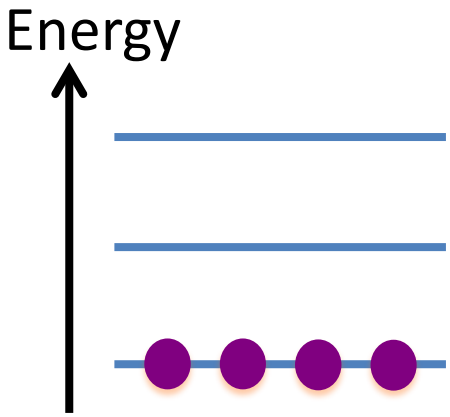
Moire Physics in Semiconductors

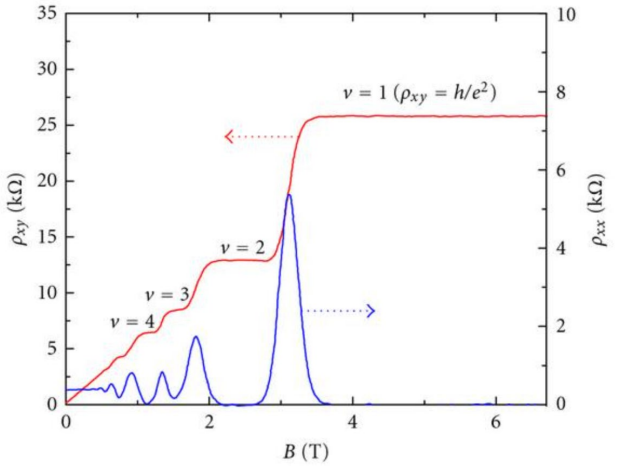
Topology with and without Flat Bands

Liang Fu

2023 Theory Winter School at MagLab

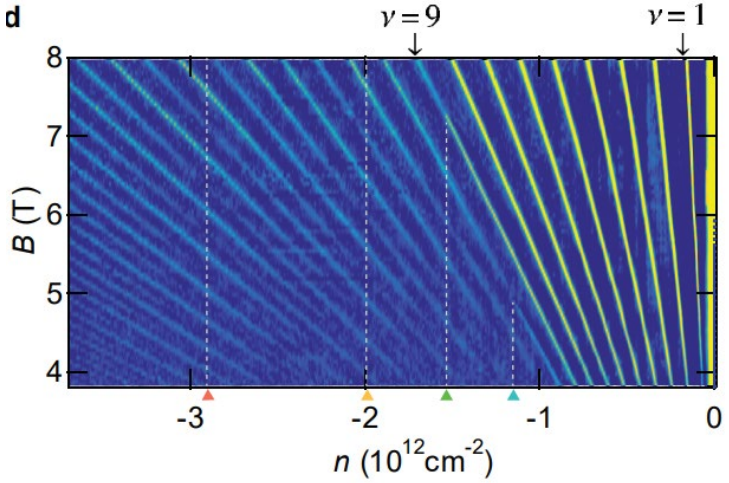
Landau Levels





$$\sigma_{xy} = N\frac{e^2}{h}$$

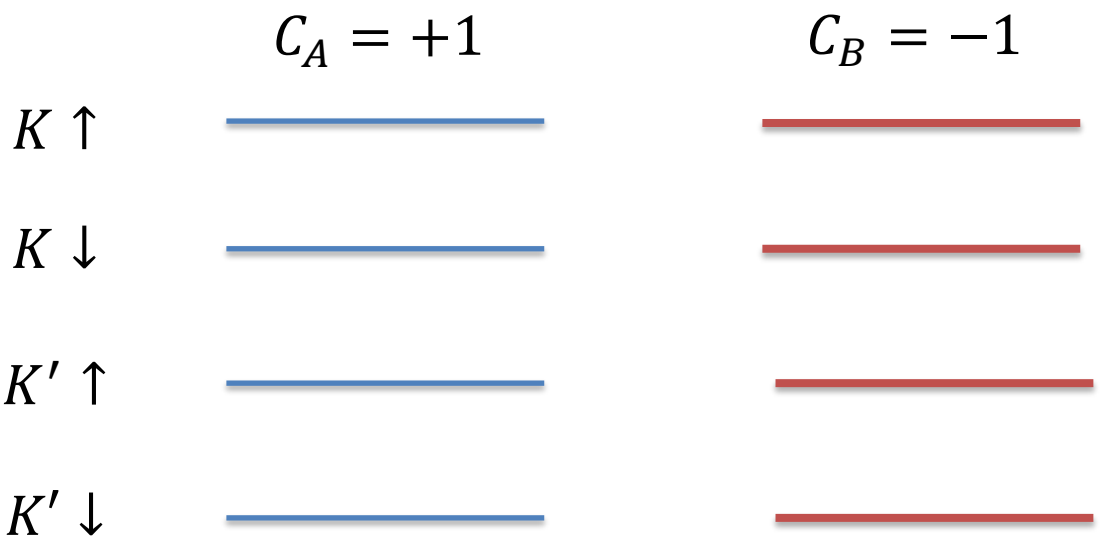
$$\frac{dn}{dB} = N\frac{e}{h}$$



Magic-Angle Twisted Bilayer Graphene

flat band from Dirac fermion with spatially varying interlayer tunneling (AA, BB, AB, BA)

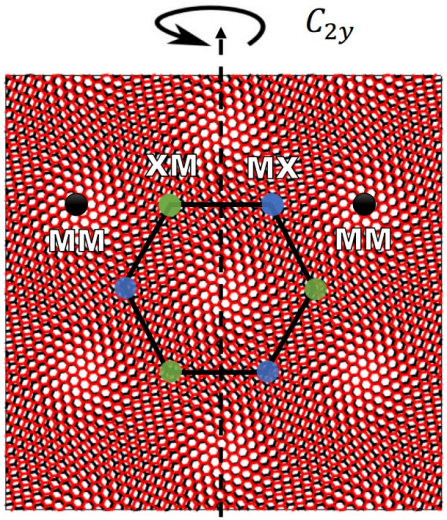
chiral limit: 8 flat Chern bands at $E = 0$

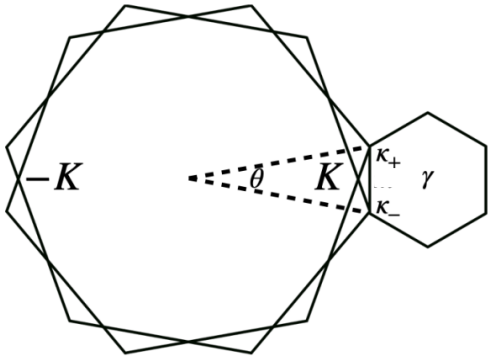


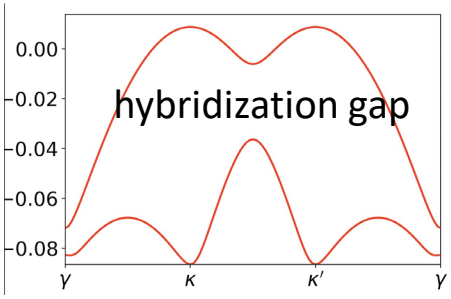
Topological Insulators in Twisted Transition Metal Dichalcogenide Homobilayers

Fengcheng Wu,[1,2] Timothy Lovorn,[3] Emanuel Tutuc,[4] Ivar Martin,[1] and A. H. MacDonald[3]

$\theta \sim 0$ (AA stacking)







$$\mathcal{H}_\uparrow = \begin{pmatrix} -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_b(\boldsymbol{r}) & \Delta_T(\boldsymbol{r}) \\ \Delta_T^\dagger(\boldsymbol{r}) & -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_t(\boldsymbol{r}) \end{pmatrix}$$

$$\boldsymbol{\Delta}(\boldsymbol{r}) = (\Delta_x, \Delta_y, \Delta_z) \equiv (\mathrm{Re}\Delta_T^\dagger, \mathrm{Im}\Delta_T^\dagger, \frac{\Delta_b - \Delta_t}{2})$$

- moire potential $V(\boldsymbol{r})$ and complex-valued interlayer tunneling $w(\boldsymbol{r})$
- $w(\boldsymbol{r})$ vanishes at XM & MX due to atomic-scale interference of K-point w.f.

Band Topology from Skrymion Lattice

$$\mathcal{H}_{\uparrow} = \begin{pmatrix} -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{\kappa}_+)^2}{2m^*} + \Delta_{\mathfrak{b}}(\boldsymbol{r}) & \Delta_T(\boldsymbol{r}) \\ \Delta_T^{\dagger}(\boldsymbol{r}) & -\frac{\hbar^2(\boldsymbol{k}-\boldsymbol{\kappa}_-)^2}{2m^*} + \Delta_{\mathfrak{t}}(\boldsymbol{r}) \end{pmatrix}$$

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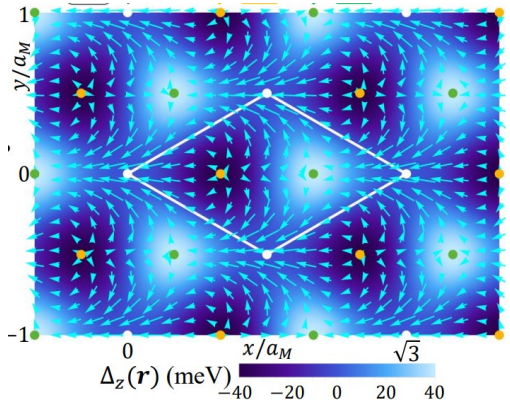
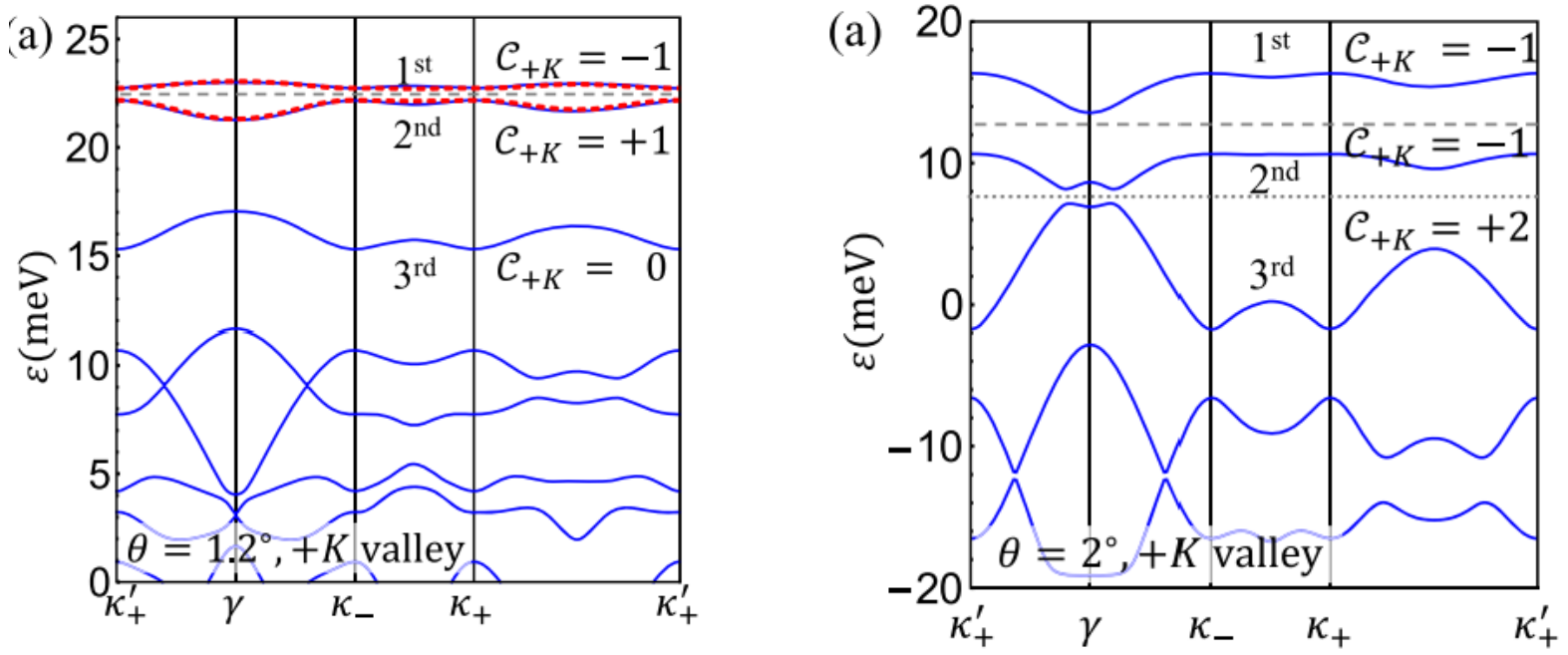


Layer-pseudospin Zeeman field forms skrymion lattice!

Wu, Lovorn, Tutuc, Martin and MacDonald, PRL (2019)

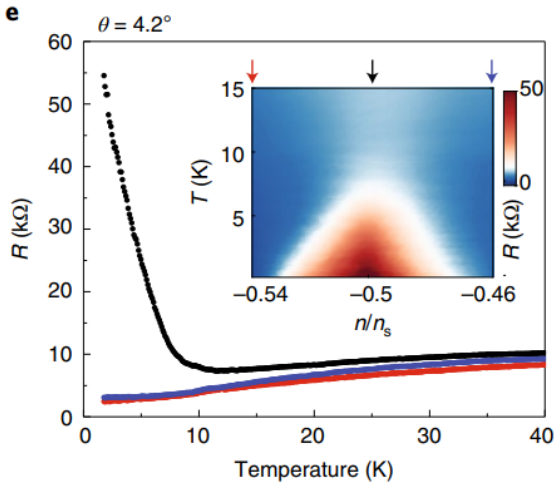
Band Topology from Skrymion Lattice

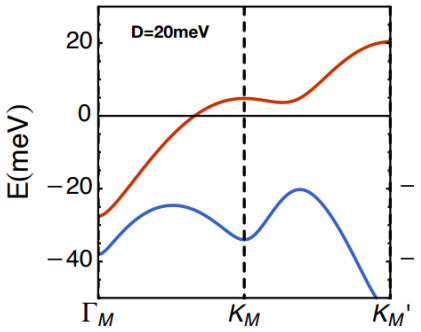


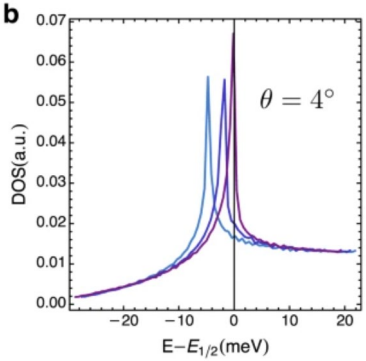
Wu, Lovorn, Tutuc, Martin and MacDonald, PRL (2019)

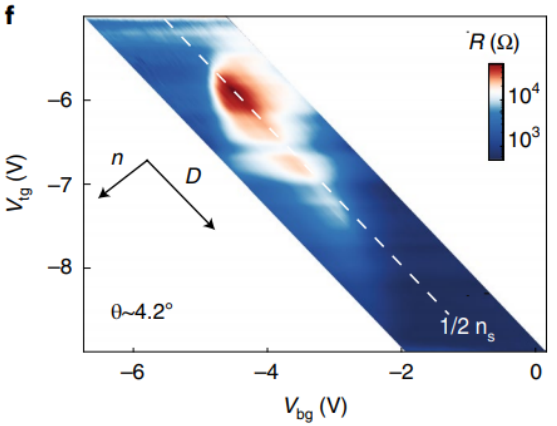
Twisted WSe_2 at $\theta \sim 4°$

Metal-insulator transition tuned by E field









Correlated insulator at n=1:

- valley-polarized (Ising) ferromagnet
- <u>intervalley coherent (xy) antiferromagnet</u>

Wang et al, Nature Materials (2020)

Bi & LF, Nature Communications (2021)

Twisted WSe_2 at $\theta \sim 4°$

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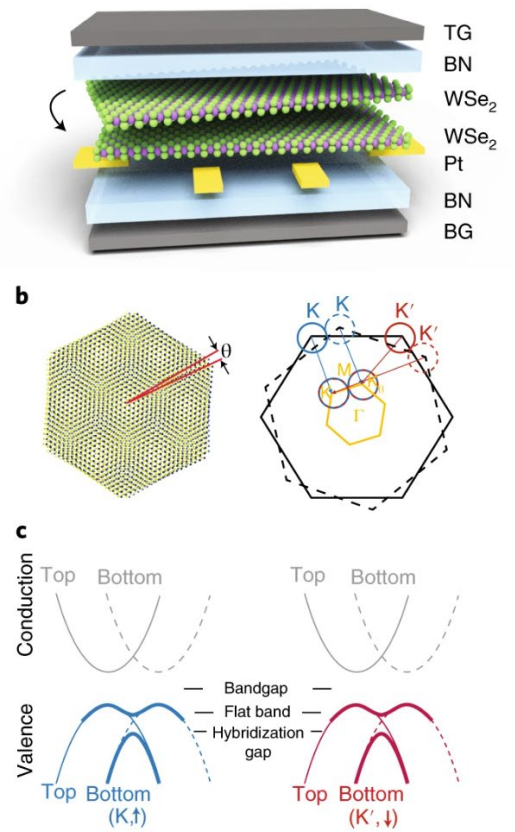
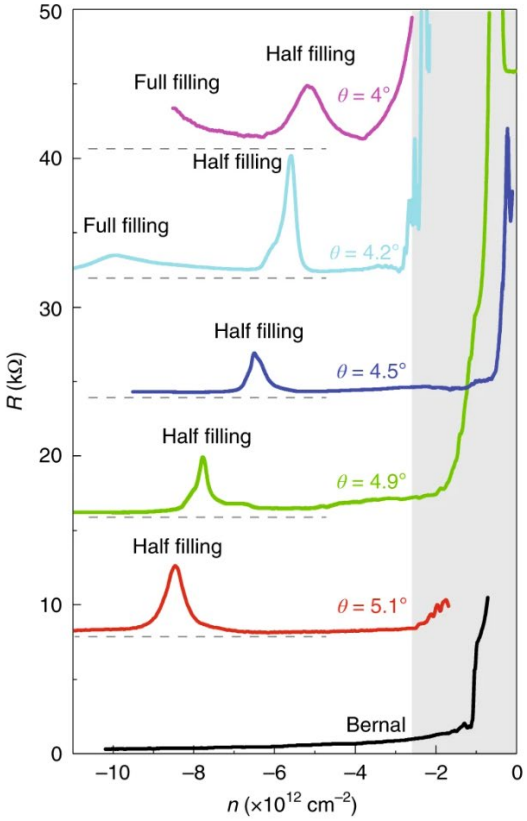
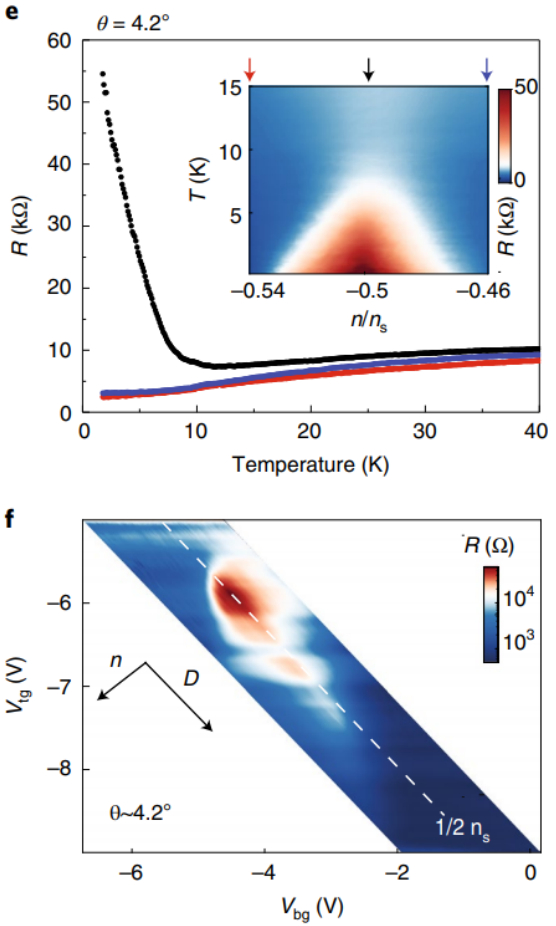
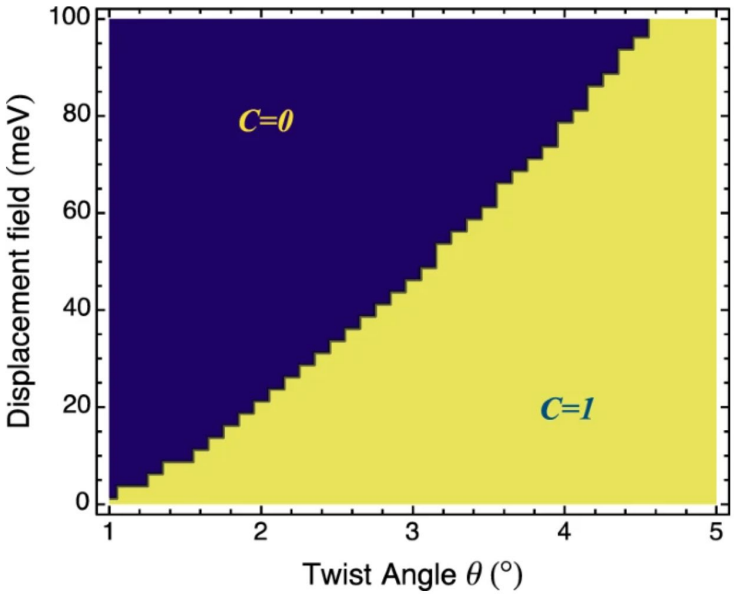


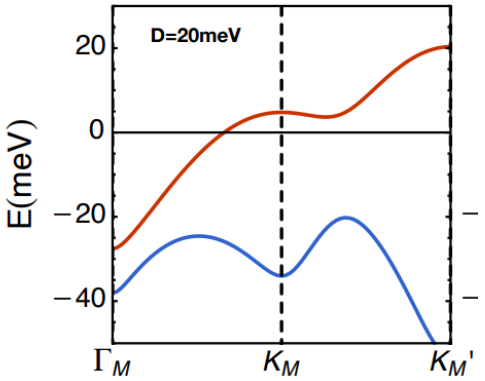


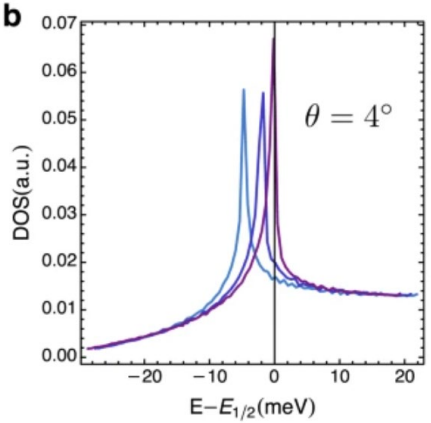


Wang et al, Nature Materials (2020)

Twisted WSe_2





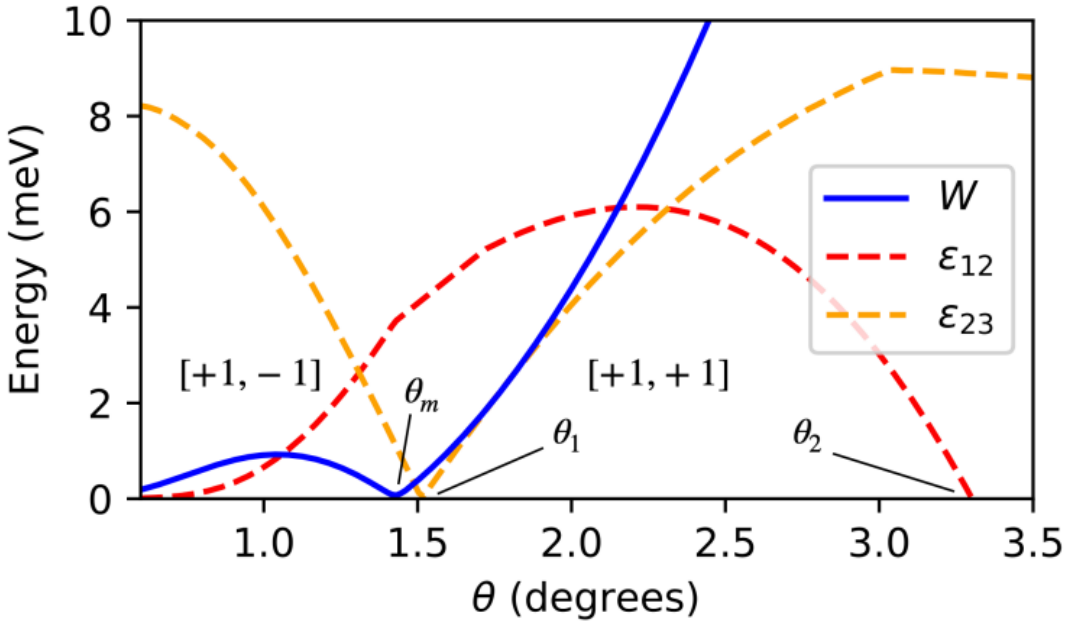


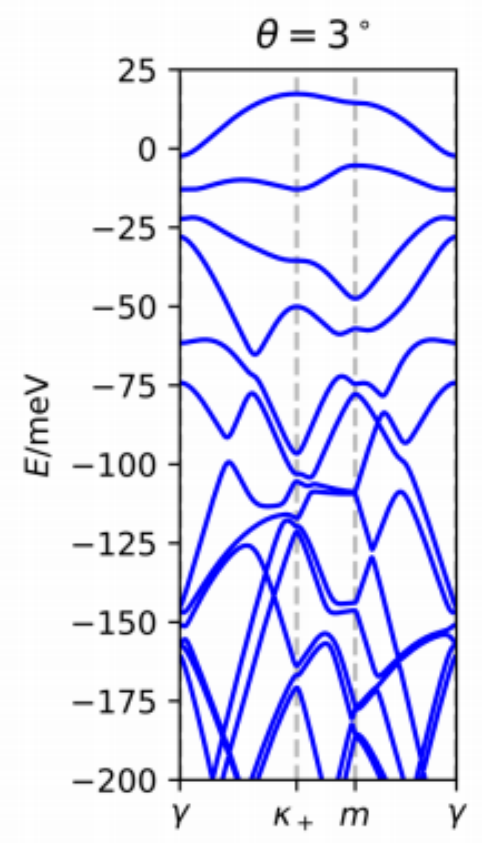
Correlated insulator at n=1:

- valley-polarized (Ising) ferromagnet
- <u>intervalley coherent (xy) antiferromagnet</u>

Bi & LF, Nature Communications (2021)
See also Cano & Millis, Das Sarma ...

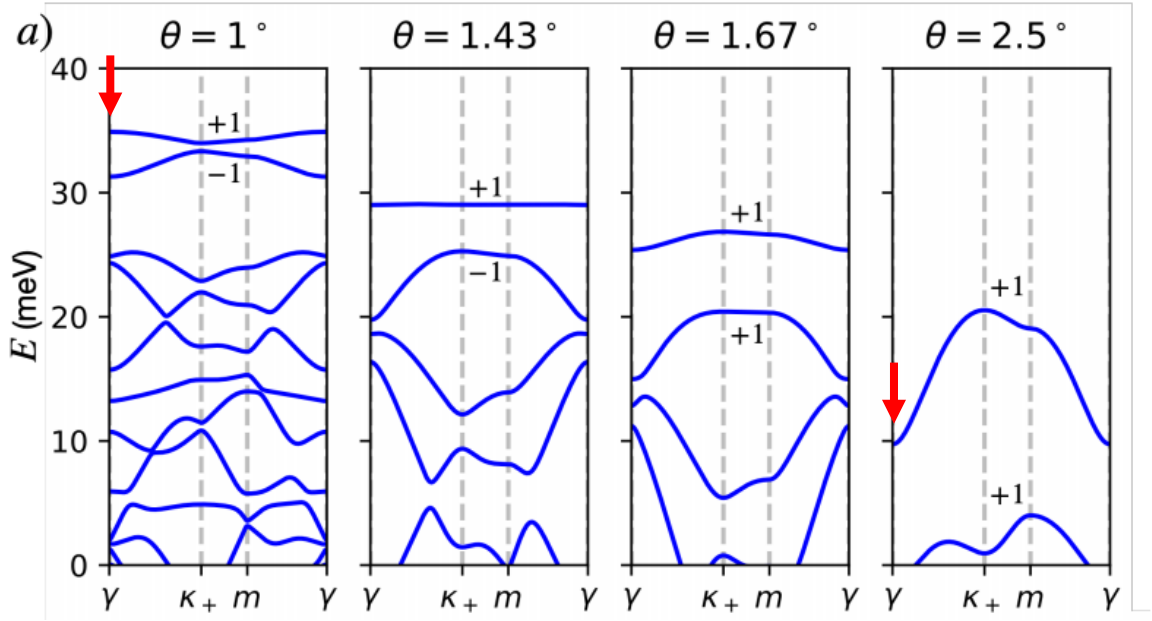
Isolated Topological Bands





Devakul, Crepel, Zhang & LF, Nature Communications (2021)

$\theta \sim 1.4°$: Magic *Flat* Band



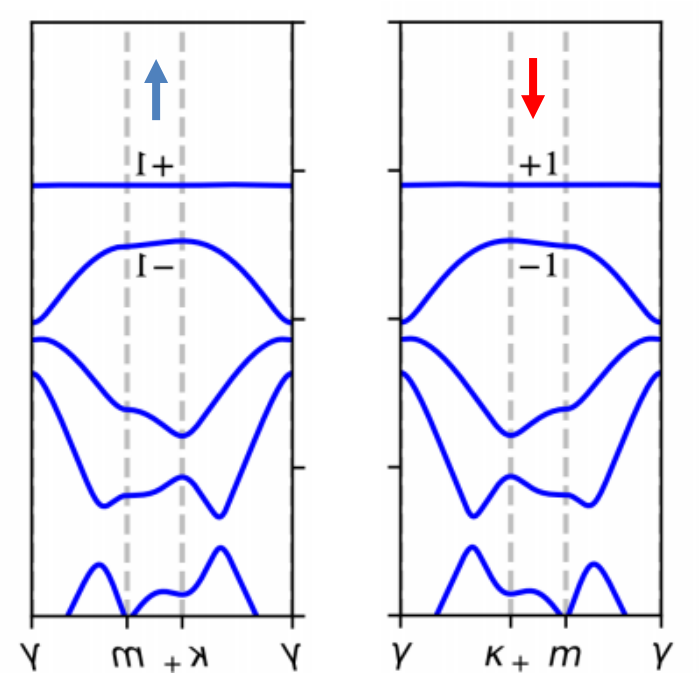
Analytical formula for magic angle based on diverging band mass at γ

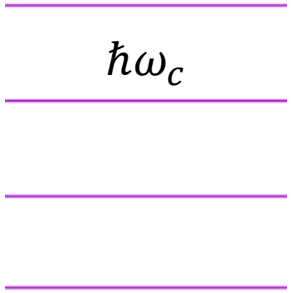
$$\tilde{\theta}_m^{-2} = \frac{8\pi^2}{9m^* a_0^2}\left(\frac{1}{\mathcal{E}_{n_0} - \mathcal{E}_{n_0+1}} + \frac{1}{\mathcal{E}_{n_0} - \mathcal{E}_{n_0-1}}\right)$$

$$\text{where } \mathcal{E}_n = 2w\cos(\pi n/3) + 2V\cos(2\pi n/3 - \psi),$$

Magic flat band: bandwidth 0.1meV, topological gap 4meV

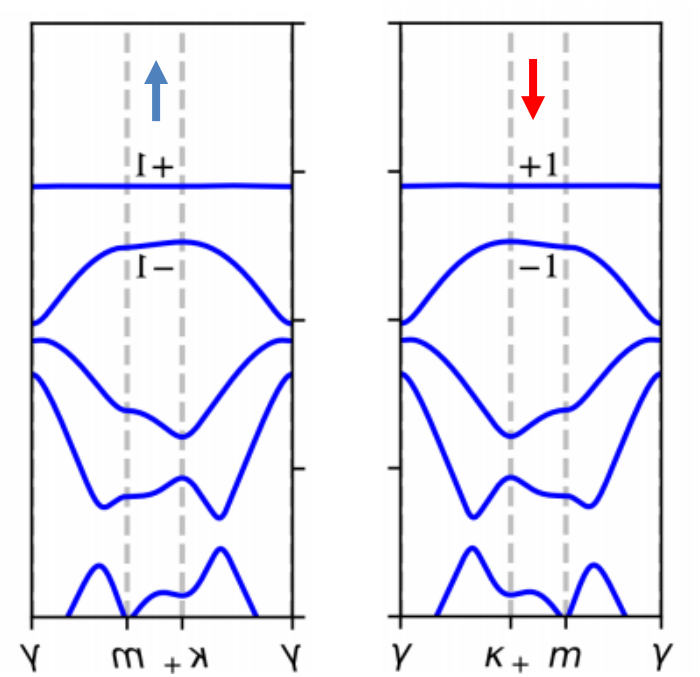
Comparison with Landau Level

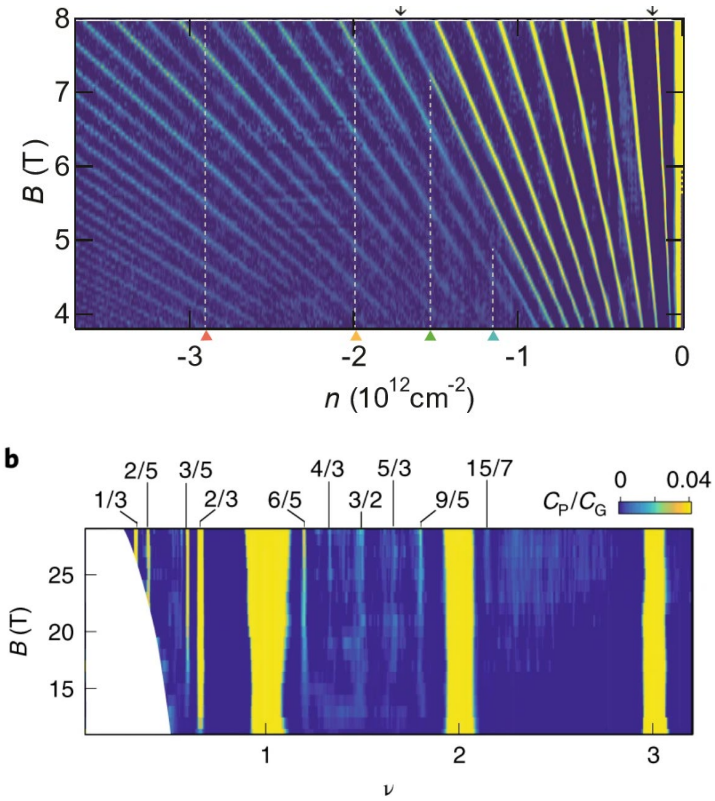




Topological gap 4meV $\Leftrightarrow$ $B = 18$T in monolayer WSe_2

Comparison with Landau Level



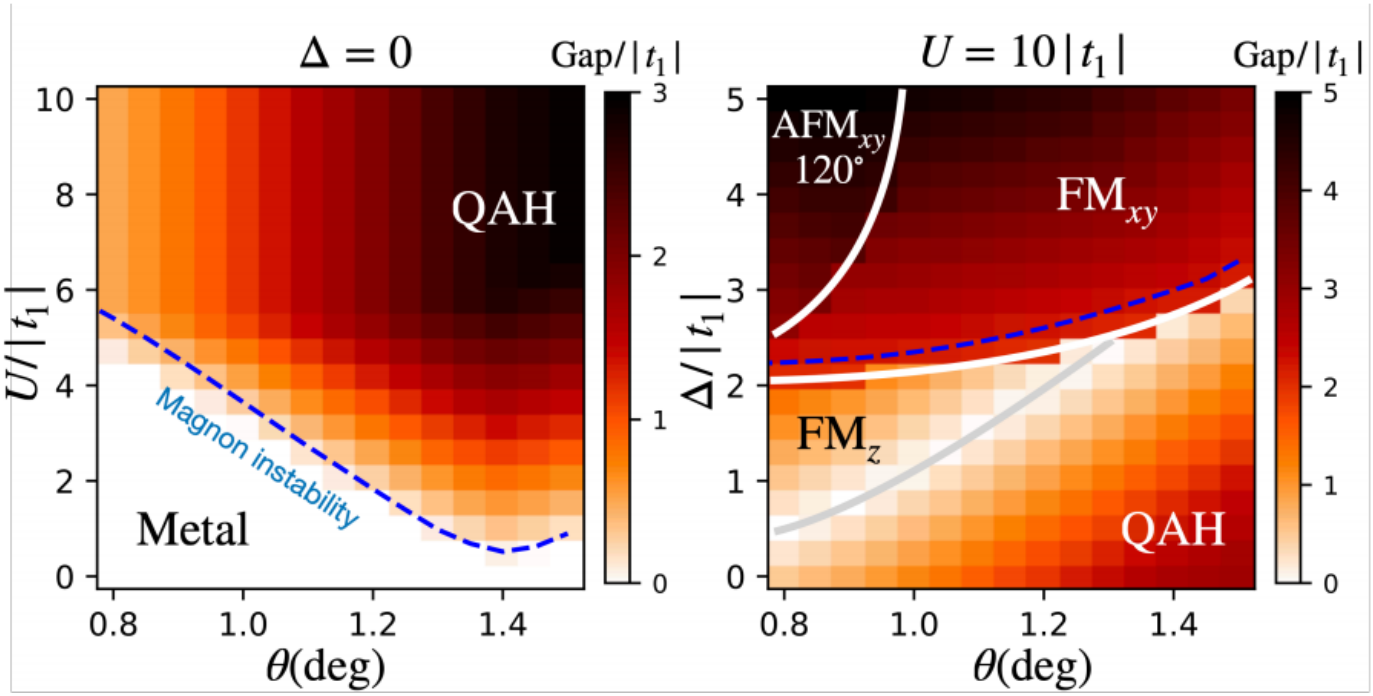


Shi et al, Nat. Nano. 2020

Topological gap 4meV $\Leftrightarrow B = 18$T in monolayer WSe_2

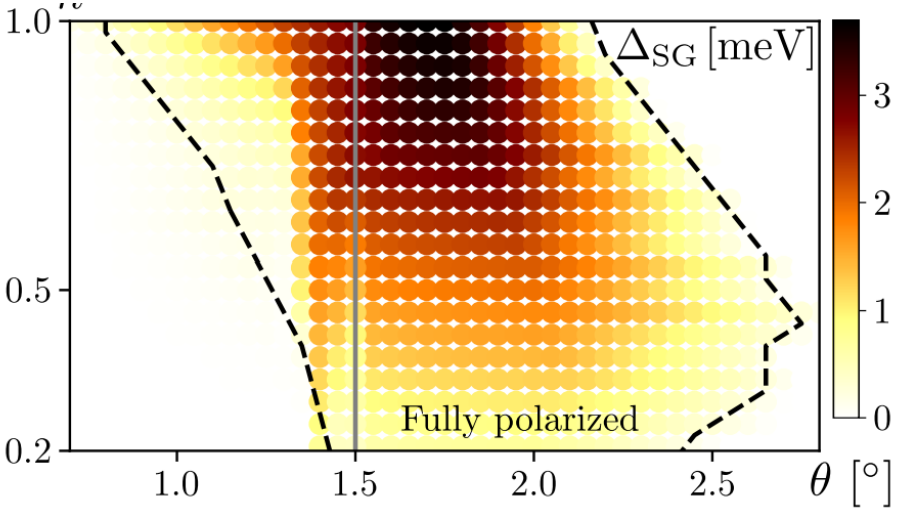
Haldane and Mott Insulators at n=1

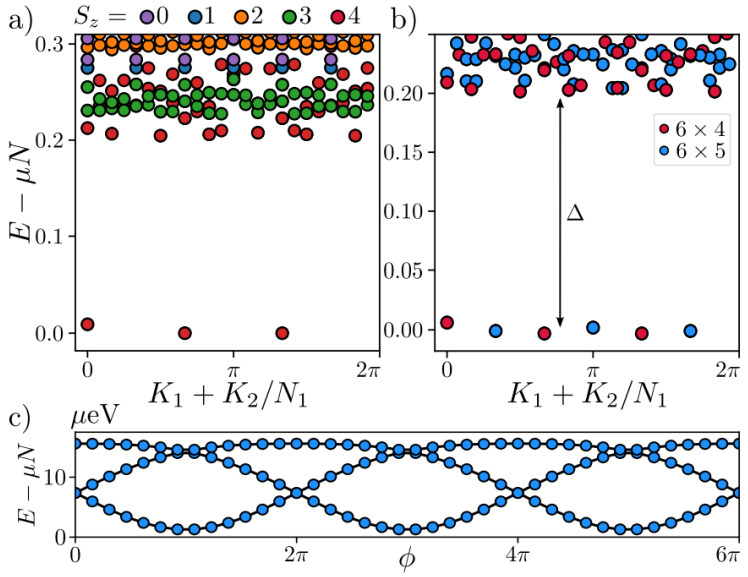
tuned by electric field



Devakul, Crepel, Zhang & LF, Nature Communications (2021)

Fractional Fillings:
Anomalous Hall Metal & Fractional Chern Insulator





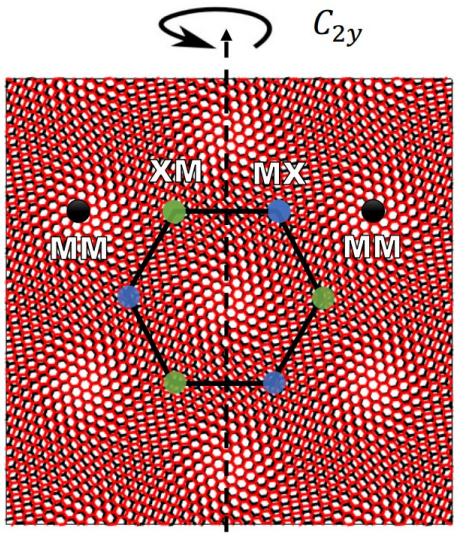
Spontaneous spin-valley polarization

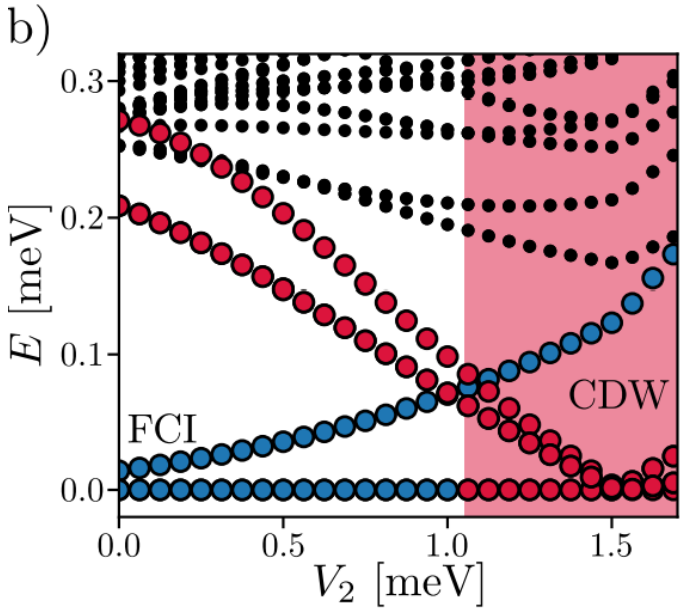
Gapped magnon due to spin-valley locking

Crepel & LF, arXiv:2207.08895

See also Li, Kumar, Sun and Lin, Physical Review Research 3, L032070 (2021).

FCI vs CDW



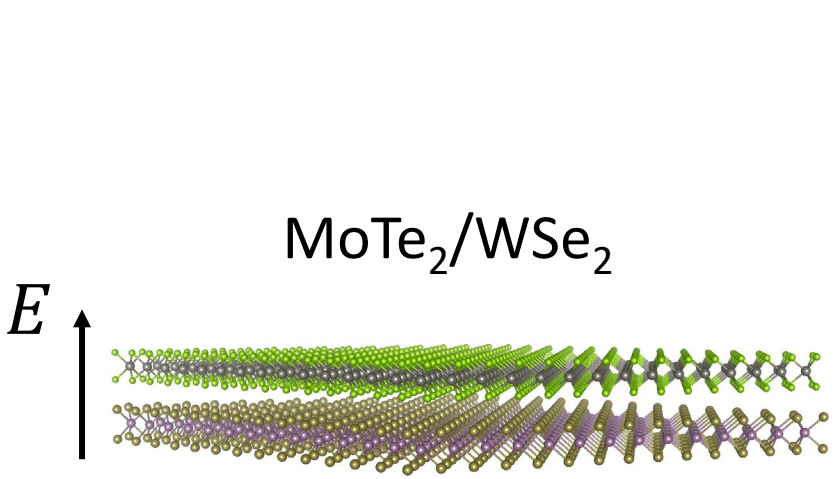


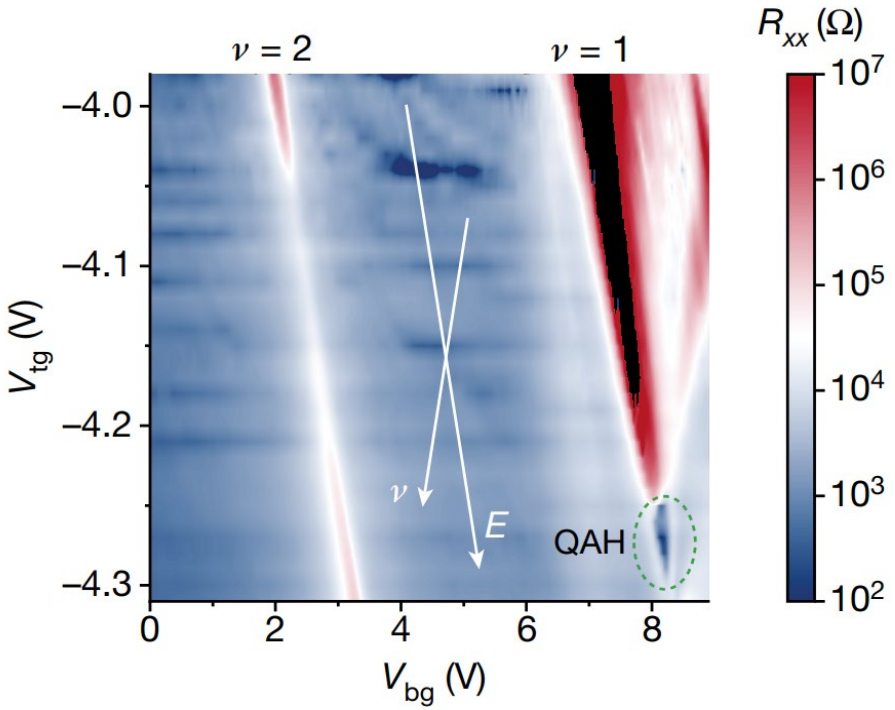
Crepel & LF, arXiv:2207.08895

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 ✉

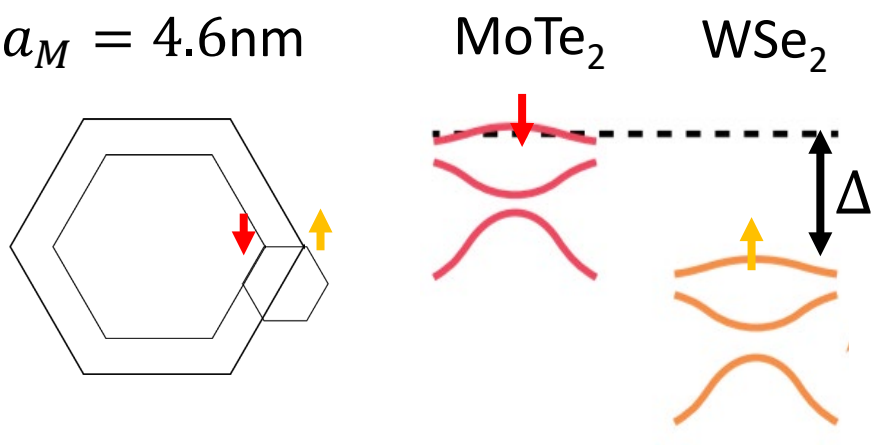




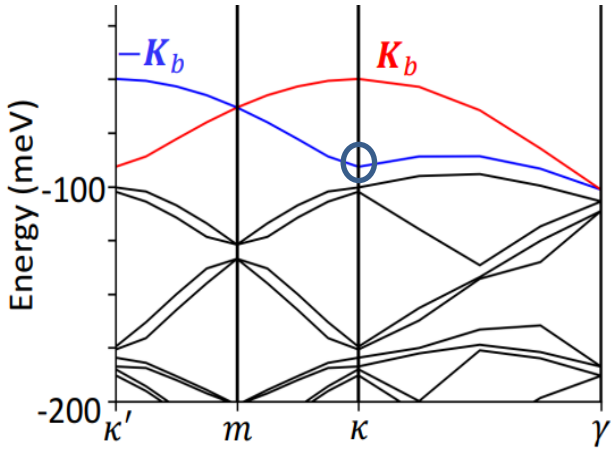
- Electric field tunes <u>interlayer</u> charge transfer

Moire Bands in $MoTe_2/WSe_2$

$a_M = 4.6\text{nm}$

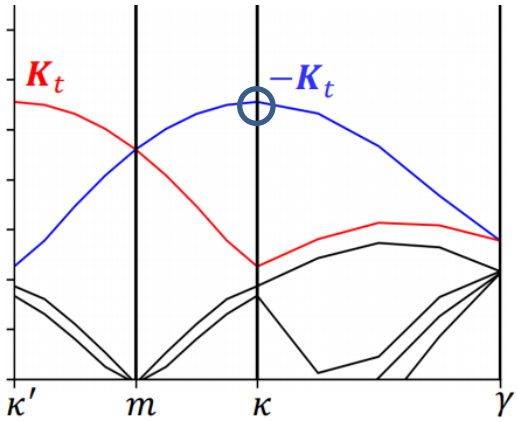


13 x13 $MoTe_2$

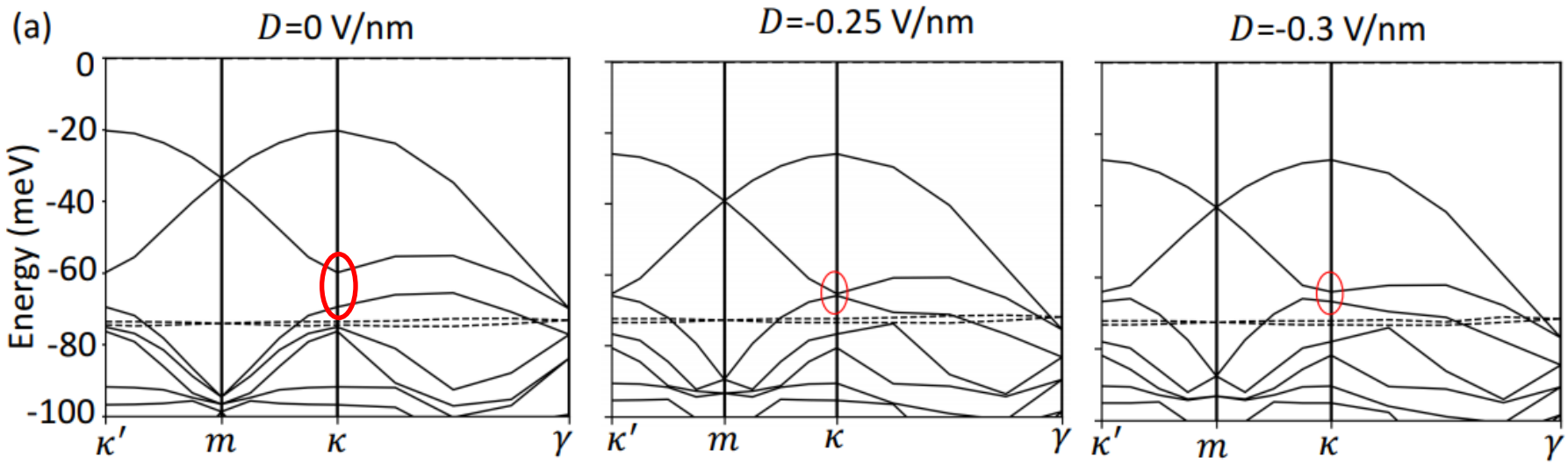


- $\Delta = 0.13\text{eV}$ at zero E field
- majority layer: $MoTe_2$
  minority layer: WSe_2
- moire band due to lattice corrugation with bandwidth ~ 50 meV

14 x14 WSe_2



E Field Tunes Band Inversion

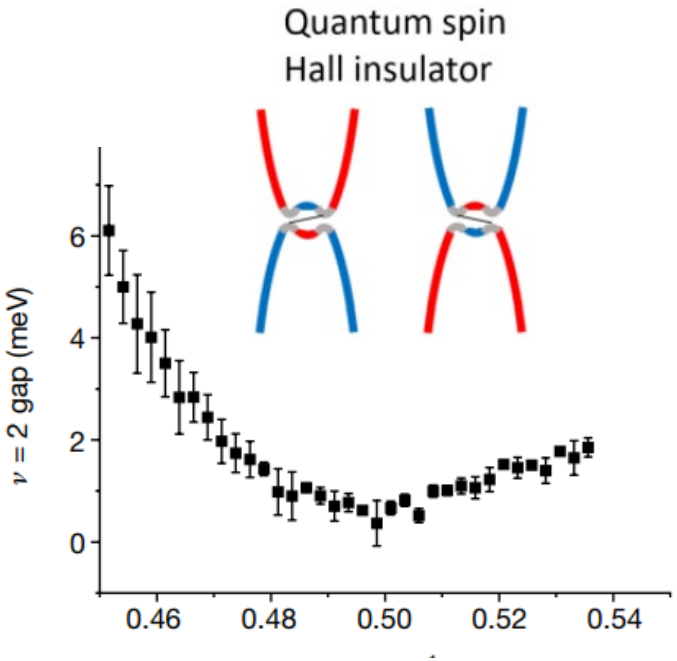


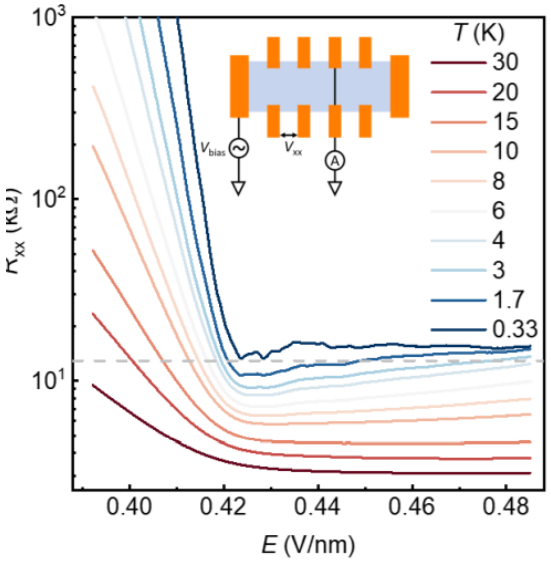
- electric field inverts minibands on two layers
- band inversion + p-wave interlayer tunneling => valley Chern number

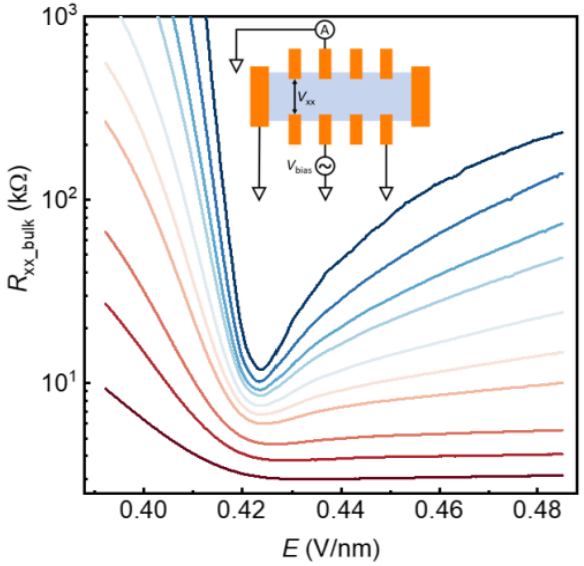
Prediction: E field induced quantum spin Hall insulator at n=2

Zhang, Devakul & LF, PNAS (2021)

Edge Transport in $MoTe_2/WSe_2$





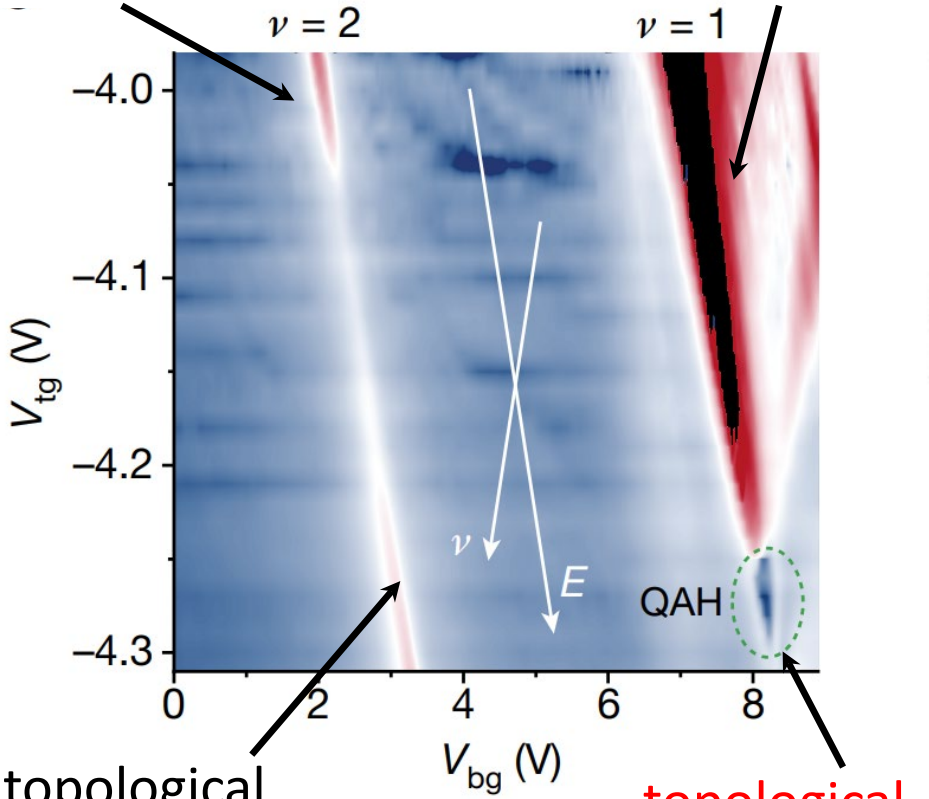


Zhao et al, arXiv:2207.02312

Quantum Anomalous Hall Effect at Half Filling

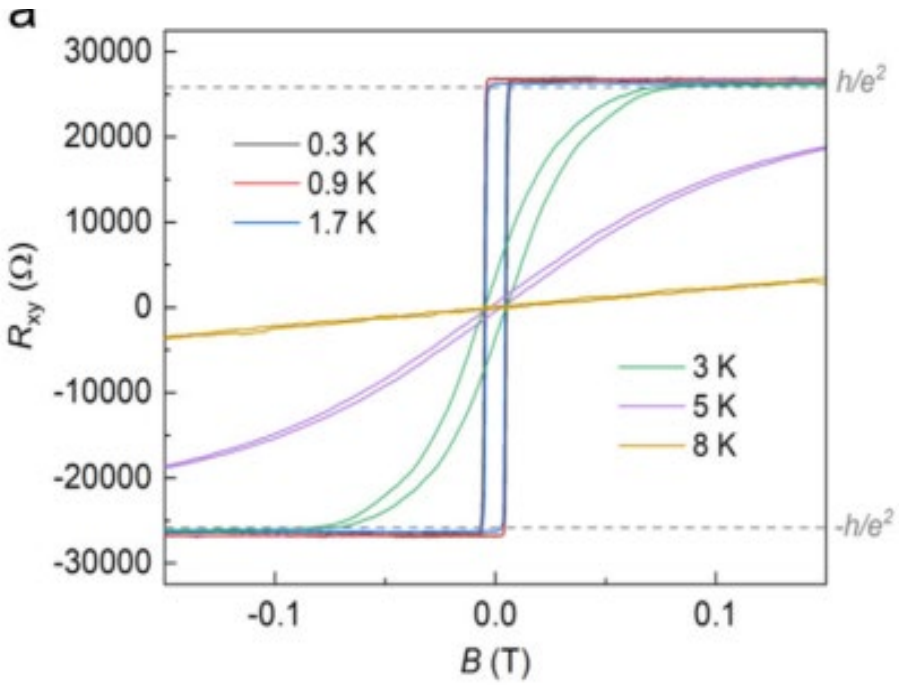
band insulator

Mott insulator

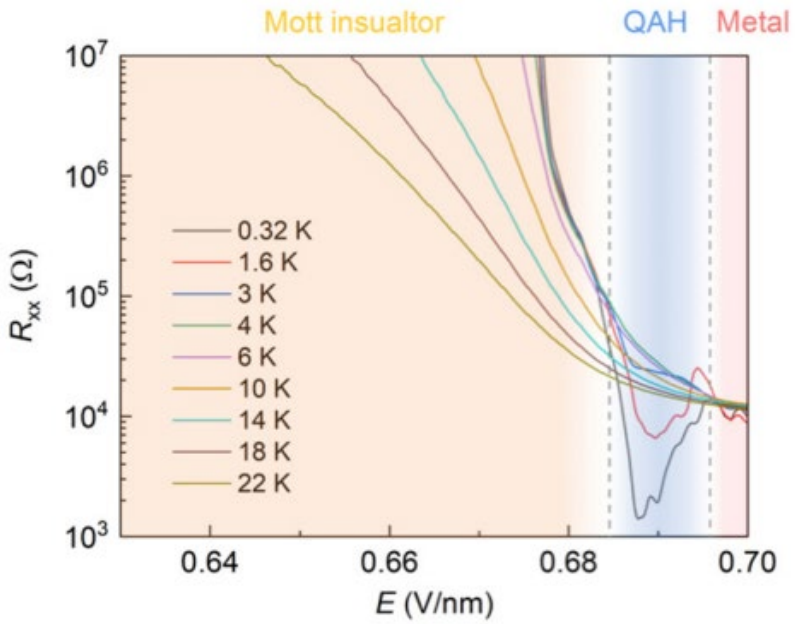


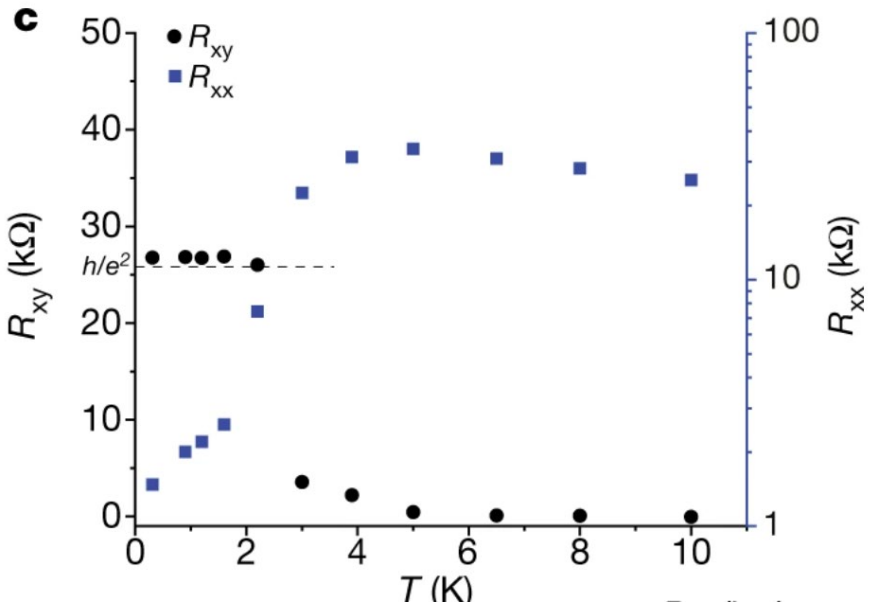
topological band insulator

topological Mott insulator



E Field Induced Mott-QAH Transition

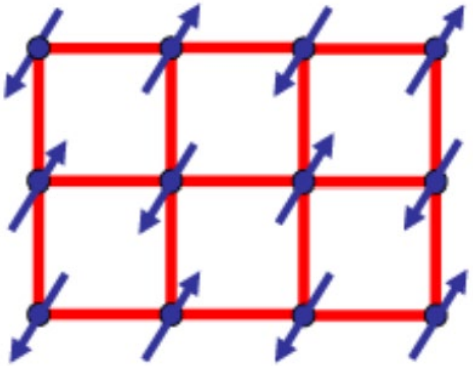


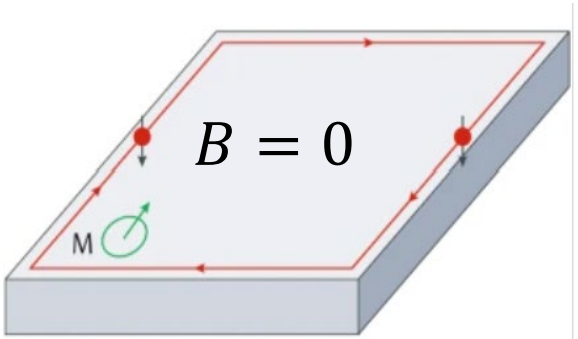


- absence of E field hysteresis
- robust and reproducible

Mottness versus Topology

dichotomy between particle and wave





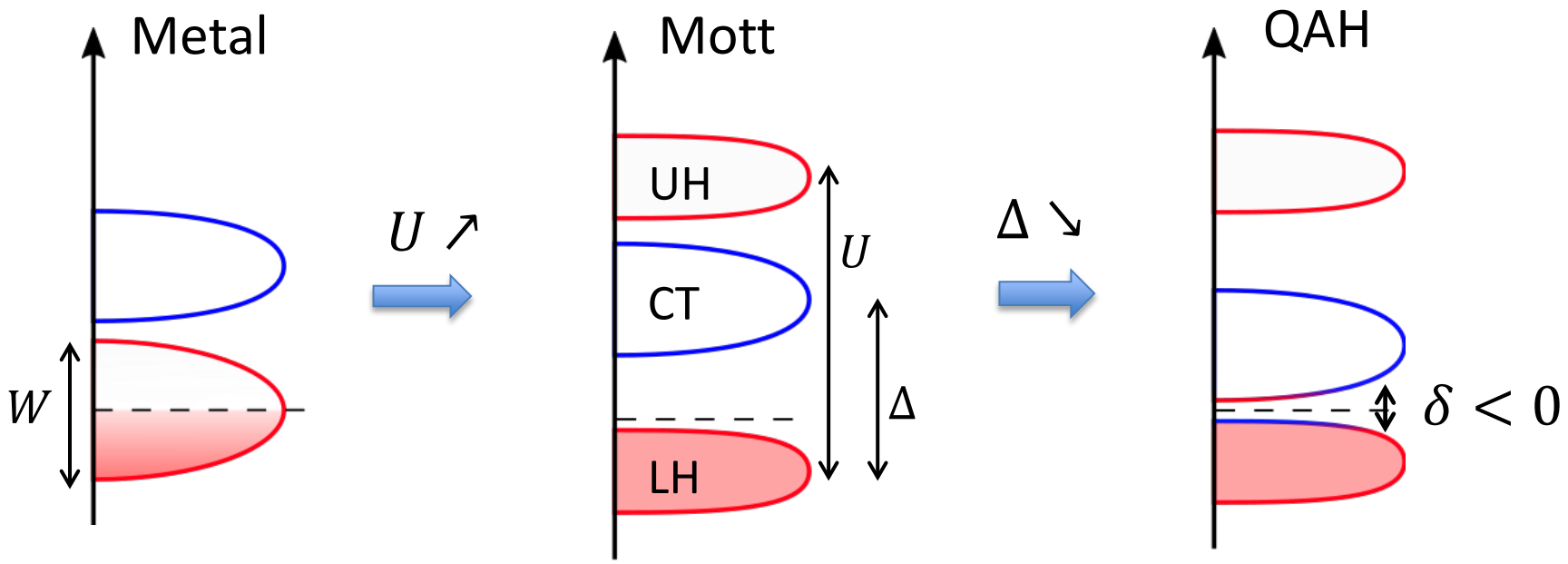

Mott
Topology

Quantum Anomalous Hall State in Antiferromagnetic Mott Insulators

Devakul & LF, PRX (2022)

Mott to QAH Insulators

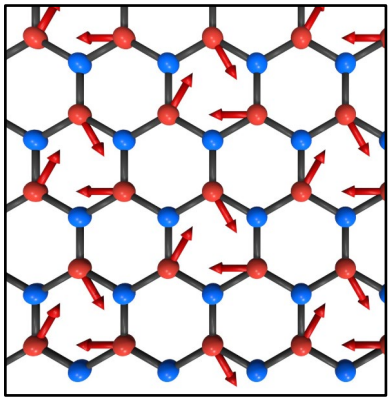
Mott-QAH transition by inverting charge transfer gap

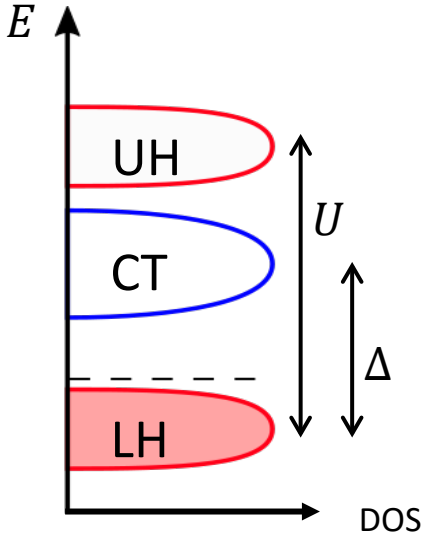


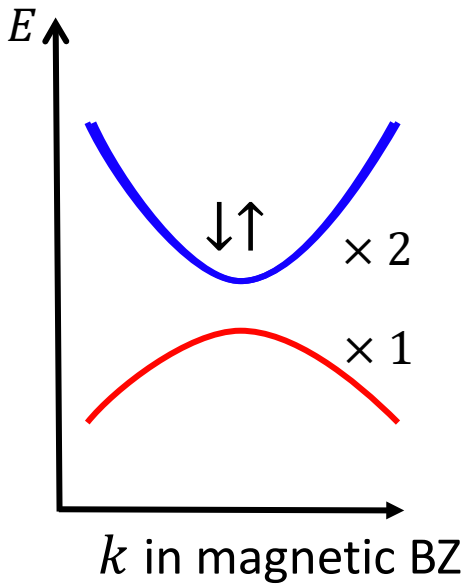
Devakul & LF, PRX (2022)

$\delta \sim \Delta - W$

120°-AFM Mott Insulator



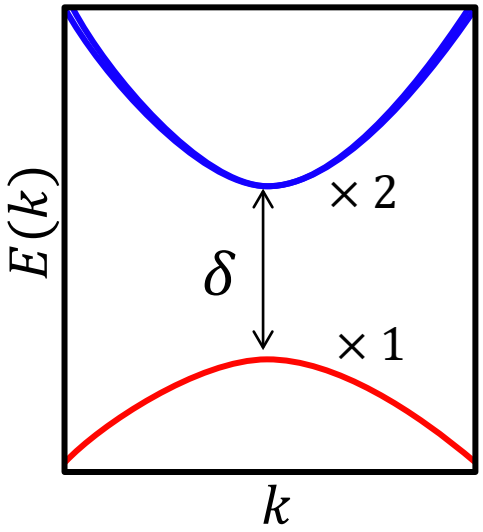




- Quasiparticle bands in magnetically ordered insulator are different from noninteracting bands.
- Low-energy states: spin-polarized holes on majority layer & spin-degenerate electrons on minority layer

Interacting Field Theory

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

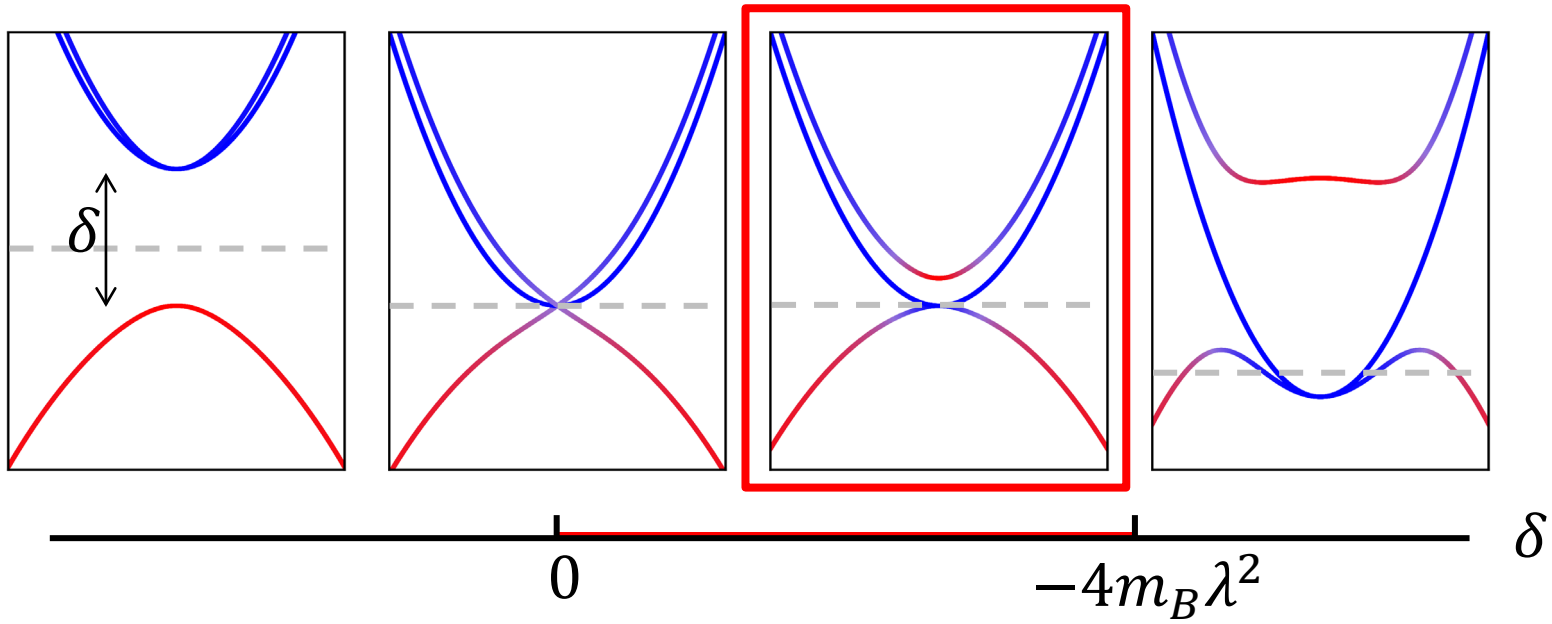


$$H_{\text{eff}} = \begin{pmatrix} -\frac{k^2}{2m_A} & \lambda(k_x + ik_y) & \lambda(k_x - ik_y) \\ " \ " & \frac{k^2}{2m_B} + \delta & 0 \\ " \ " & 0 & \frac{k^2}{2m_B} + \delta \end{pmatrix}$$

- 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

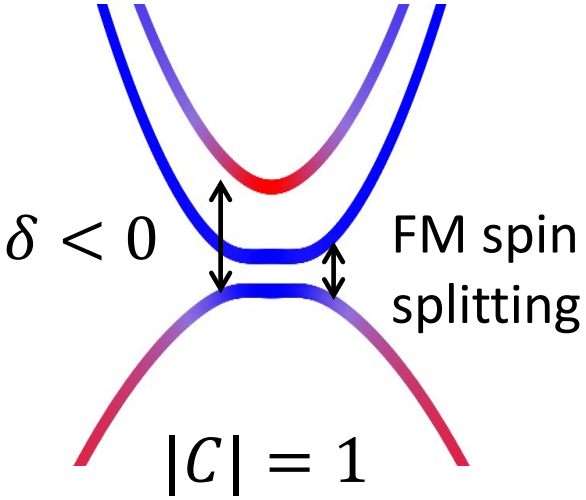
Quasiparticle band at $g = 0$

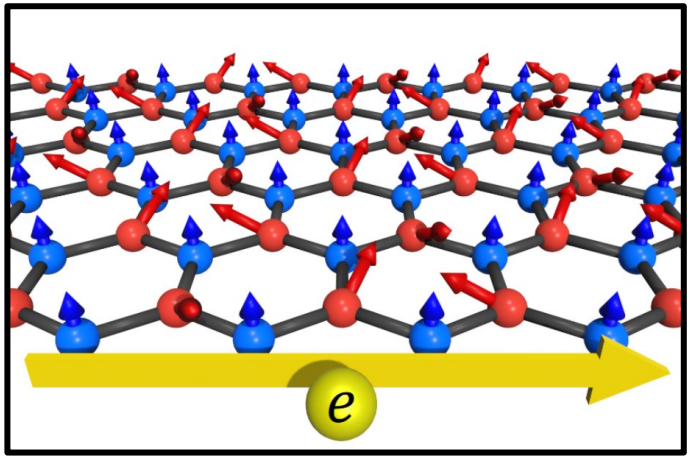


After band inversion $\delta < 0$, quadratic band touching appears at Fermi level, which is unstable to repulsion g Sun, Yao, Fradkin, Kivelson, PRL 2009

$g > 0$ changes from irrelevant to marginally relevant at band inversion, enabling an unconventional continuous Mott-QAH transition.

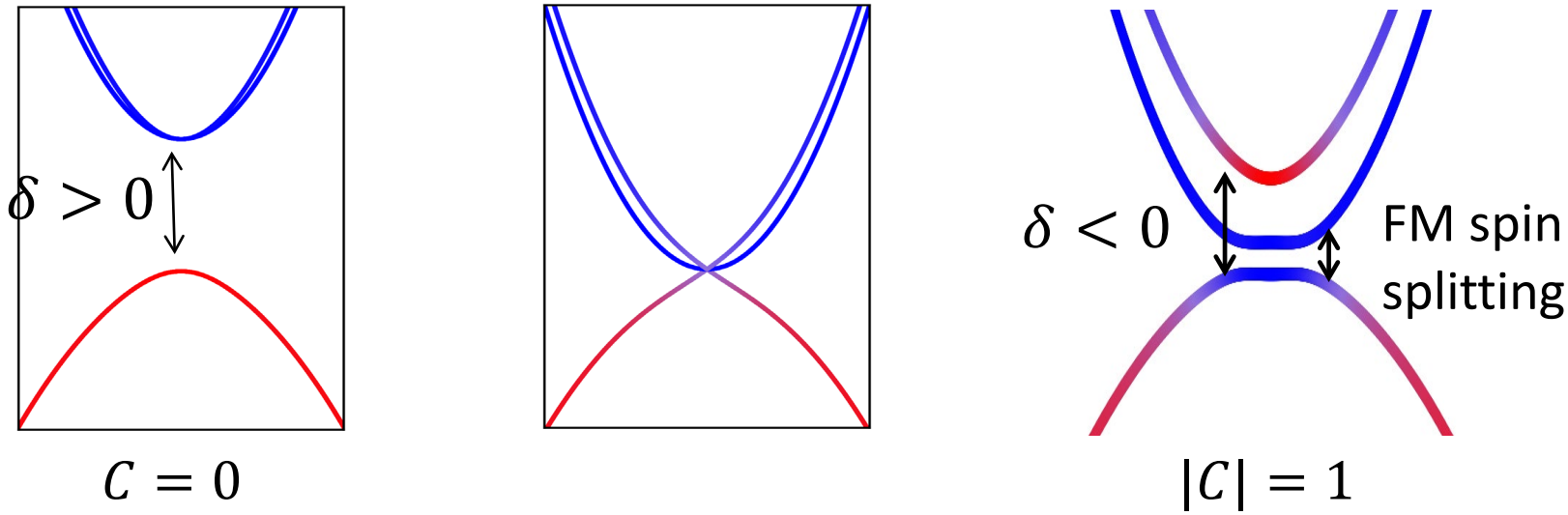
QAH with non-coplanar magnetism





- After quasiparticle band inversion, Ising FM in minority layer opens Chern gap at quadratic band touching
- chiral spin order: xy-AFM in $MoTe_2$ & Ising FM in WSe_2
- canting of xy-AFM allowed by symmetry

Continuous Mott-Chern Transition

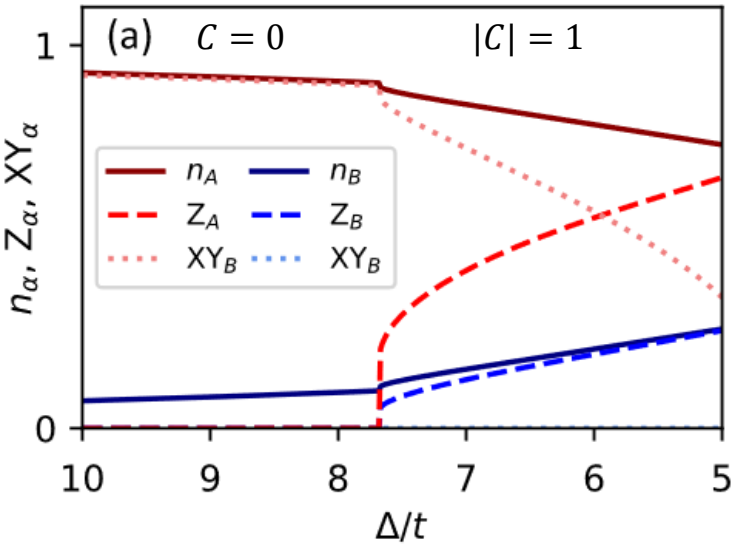


Inverting charge transfer gap induces <u>simultaneous</u> change of magnetism & topology.

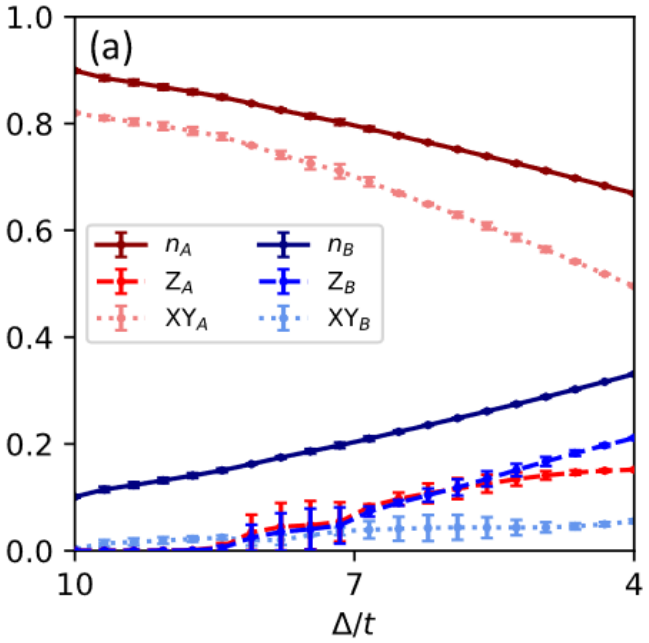
Devakul & LF, PRX (2022)

Numerical Results

Self-consistent Hartree-Fock



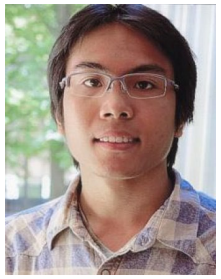
DMRG

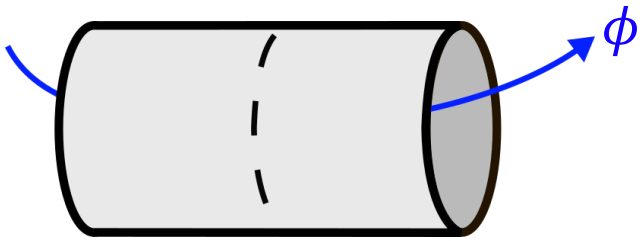


Honeycomb Hubbard model

$$H = H_A + H_B + H_{AB} + H_\Delta + H_U$$

Topology in DMRG

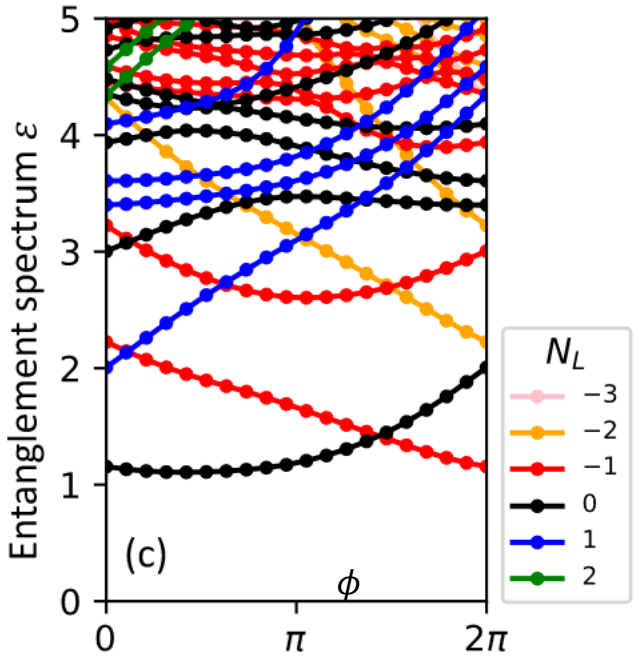




Laughlin 1981.

Charge pumping argument

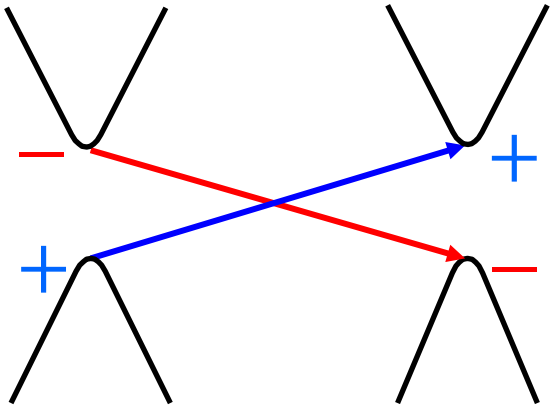
$$\sigma_{xy} = \frac{I_x}{V_y} = \delta_{N_L} \frac{e^2}{h} \Longrightarrow |C| = 1$$



$$\phi \rightarrow \phi + 2\pi$$
$$N_L \rightarrow N_L - 1$$

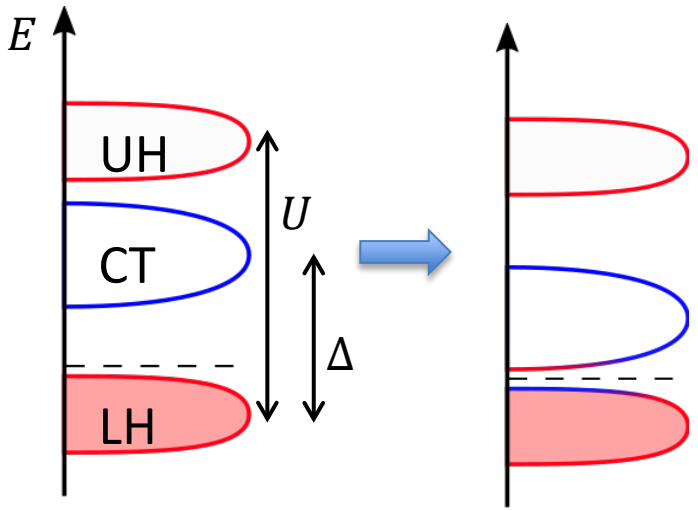
Topological Band & Mott Insulators

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

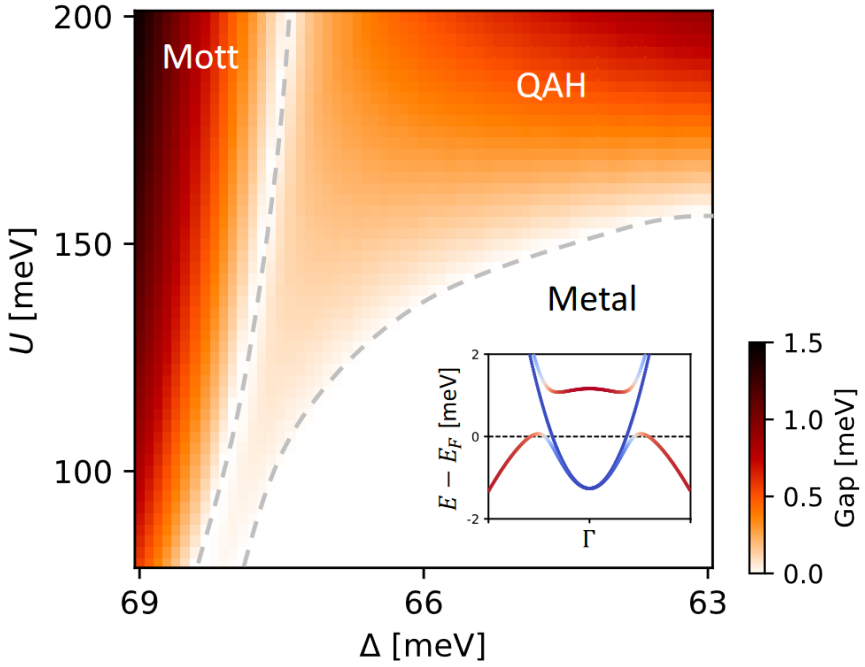
$C_K = +1$ $C_{K'} = -1$

Zhang & Senthil, MacDonald, Xie et al, Pan et al …

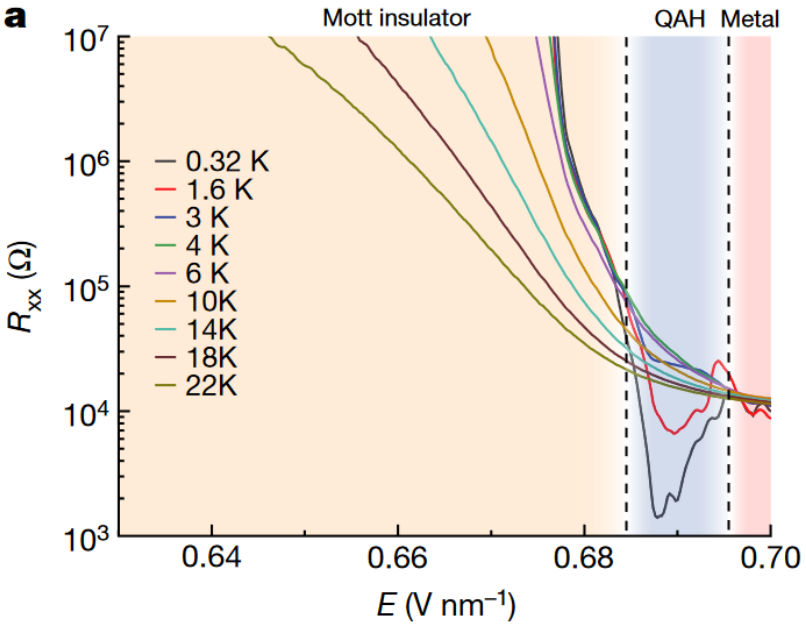
QAH in $MoTe_2/WSe_2$ differs fundamentally from flat band FM.

Comparison with Experiment

Hartree-Fock Phase Diagram



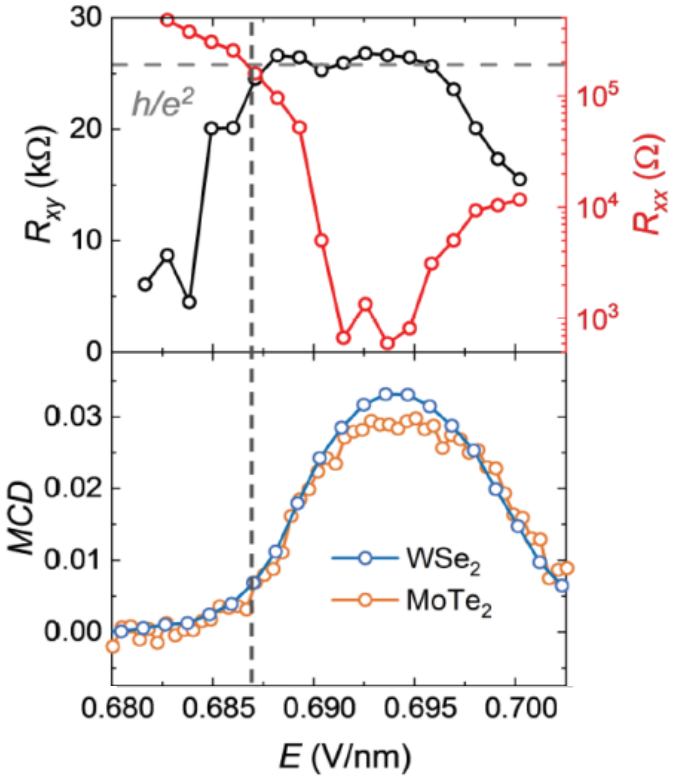
$MoTe_2/WSe_2$

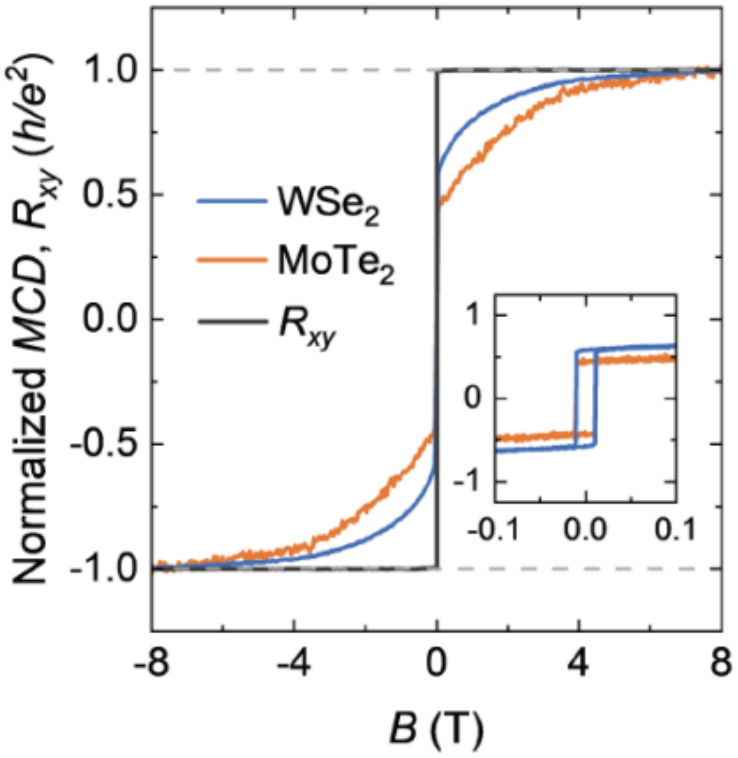


Prediction for Magnetism

- 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

Theory

Yang Zhang

Noah Yuan

Bi Zhen

Hiroki Isobe

Trithep Devakul

Philip Crowley

Nisarga Paul

Valentin Crepel

Margarita Davydova

Aidan Reddy

Kevin Slagle (Caltech)

Junkai Dong (Cornell)

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Experiment

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