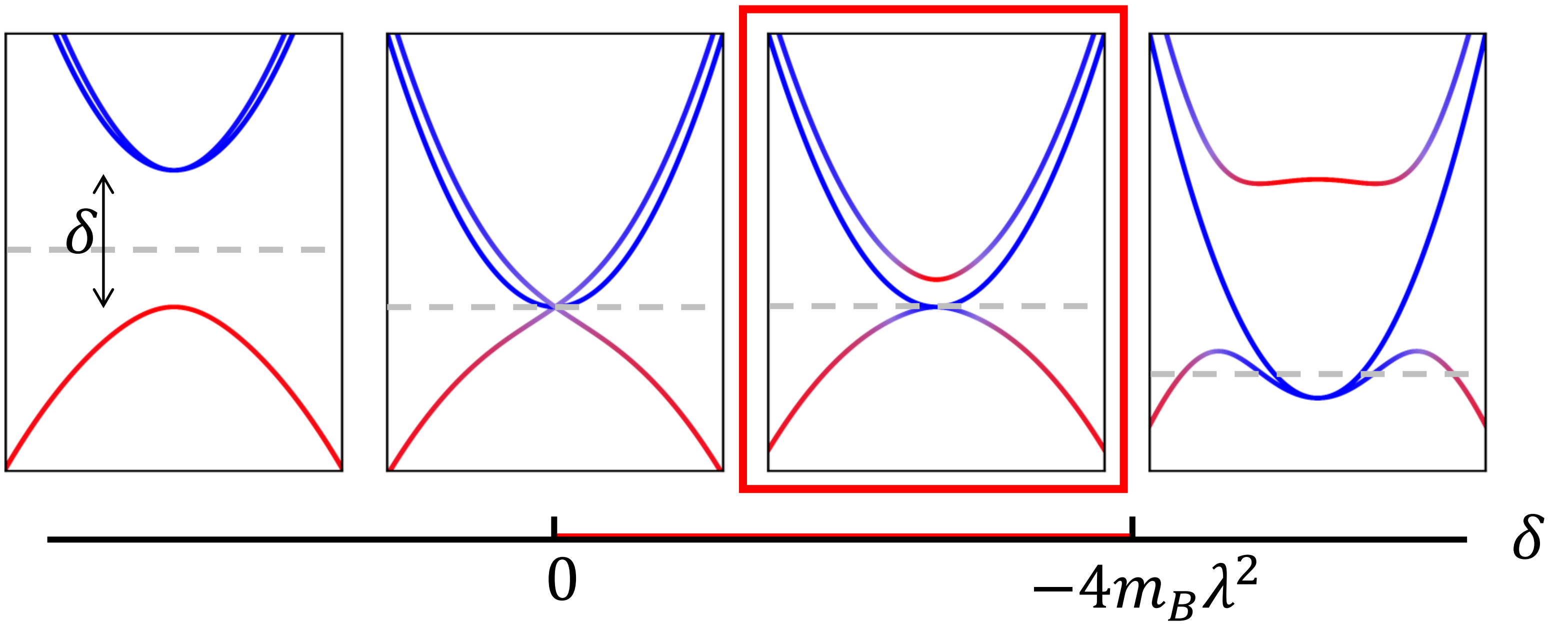


$$H_{\text{eff}} = \begin{pmatrix} -\frac{k^2}{2m_A} & \lambda(k_x + ik_y) & \lambda(k_x - ik_y) \\ \text{" "} & \frac{k^2}{2m_B} + \delta & 0 \\ \text{" "} & 0 & \frac{k^2}{2m_B} + \delta \end{pmatrix}$$

- spin degeneracy at k=0 on minority layer protected by C_3 & Ts_z
- p-wave hybridization dictated by band symmetry
- g: electron repulsion on minority layer

Interacting Field Theory

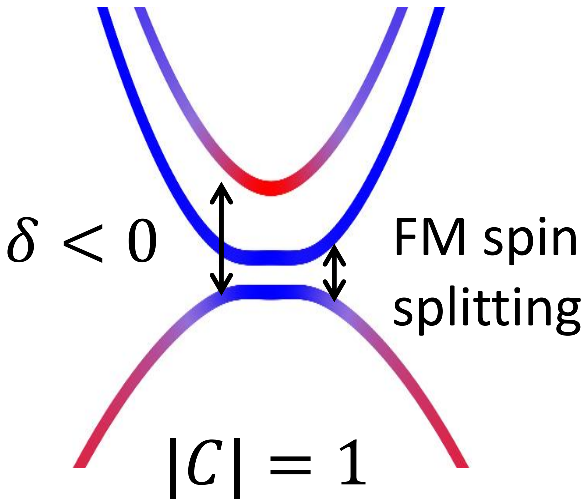
Quasiparticle band at $g = 0$

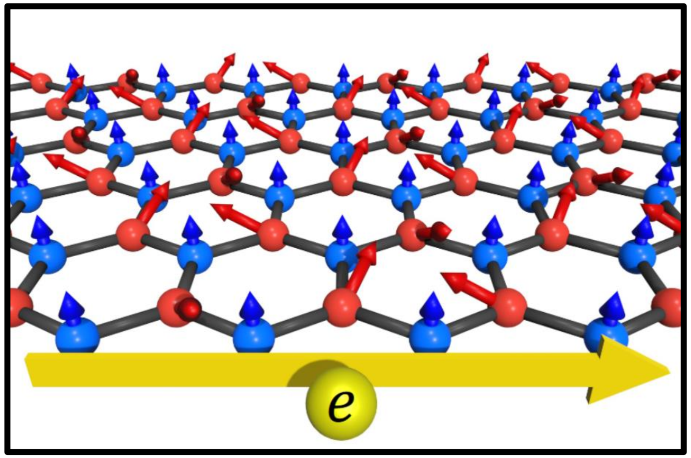


After band inversion $\delta < 0$, quadratic band touching appears at Fermi level, which is unstable to repulsion g Sun, Yao, Fradkin, Kivelson, PRL 2009

$g > 0$ changes from irrelevant to marginally relevant at band inversion!

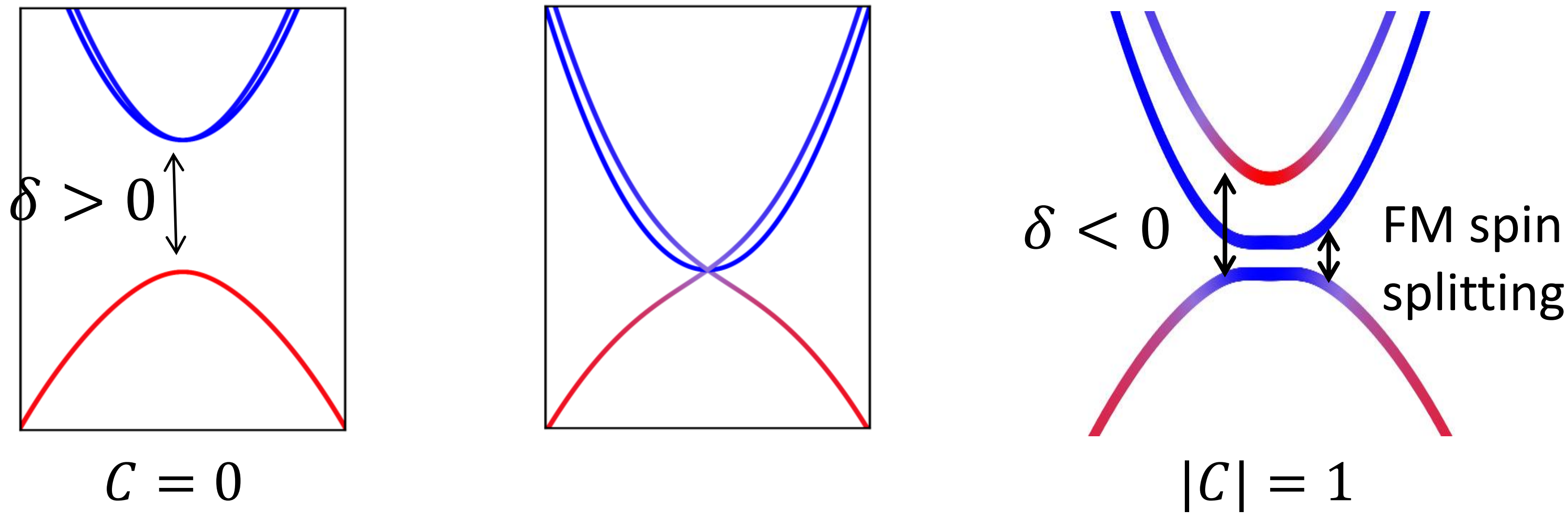
QAH with non-coplanar magnetism





- chiral spin order: (canted) xy-AFM in $MoTe_2$ & Ising FM in WSe_2
- Ising FM opens Chern gap at quadratic band touching

Continuous Mott-Chern Transition

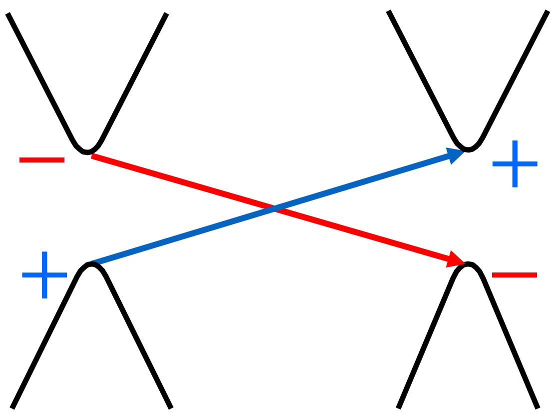


Inverting charge transfer gap induces <u>simultaneous</u> change of magnetism & topology.

Devakul & LF, PRX (2022)

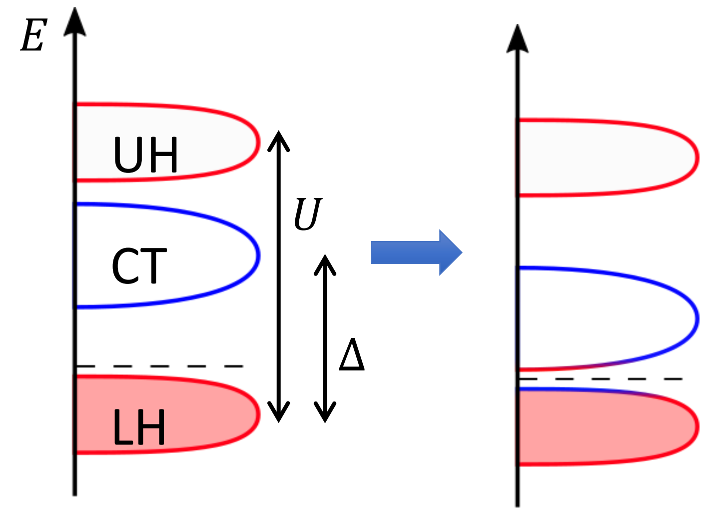
Topological Band & Mott Insulators

Inverting single-particle gap
(even-integer filling)



2007

Inverting many-body gap
(odd-integer filling)



2022

AFM Mott insulators with negative charge transfer gap:
potential route to high-temperature QAH

Bridging Mott and Chern

Comparison with Other QAH Systems

Magnetically doped TI film Chang et al (2013)

- FM of dopant opens Chern gap at surface Dirac point
- even integer filling

Magic-angle graphene Sharpe et al, Serlin et al (2019)

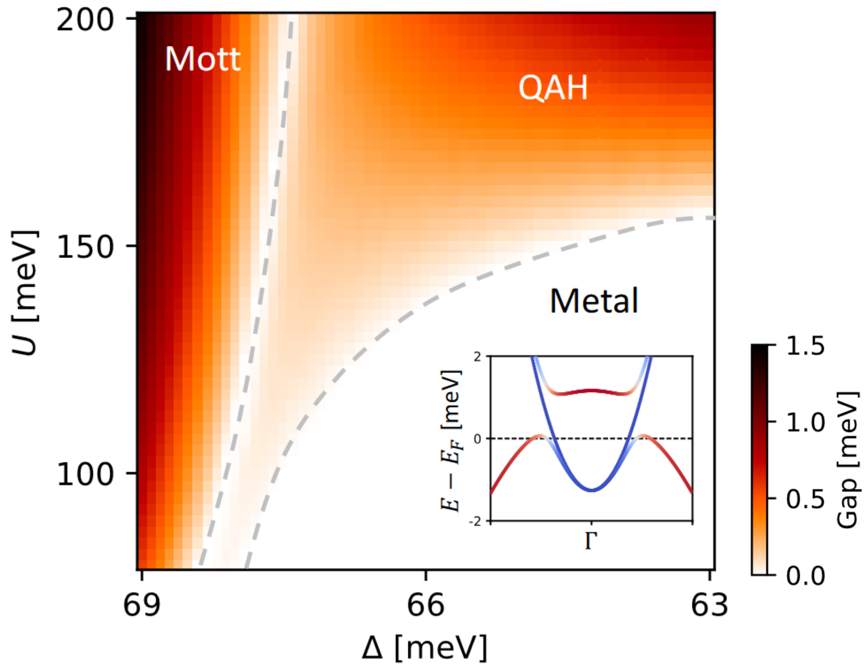
- fully valley-polarized flat Chern band

$C_K = +1$ $C_{K'} = -1$ Zhang & Senthil, MacDonald, Xie et al, Pan et al …

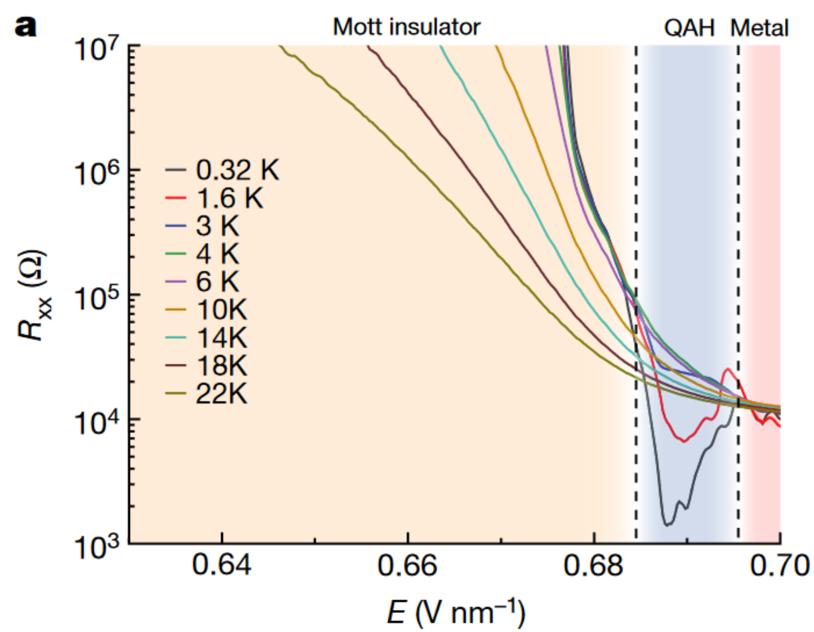
QAH in $MoTe_2/WSe_2$ differs fundamentally from flat band FM.

Comparison with Experiment

Hartree-Fock Phase Diagram



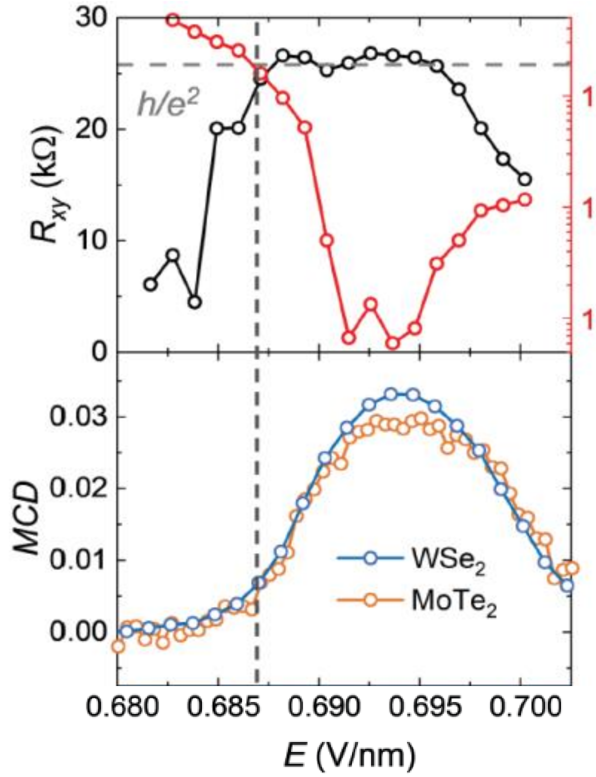
$MoTe_2/WSe_2$

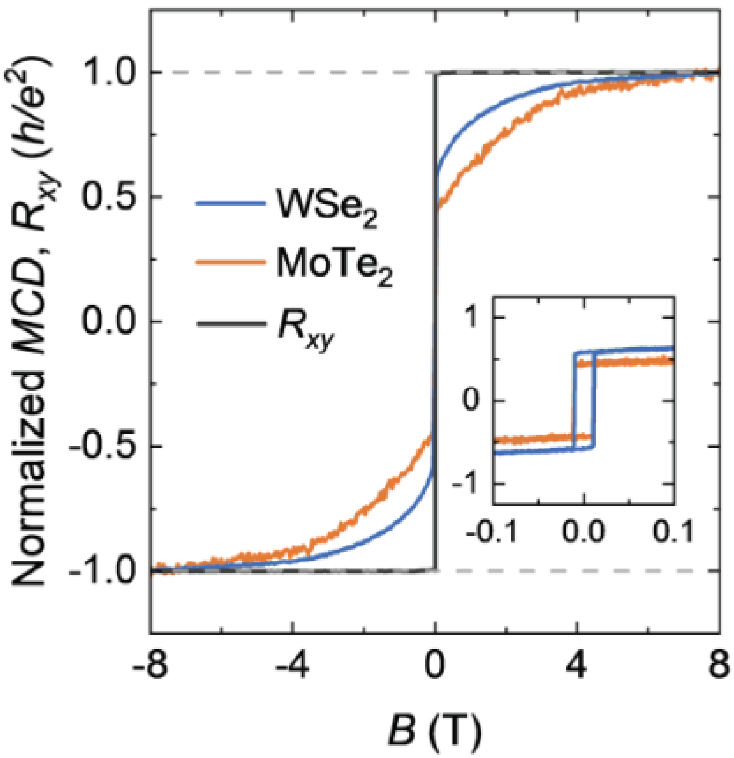


Prediction for Magnetism

- Mott: **zero** spin S_z polarization
- QAH: **finite but incomplete** spin S_z polarization increasing with B field and E field
- Intervalley *XY* magnetic order: **gapless** magnon

Evidence for Canted Spin Texture in QAH





Tao et al, arXiv: 2208.07452

Outlook

- charge gap across Mott-Chern transition
- spin superfluidity
- critical exponents
- inverting quantum spin liquid