Slide 1

Intrinsic magnetic topological states in $MnBi_2Te_4$

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2D van der Waals spin systems, SPICE

Outline

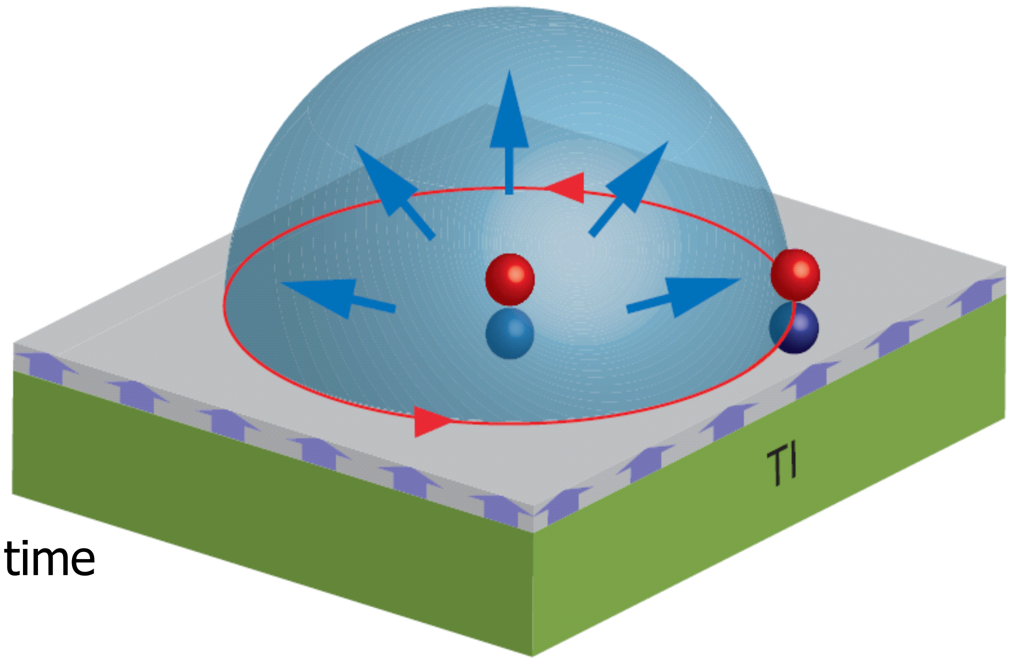
Slide 2

1. Axion response from topological insulators
2. Quantized anomalous Hall effect vs Topological magnetoelectric effect
3. Intrinsic magnetic topological state in MnBi2Te4
4. Flat Chern band in twisted bilayer MnBi2Te4

General theory of topological insulators

• Topological field theory of topological insulators. Generally valid for interacting and disordered systems. Directly measurable physically. Quantized magneto-electric effect (Qi, Hughes and Zhang, Wilczek)

$$S_0 = \frac{1}{8\pi}\int d^3x\,dt\left(\varepsilon \mathbf{E}^2 - \frac{1}{\mu}\mathbf{B}^2\right)$$



• For a periodic system, the system is time reversal symmetric only when
$\theta=0$ => trivial insulator
$\theta=\pi$ => non-trivial insulator

$$S_\theta = \left(\frac{\theta}{2\pi}\right)\left(\frac{\alpha}{2\pi}\right)\int d^3x\,dt\,\mathbf{E}\cdot\mathbf{B}$$

$$\alpha = \frac{e^2}{\hbar c}$$

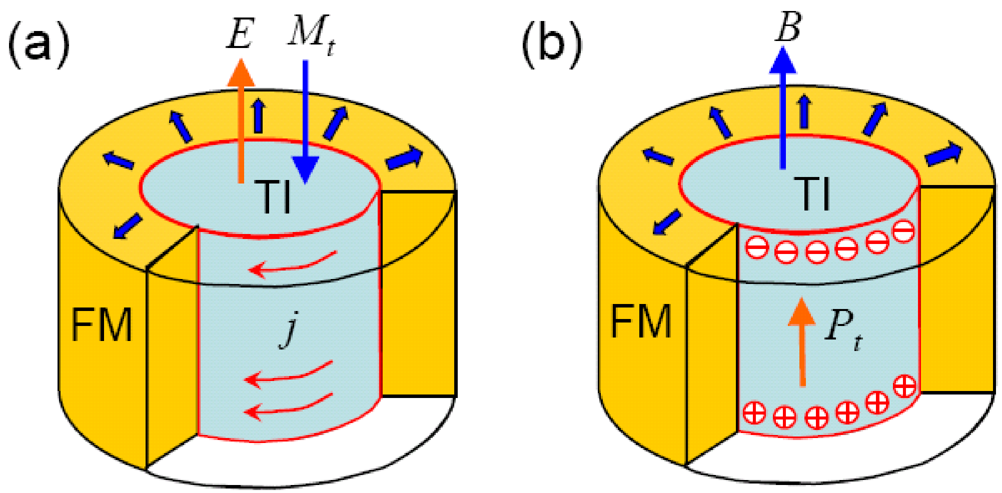
• Topological band theory based on Z2 topological band invariant of single particle states.
(Fu, Kane and Mele, Moore and Balents, Roy)

$$S_\theta = \frac{\theta}{2\pi}\frac{\alpha}{16\pi}\int d^3x\,dt\,\epsilon_{\mu\nu\rho\tau}F^{\mu\nu}F^{\rho\tau} = \frac{\theta}{2\pi}\frac{\alpha}{4\pi}\int d^3x\,dt\,\partial^\mu(\epsilon_{\mu\nu\rho\sigma}A^\nu\partial^\rho A^\tau)$$

The Topological Magneto-Electric (TME) effect

Slide 4

• Equations of axion electrodynamics predict the robust TME effect.



$4\pi\mathbf{M}=\alpha\,\theta/2\pi\,\mathbf{E}$ $\quad$ $4\pi\mathbf{P}=\alpha\,\theta/2\pi\,\mathbf{B}$

$$\begin{aligned}
\nabla\cdot\mathbf{D} &= 4\pi\rho \\
\nabla\cdot\mathbf{B} &= 0 \\
\nabla\times\mathbf{E} &= -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t} \\
\nabla\times\mathbf{H} &= \frac{4\pi}{c}\mathbf{J}+\frac{1}{c}\frac{\partial\mathbf{D}}{\partial t} \\
\mathbf{D} &= \mathbf{E}+4\pi\mathbf{P}-2P_3\alpha\mathbf{B} \\
\mathbf{H} &= \mathbf{B}-4\pi\mathbf{M}+2P_3\alpha\mathbf{E}
\end{aligned}$$

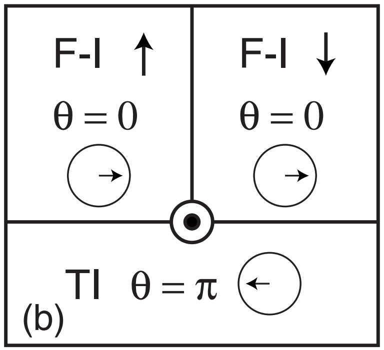
Wilzcek, axion electrodynamics

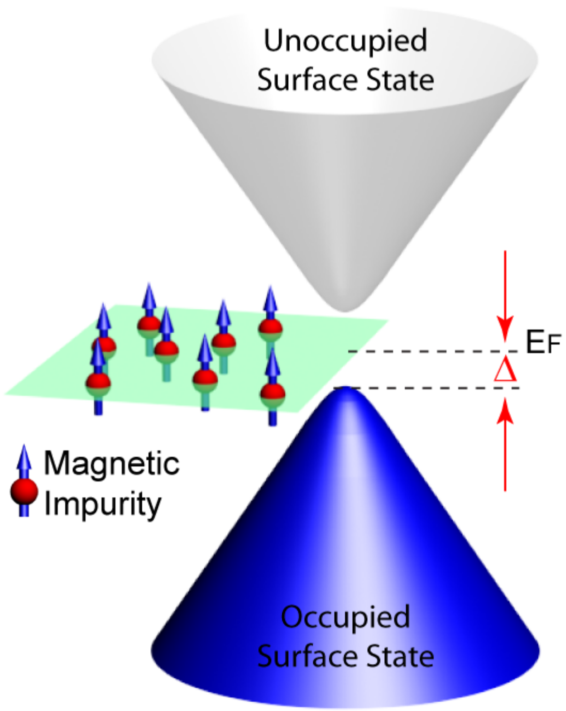
• $P_3=\theta/2\pi$ is the electro-magnetic polarization, microscopically given by the CS term over the momentum space. Change of P_3=2nd Chern number!

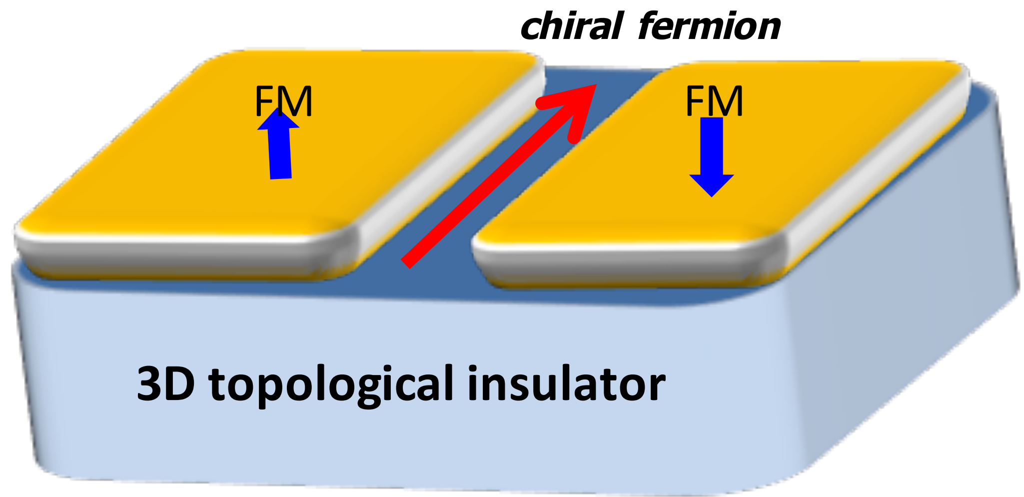
$$P_3(\theta_0)=\int d^3k\mathcal{K}^\theta$$

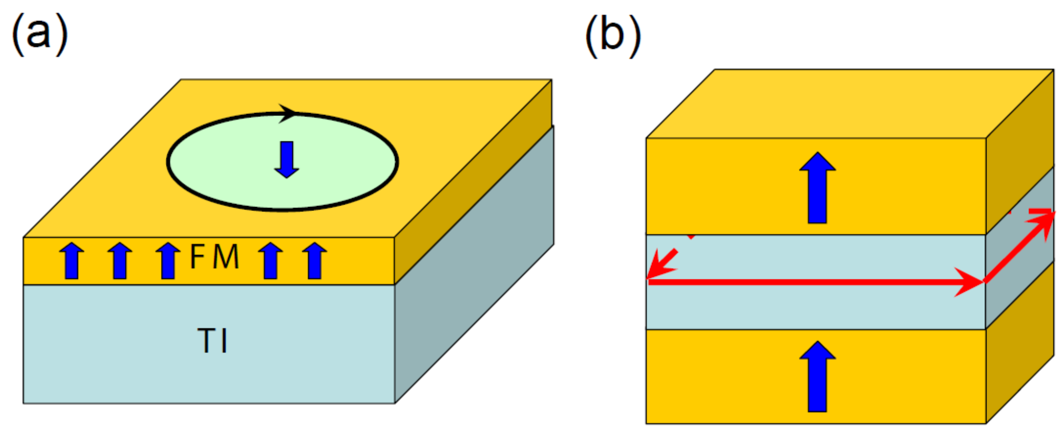
$$=\frac{1}{16\pi^2}\int d^3k\epsilon^{\theta ijk}\,\mathrm{Tr}\left[\left(f_{ij}-\frac{1}{3}[a_i,a_j]\right)\cdot a_k\right]$$

Gapped Dirac fermions on the surface, chiral fermions on the domain wall



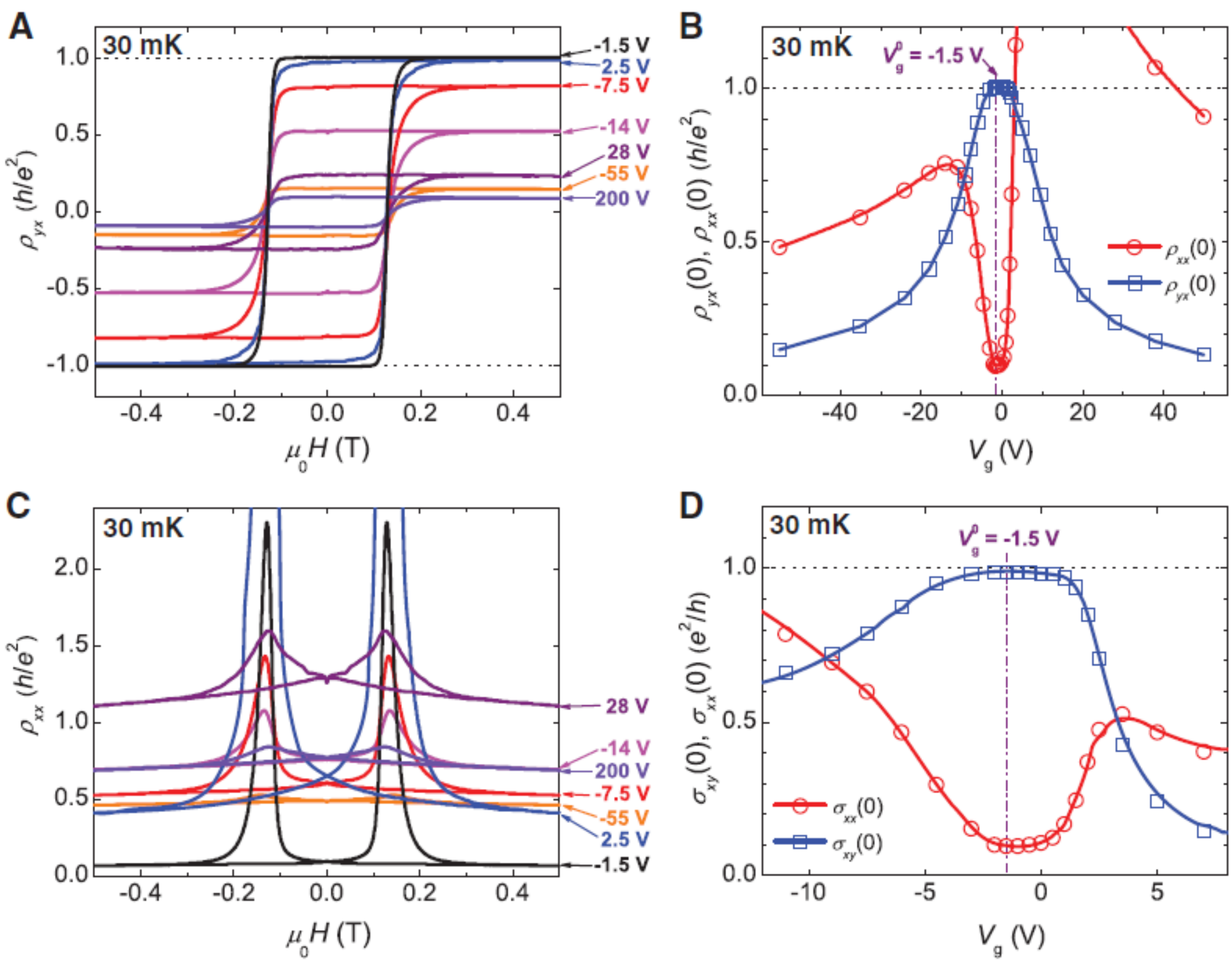






QAH can be realized in ferromagnetic TI (Qi, Hughes, Zhang, PRB 2008)

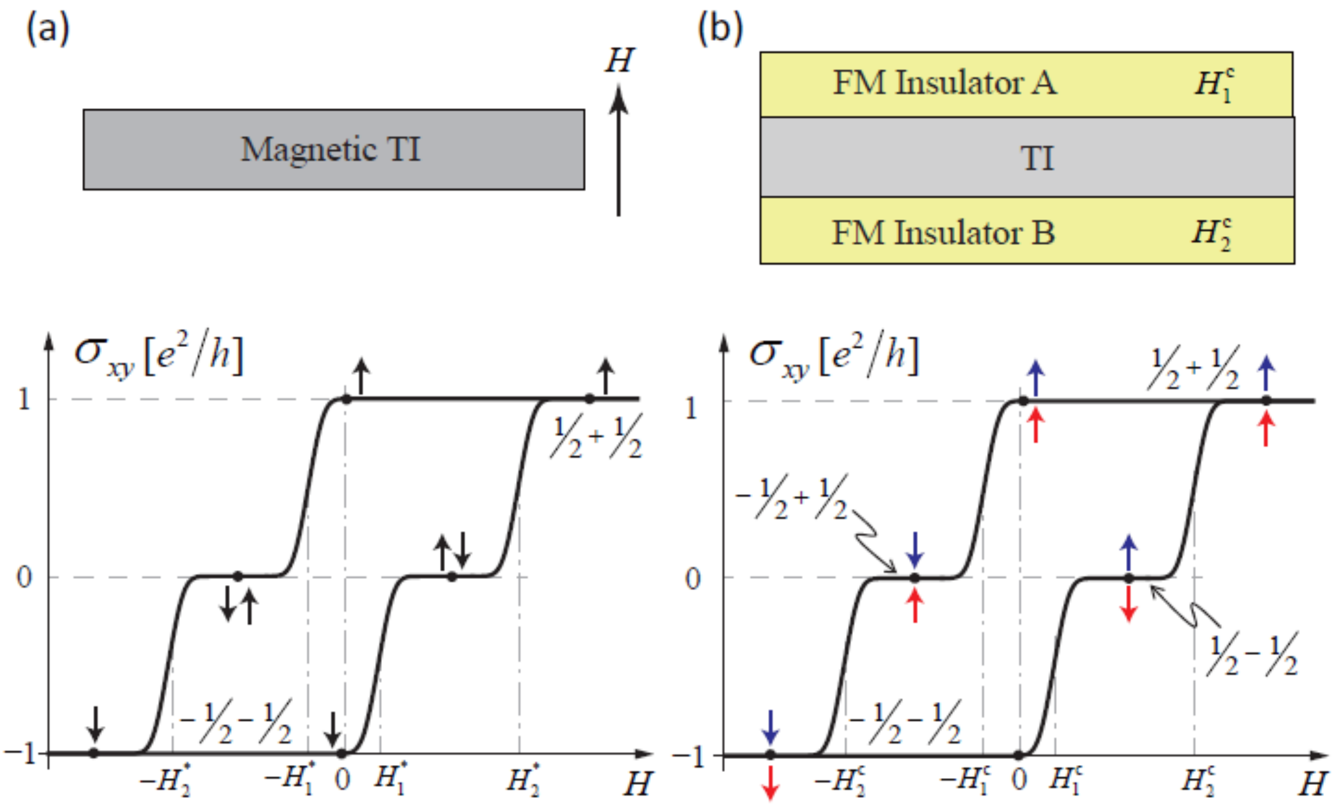
Experimental observation of the QAH effect in 5 QL CrBiSbTe at 20 mK (Science 2013)



Topological magnetoelectric effect in TIs and QAHE

$$\mathcal{S}_\theta = \frac{\theta}{2\pi}\frac{e^2}{h}\int d^3x dt \mathbf{E}\cdot\mathbf{B},$$

1. T-breaking surface gap
2. Fully insulating
3. Finite size

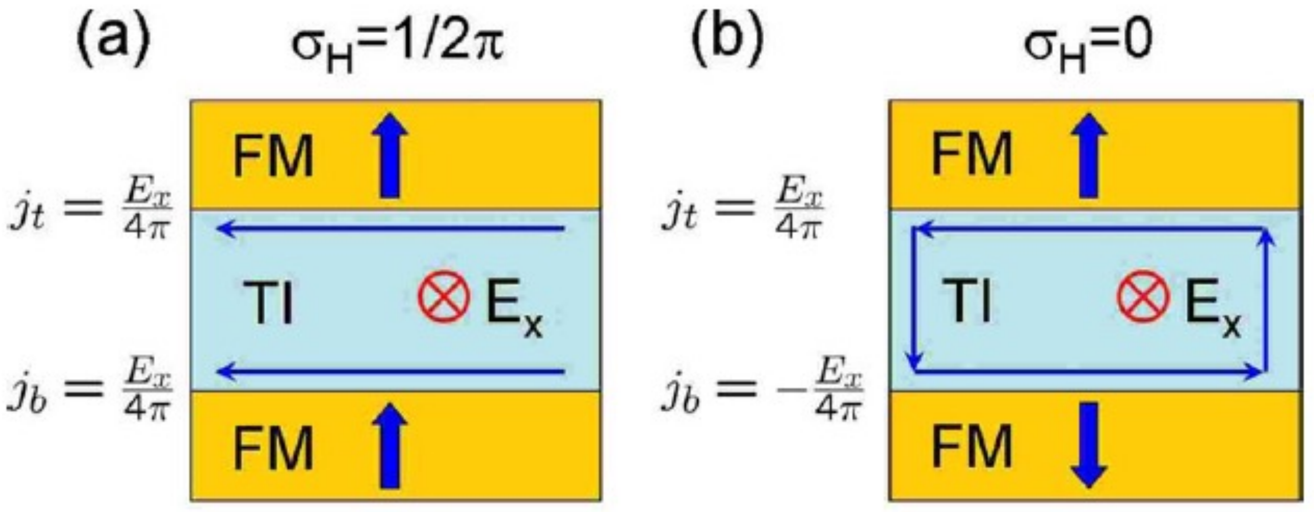


J Wang, B Lian, XL Qi, SC Zhang, PRB 92, 081107 (2015)

QAH effect vs TME effect

QAH insulator

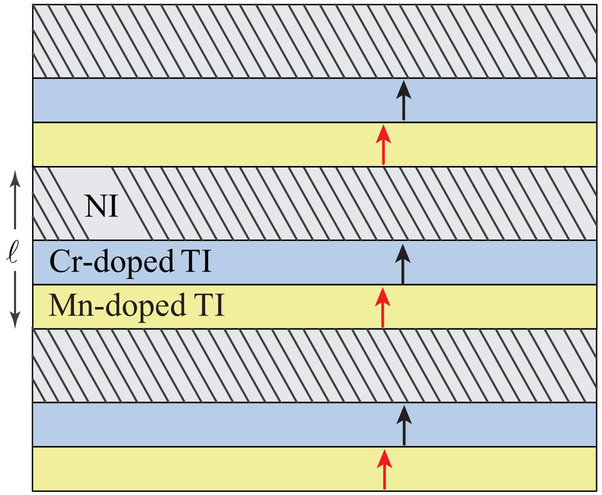
Axion insulator

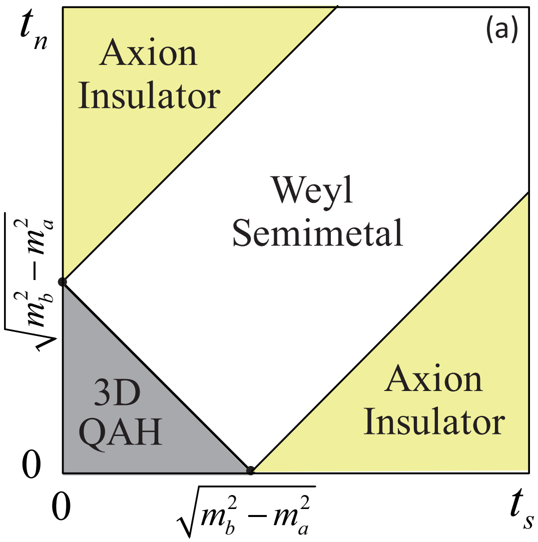


- T-breaking surfaces
- With magnetic domain
- Gapless edge mode at domain wall
- Fully insulating
- 2D system, need finite size

- T-breaking surfaces
- Without magnetic domain
- No gapless edge/hinge mode
- Fully insulating
- 3D system, finite size effect in 2D

Multiple types of topological states in superlattice





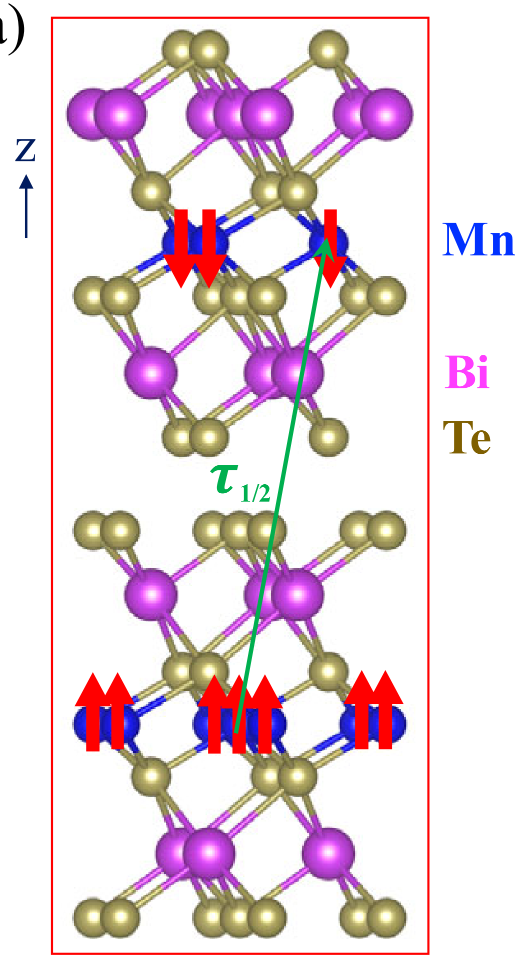
$$\mathcal{H} = \sum_{\mathbf{k}_\parallel, i, j} \Big[v_F \tau^z (\hat{\mathbf{z}} \times \boldsymbol{\sigma}) \cdot \mathbf{k}_\parallel \delta_{i,j} + m_a \tau^z \sigma^z \delta_{i,j} + m_b \sigma^z \delta_{i,j} + t_s \tau^x \delta_{i,j} + \frac{t_n}{2} \tau^+ \delta_{i+1,j} + \frac{t_n}{2} \tau^- \delta_{i-1,j} \Big] c^\dagger_{\mathbf{k}_\parallel i} c_{\mathbf{k}_\parallel j}, \qquad (2)$$

JW, B Lian, SC Zhang, PRB 93, 045115 (2016)

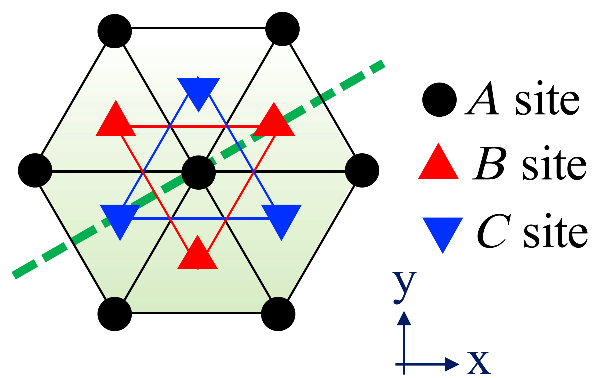
Hydrogen atom of magnetic TI: MnBi2Te4

$$\mathcal{S} = \Theta\tau_{1/2}$$

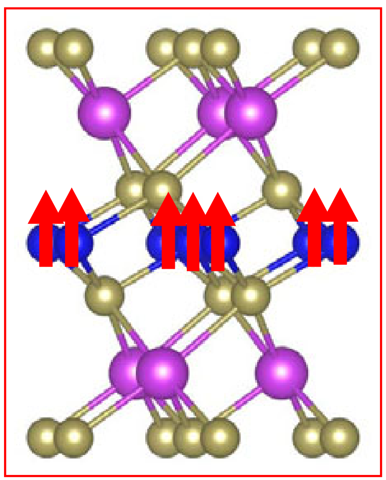
(a)



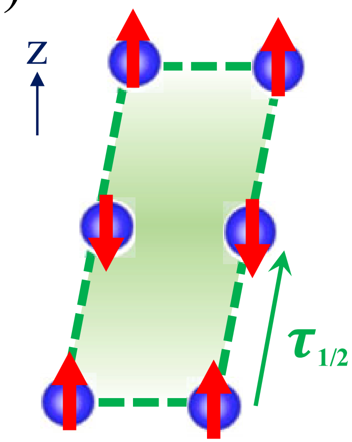
(b)



(c)



(d)

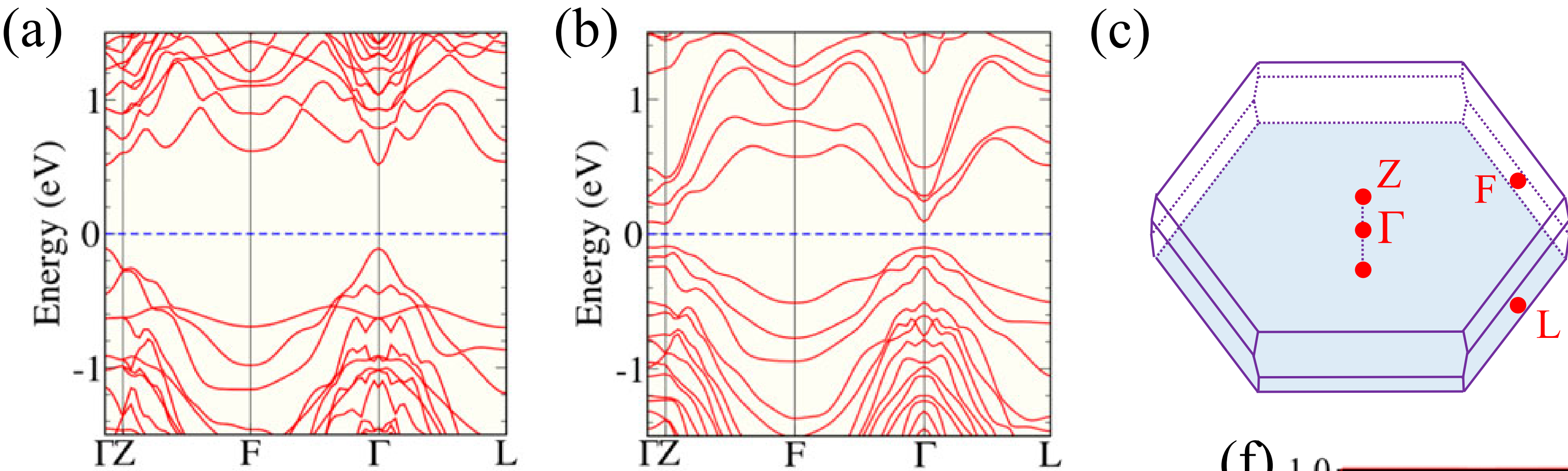


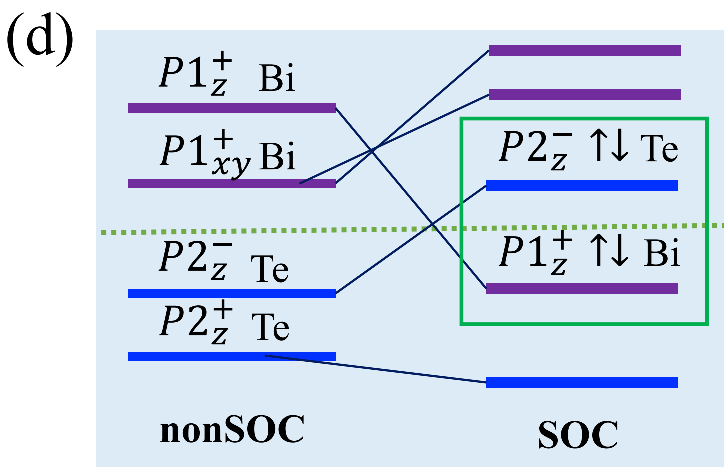
(e)

Phase	Energy
AFM1	0.0000eV
AFM2	0.0017eV
FM1	0.0460eV
FM2	0.0464eV

Wang *et al*, Phys. Rev. Lett. 122, 206401 (2019)

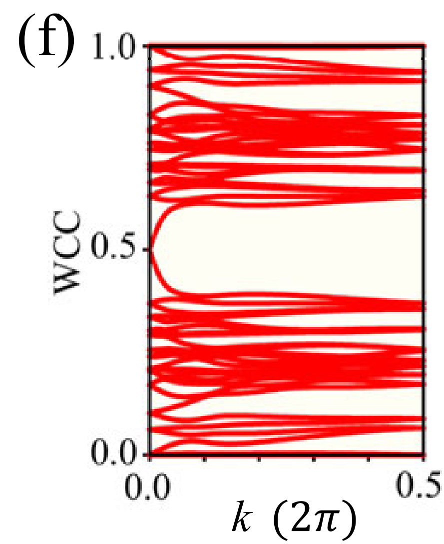
Electronic band structure of AFM MnBi2Te4





(e)

TRIM $\bar{G}$ $\bar{G} \cdot \tau_{1/2}$=nπ	Parity product
Γ(000)	−
3$F(\pi\pi 0)$	3 +
$\mathcal{Z}_2$	1



Moore *et al*, PRB 2010

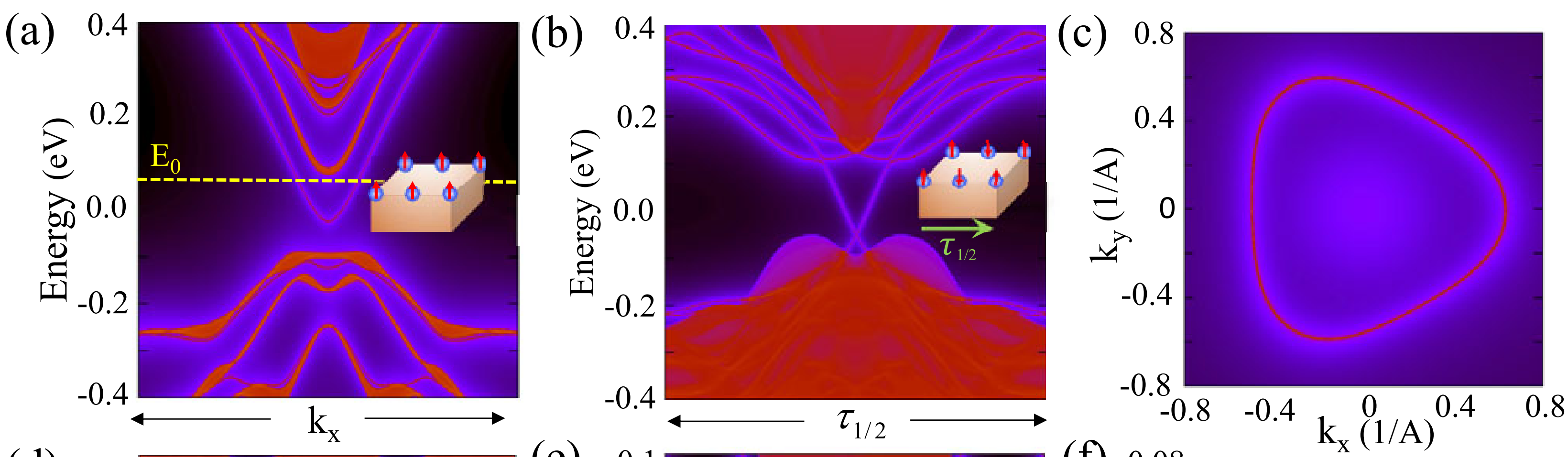
Model for AFM topological insulator MnBi2Te4

$\mathcal{I}$, C_{3z} and $\mathcal{S}$

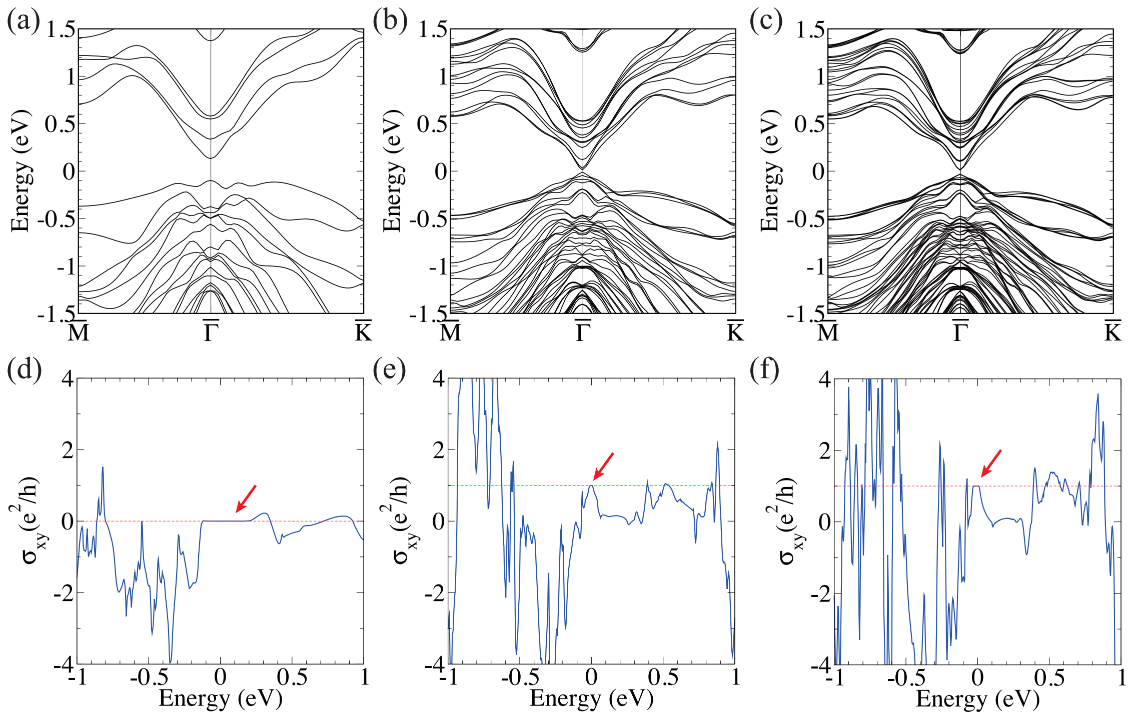
$$H(\mathbf{k}) = \epsilon_0(\mathbf{k})\mathrm{I}_{4\times 4} + \begin{pmatrix} \mathcal{M}(\mathbf{k}) & A_1 k_z & 0 & A_2 k_- \\ A_1 k_z & -\mathcal{M}(\mathbf{k}) & A_2 k_- & 0 \\ 0 & A_2 k_+ & \mathcal{M}(\mathbf{k}) & -A_1 k_z \\ A_2 k_+ & 0 & -A_1 k_z & -\mathcal{M}(\mathbf{k}) \end{pmatrix} + o(\mathbf{k}^2)$$

Pz+, up, Pz-, up, Pz+, down, Pz-, down

Single Gapped Dirac cone on the surface of MnBi2Te4



QAH and Zero plateau in MnBi2Te4 odd and even layers



Even layer, conserved $\mathcal{I}\Theta$

$$\sigma_{xy} = 0$$

Odd layer, broken $\mathcal{I}\Theta$, with band inversion

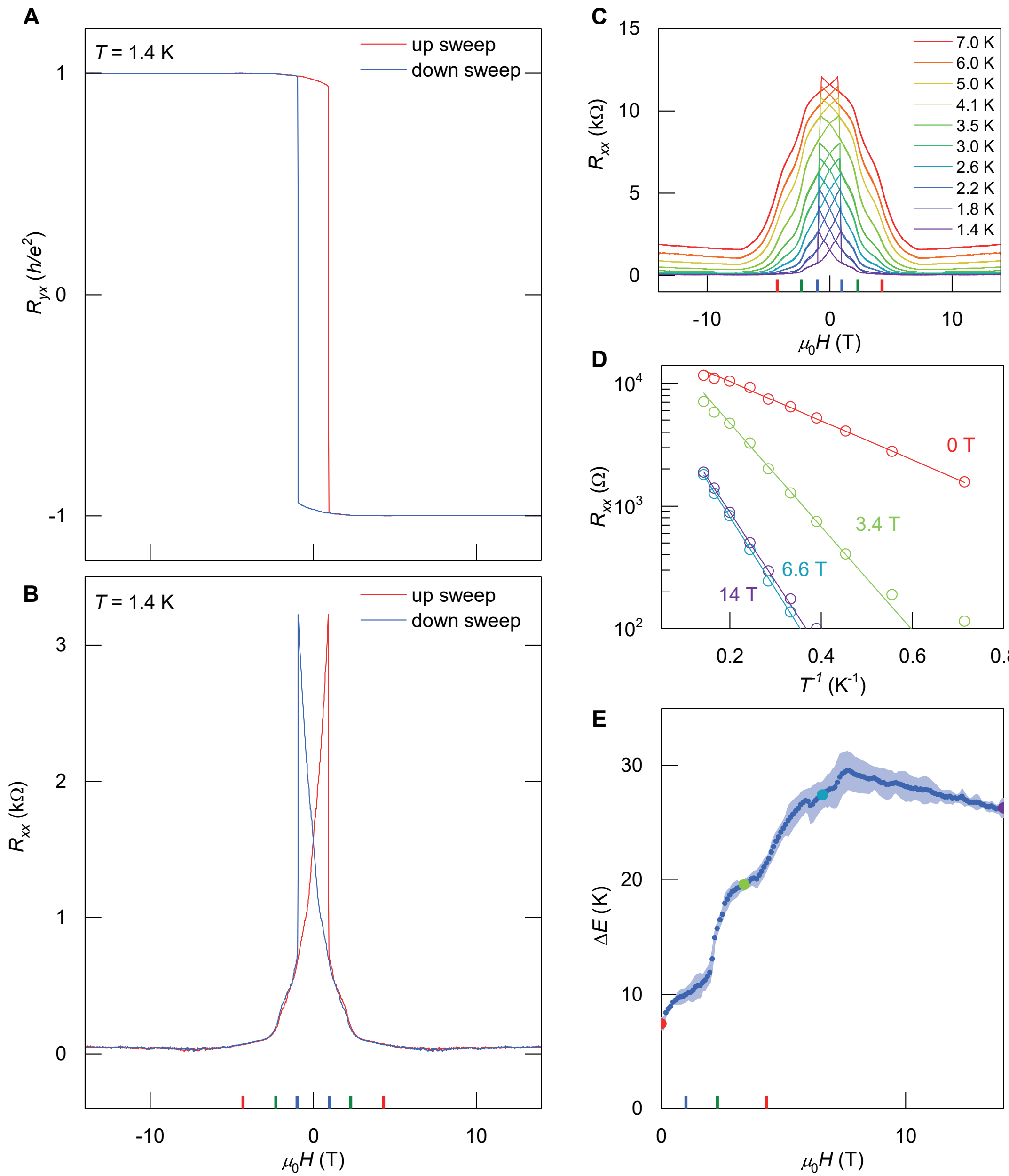
$$\sigma_{xy} = \pm e^2/h$$

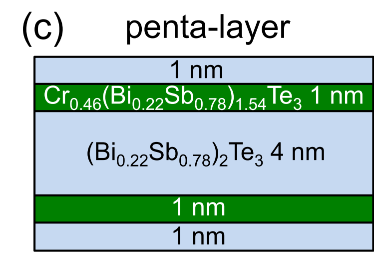
Thickness (SL)	Topology	Bandgap (meV)
1	Trivial	321
2	ZPQAH	107
3	QAH	66
4	ZPQAH	97
5	QAH	77
6	ZPQAH	87
7	QAH	85
$\propto$ (bulk)	3D AFM TI	225

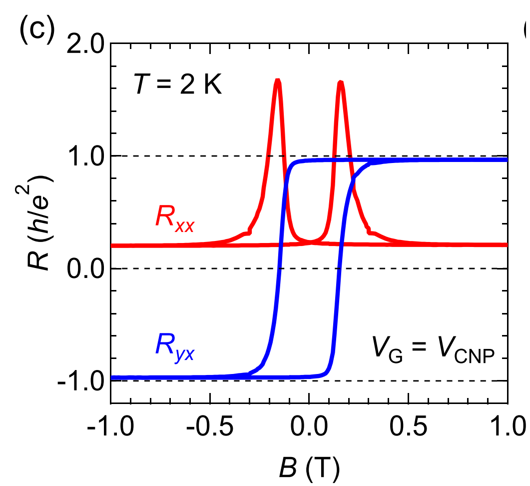
Zhang, Wang *et al*, Phys. Rev. Lett. 122, 206401 (2019)

Observation of zero-field QAH in 5 SL layer (Yuanbo Zhang Group)

Deng *et al*, Science 367, 895 (2020)



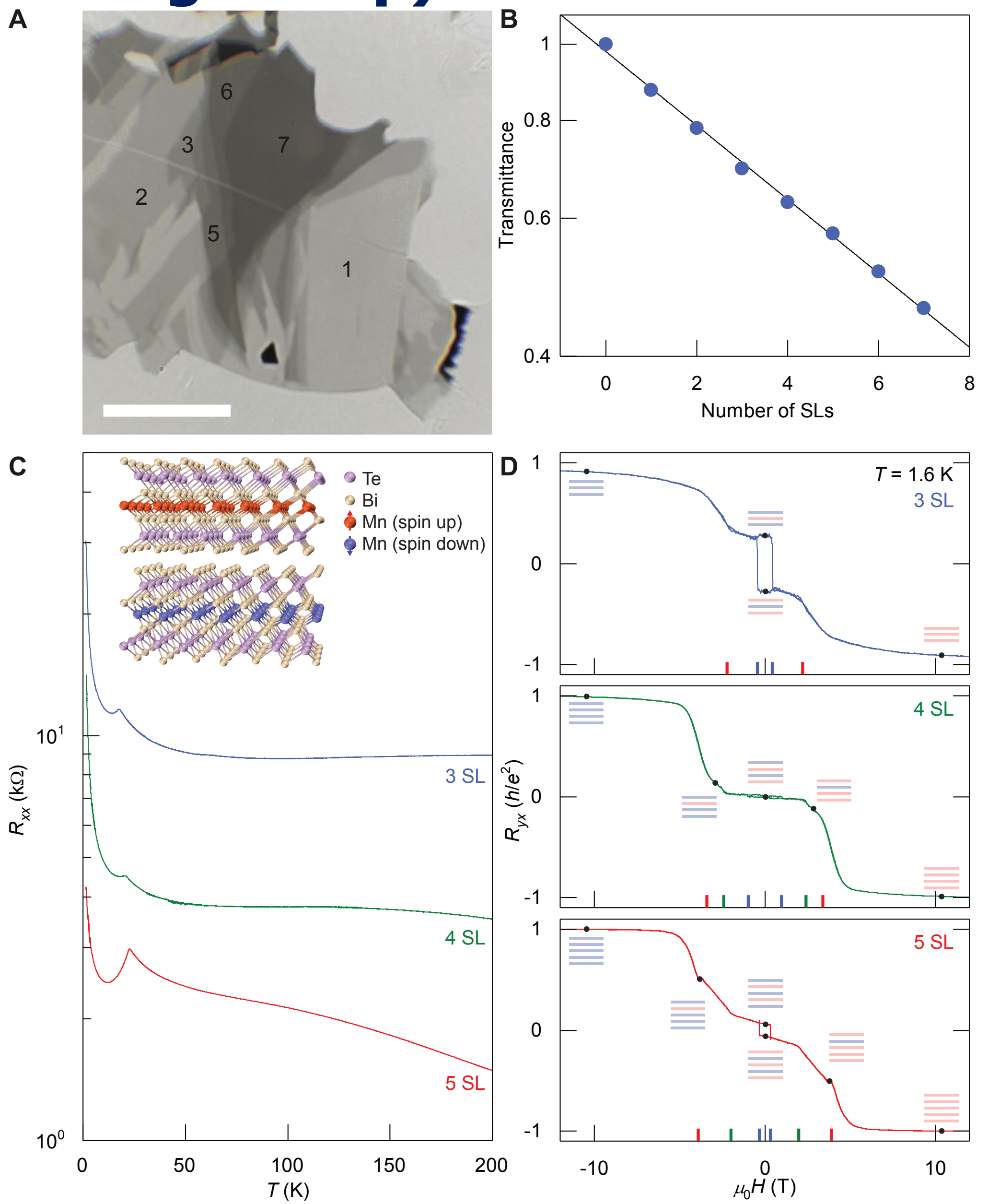




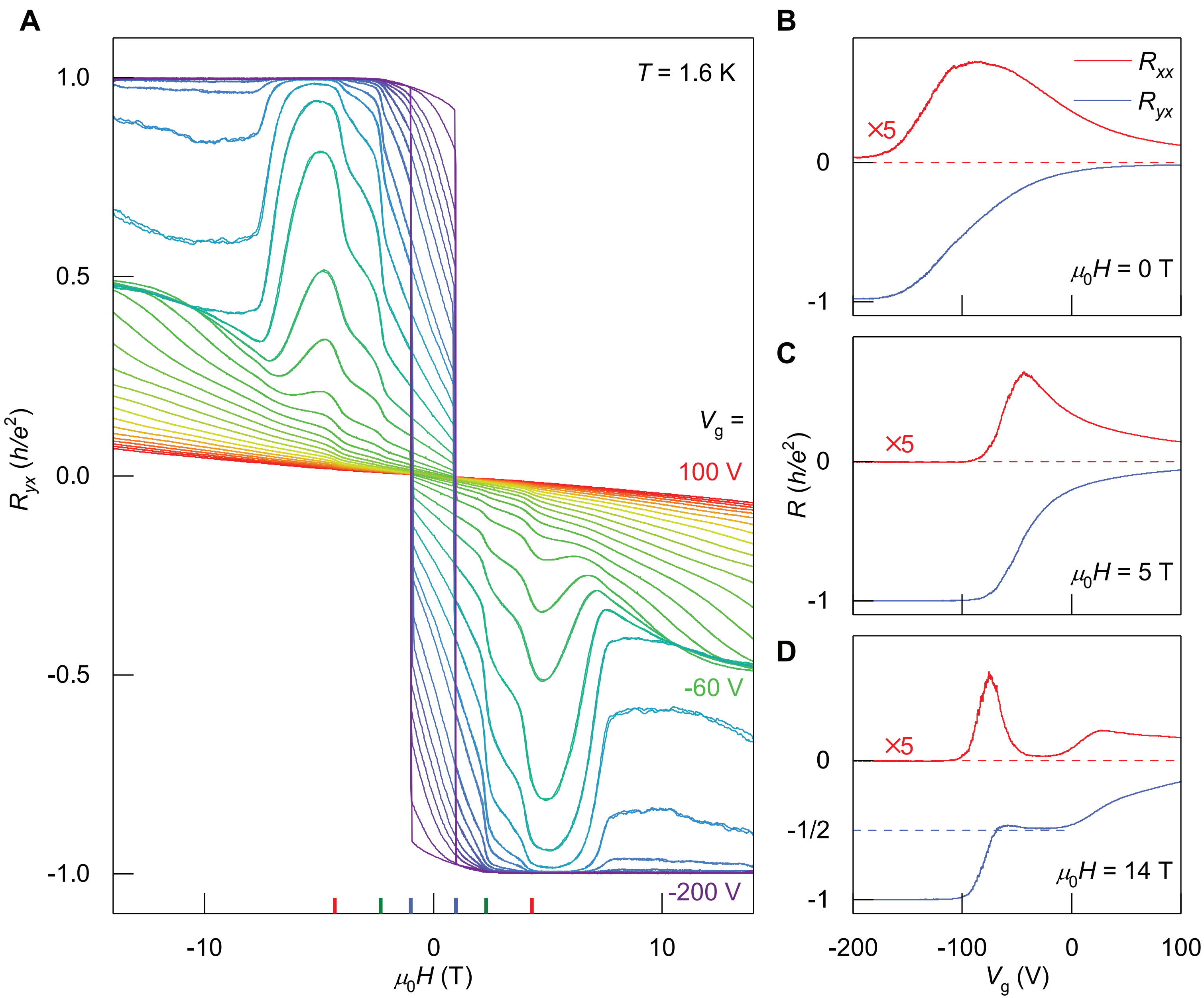
Tokura group 2015

Observation of QAH in 5 SL and possible AI in 4 SL (Yuanbo Zhang Group)

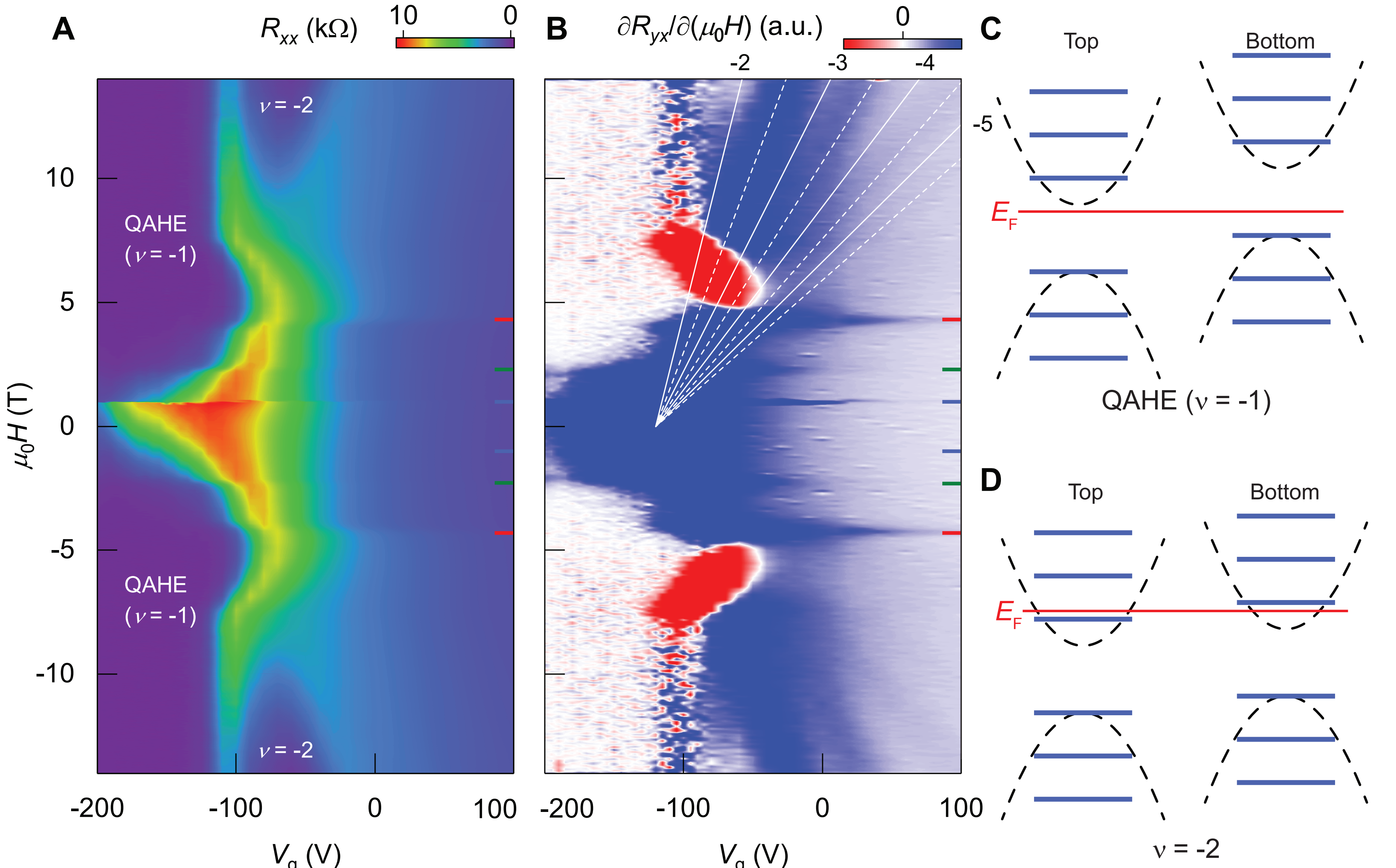
Deng *et al*, Science 367, 895 (2020)



Coexitence of QAH and QHE in odd layer



Phase diagrams of H and gate voltage



Higher plateau QAH: multi-channel chiral edge states

Basic physics (realization of $\sigma_{xy} = n\frac{e^2}{h}$) :

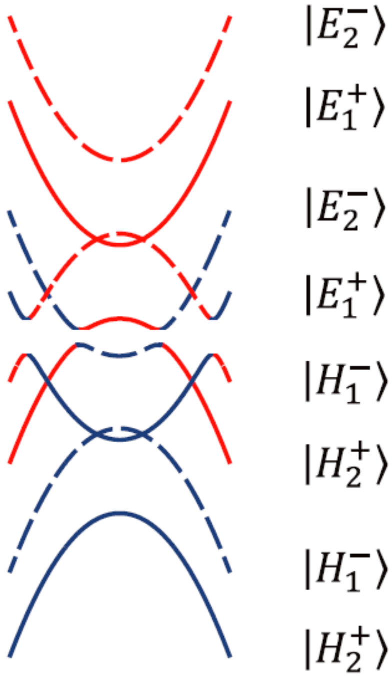
System: thin film of 3D TI with magnetic dopping.

1) Dopping induced exchange field Δ splits the 3D bulk bands with spin $\uparrow$ and $\downarrow$, and only one pair of bulk bands ($s\uparrow, p\downarrow$) are inverted, while the other are not ($s\downarrow, p\uparrow$).

2) Make 3D TI into a thin film (compactify the z direction), so that

$$\text{3D bulk bands } (s\uparrow, p\downarrow) \xrightarrow{k_z\ discrete} \text{2D sub-bands.}$$

If the lowest n 2D sub-bands are inverted, we get a QAH with Chern number n .



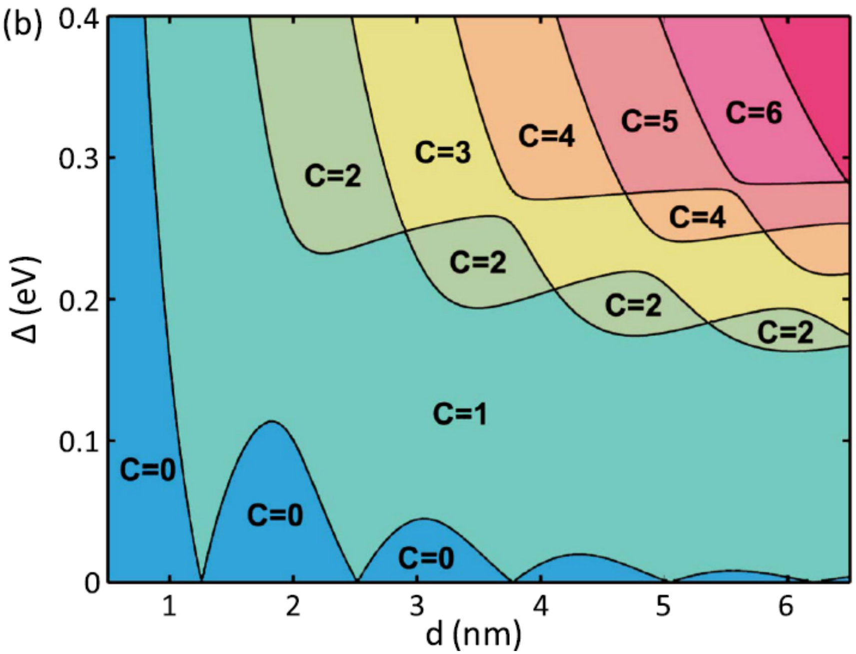
QAH with $n = 2$

Wang *et al*, Phys. Rev. Lett. 111, 136801 (2019)

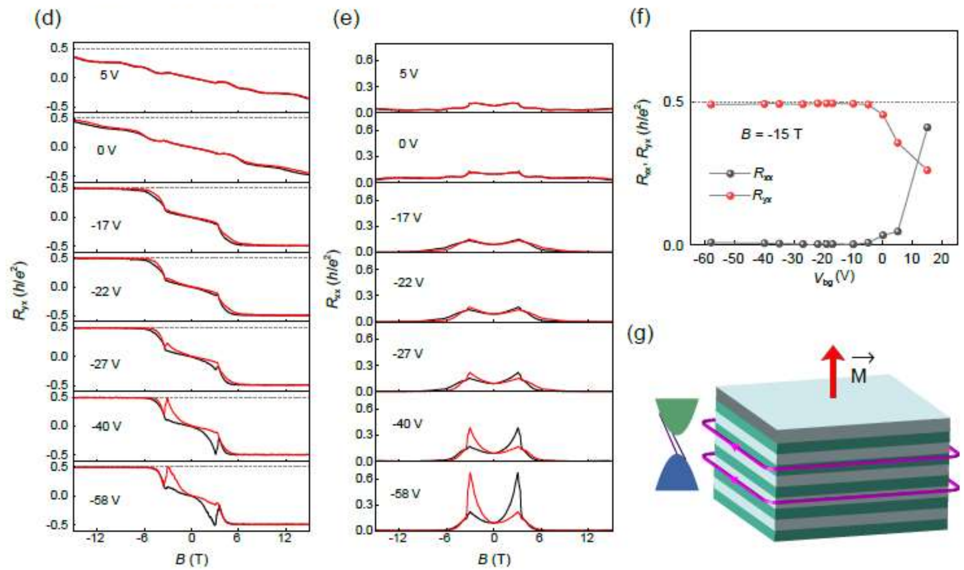
Higher plateau QAH: multi-channel chiral edge states

Theoretical phase diagram of QAH (thickness d , exchange field Δ)

Promising to realize in FM MnBi2Te4



10 SL FM MnBi2Te4, C=2

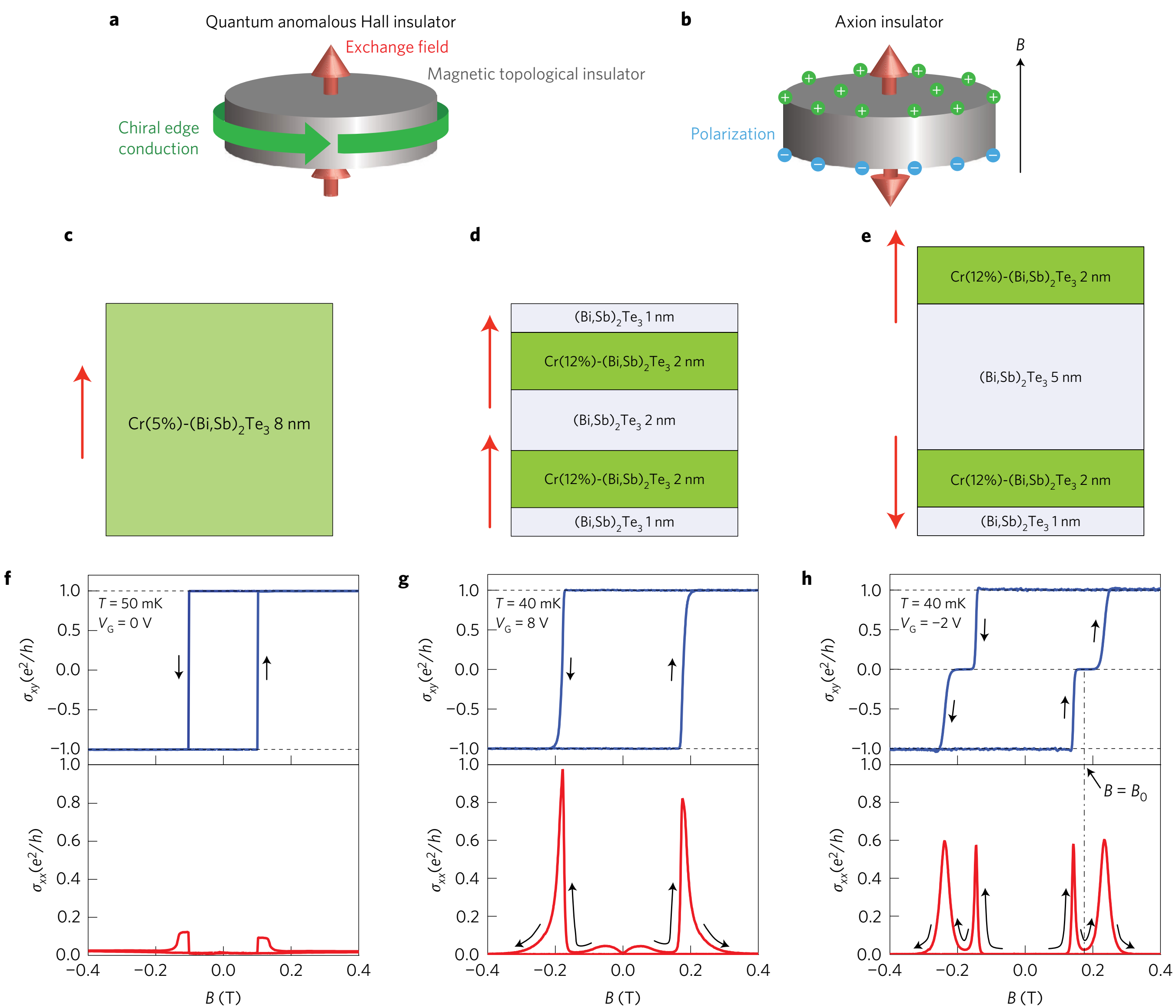


With *z* direction SOC

$$A_1 \neq 0$$

Jian Wang group. National Science Review, nwaa089 (2020)

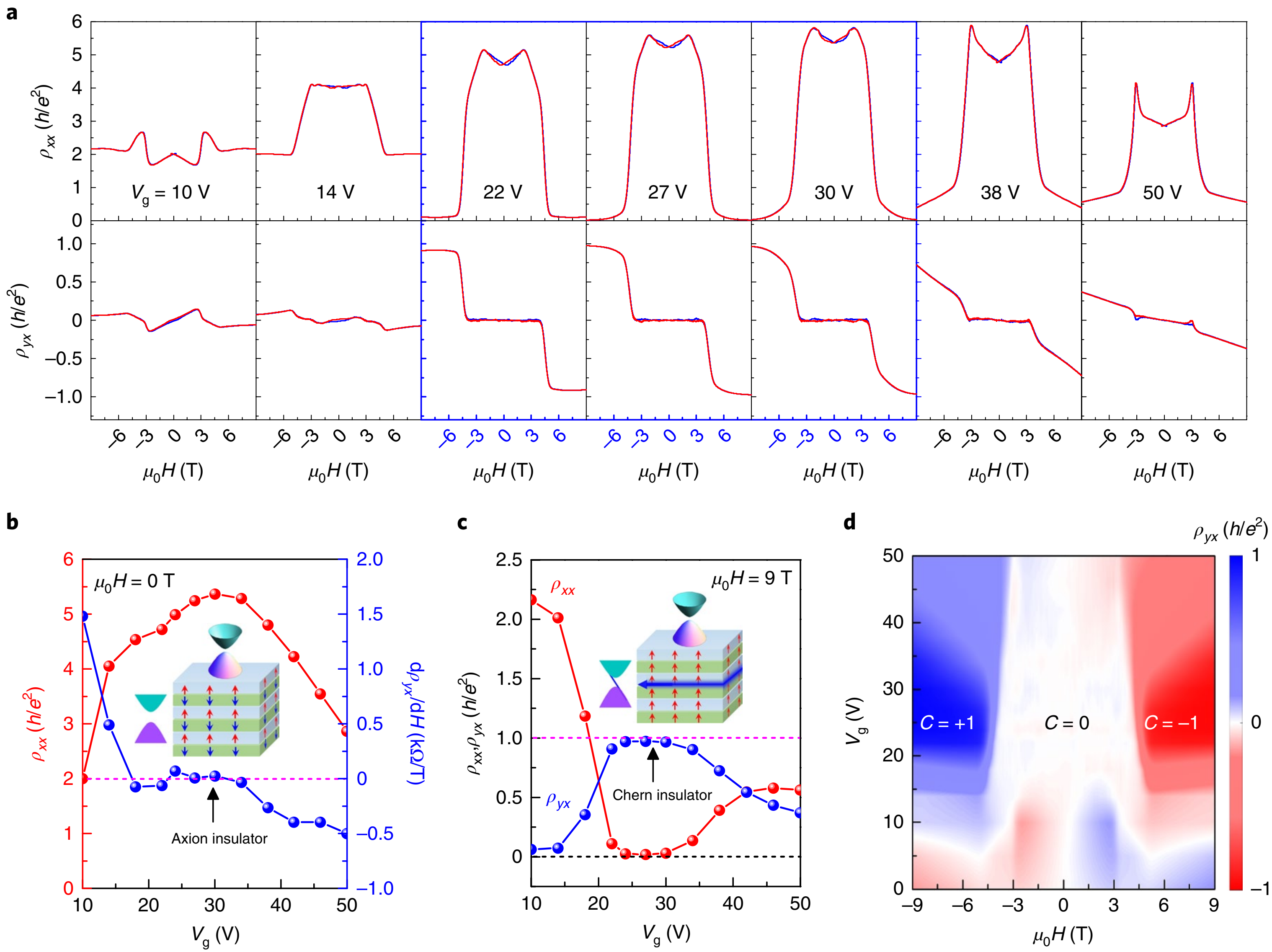
Axion state in magnetic TI heterostructure



Y Tokura *et al*, Nature Mat 16, 516 (2017)

Observation of possible AI in 6 SL $MnBi_2Te_4$ (Yayu Wang Group)

Liu *et al*, Nature Mat. 19, 522 (2020)



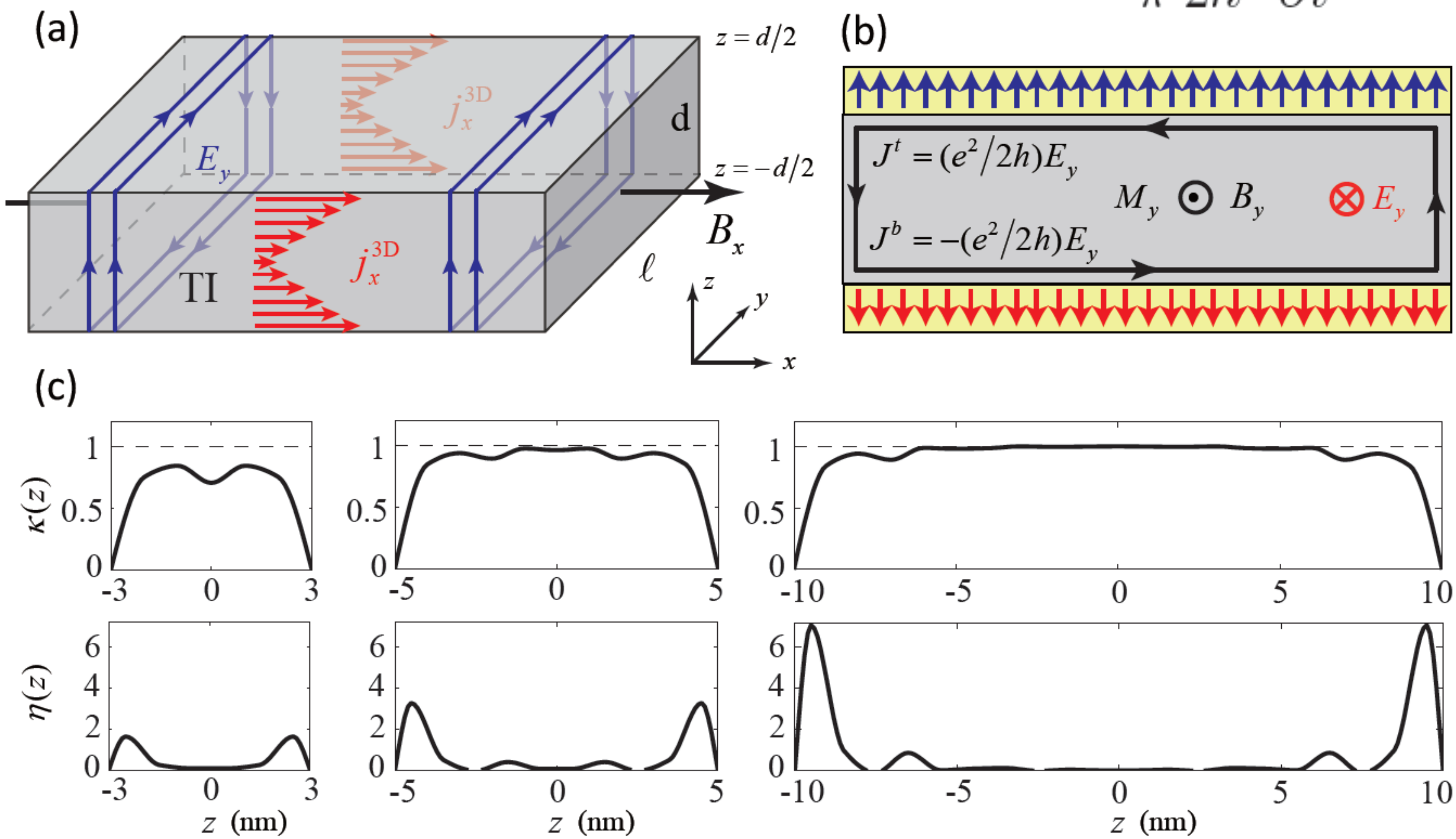
TME: ac B field induces ac current in the same direction

$$\mathbf{E}^t = -\mathbf{E}^b = (\partial B_x/\partial t)(d/2)\hat{\mathbf{y}}.$$

$$\mathbf{j}_t^{2D} = \sigma_{xy}^t \hat{\mathbf{z}} \times \mathbf{E}^t \quad \mathbf{j}_b^{2D} = \sigma_{xy}^b \hat{\mathbf{z}} \times \mathbf{E}^b.$$

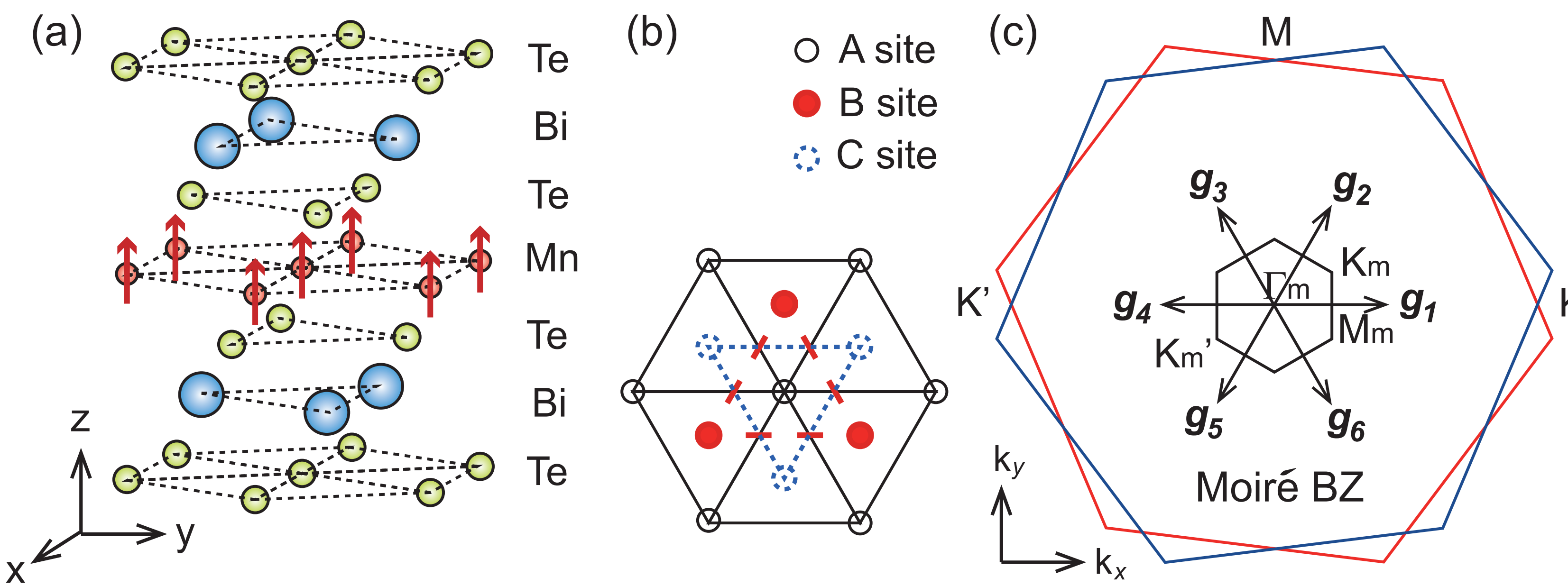
$$\mathcal{J} = \mathbf{j}^{2D}\ell = \mathcal{J}\hat{\mathbf{x}},$$

$$\mathcal{J} = \frac{\theta}{\pi}\frac{e^2}{2h}\frac{\partial B_x}{\partial t}\ell d.$$



Flat band from twisted 2D bilayer-SL MnBi2Te4

Motivation: to get a time-reversal breaking flat Chern band in the single particle level.



$$H = \begin{pmatrix} h_{1,\theta/2}(-i\nabla) + U_d & T(\mathbf{r}) \\ T^\dagger(\mathbf{r}) & h_{2,-\theta/2}(-i\nabla) - U_d \end{pmatrix},$$

$$T(\mathbf{r}) = T_0 + \sum_{j=1}^{6} T_j e^{i\boldsymbol{g}_j \cdot \mathbf{r}}$$

Lian, Wang *et al*, PRL 124, 126402 (2020)

Flat Chern band from twisted bilayer MnBi2Te4: FM

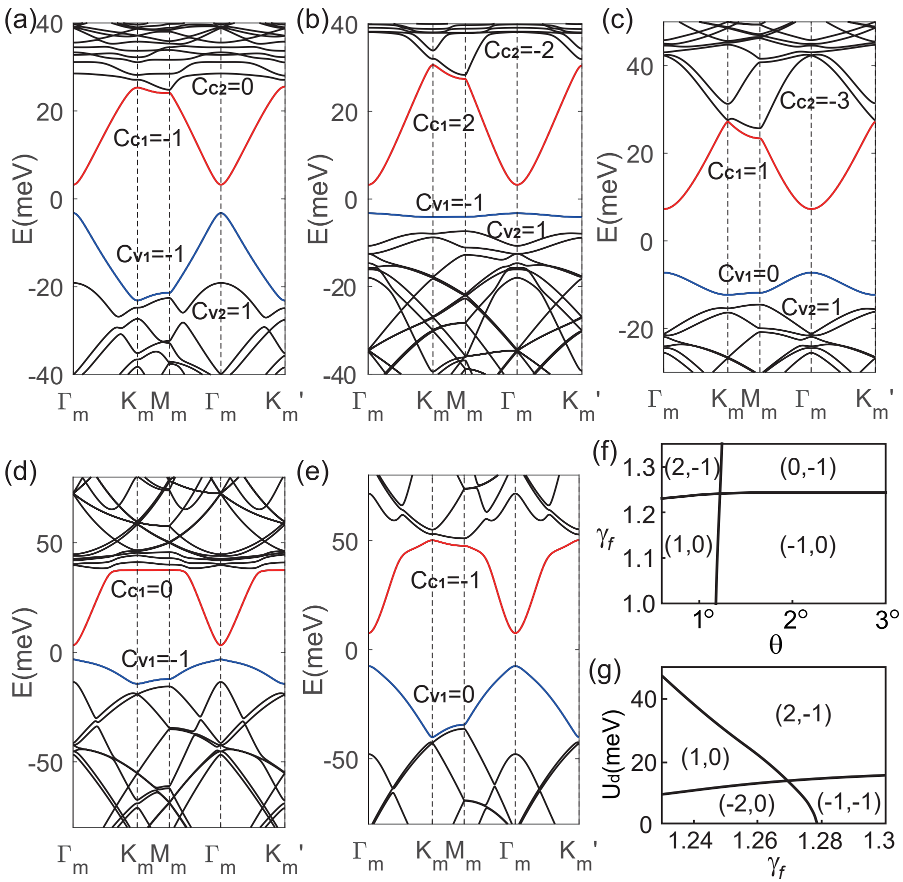
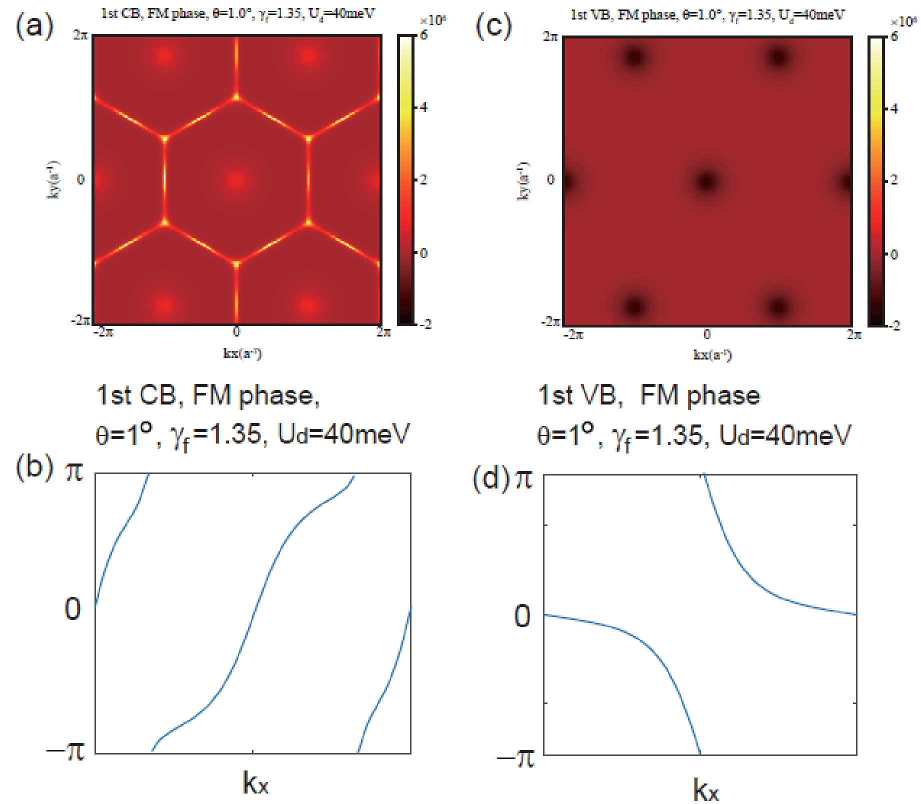


FIG. 2. The band structure of the FM tBMBT for (a) $\theta = 1^\circ$, $U_d = 10$ meV, $\gamma_f = 1.35$, (b) $\theta = 1^\circ$, $U_d = 40$ meV, $\gamma_f = 1.35$, (c) $\theta = 1^\circ$, $U_d = 40$ meV, $\gamma_f = 1$, (d) $\theta = 2^\circ$, $U_d = 40$ meV, $\gamma_f = 1.35$ and (e) $\theta = 3^\circ$, $U_d = 40$ meV, $\gamma_f = 1$. (f) Chern numbers of the lowest conduction and valence bands (C_{C1}, C_{V1}) as a function of angle θ and exchange field strength γ_f, where $U_d = 40$ meV is set. (g) (C_{C1}, C_{V1}) for $\theta = 1^\circ$ as a function of γ_f and staggered layer potential U_d.



FM: need $C_{2x}\mathcal{T}$ symmetry breaking

Staggered layer potential

Platform for fractionalized QAH

Flat Chern band from twisted bilayer MnBi2Te4: AFM

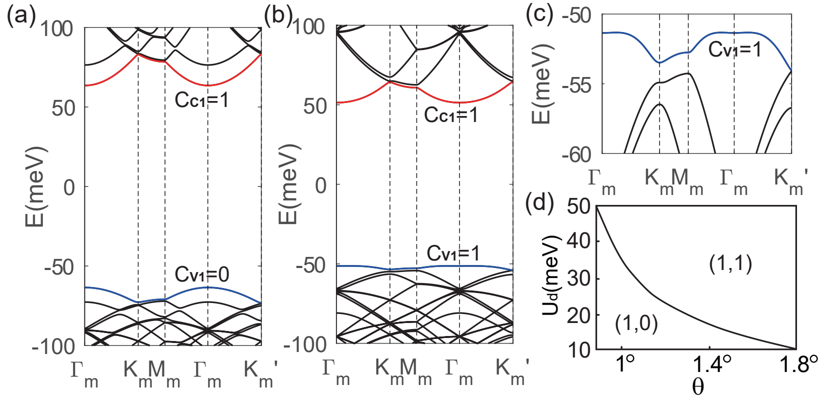
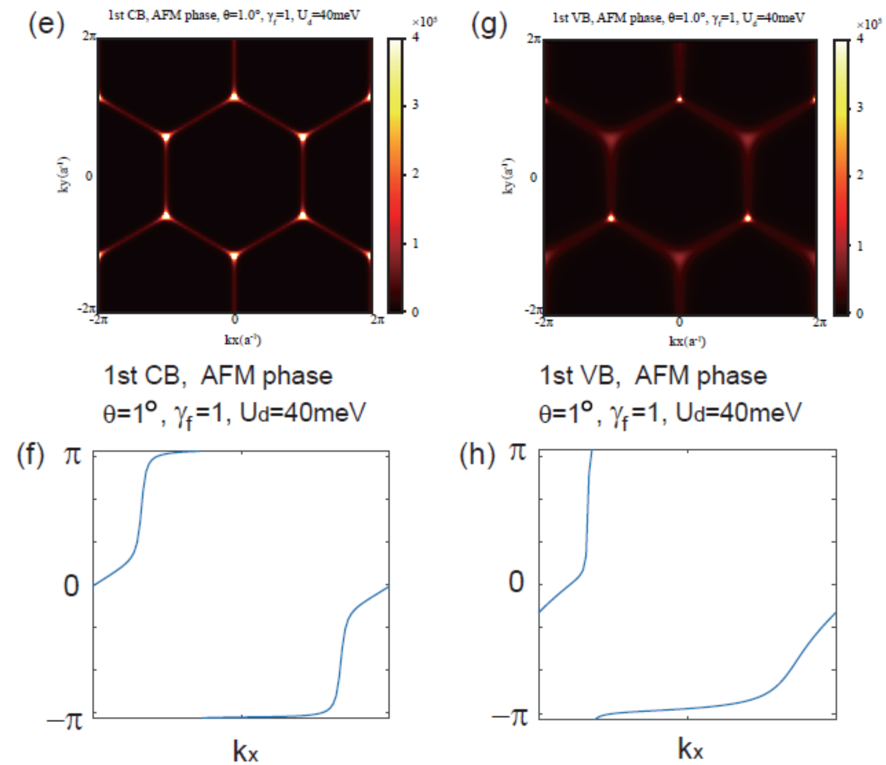
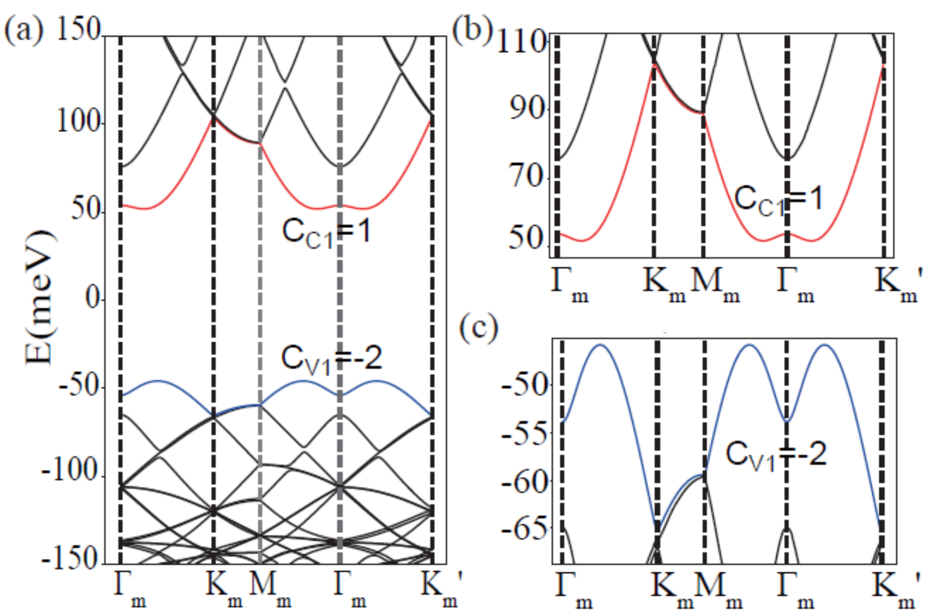


FIG. 3. The band structure of the AFM tBMBT for (a) $\theta = 1^\circ$, $\gamma_{af} = 1$, $U_d = 10$ meV, and (b) $\theta = 1^\circ$, $\gamma_{af} = 1$, $U_d = 40$ meV. (c) Zoom-in plot of the valence band structure in (b), showing the bandwidth of the first valence band. (d) (C_{C1}, C_{V1}) as a function of the twist angle θ and the staggered layer potential U_d.



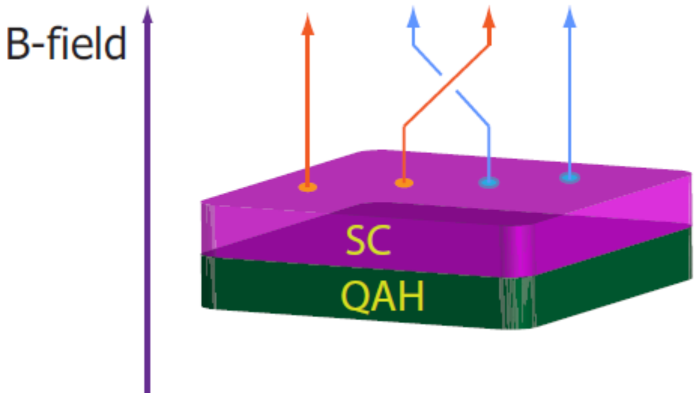


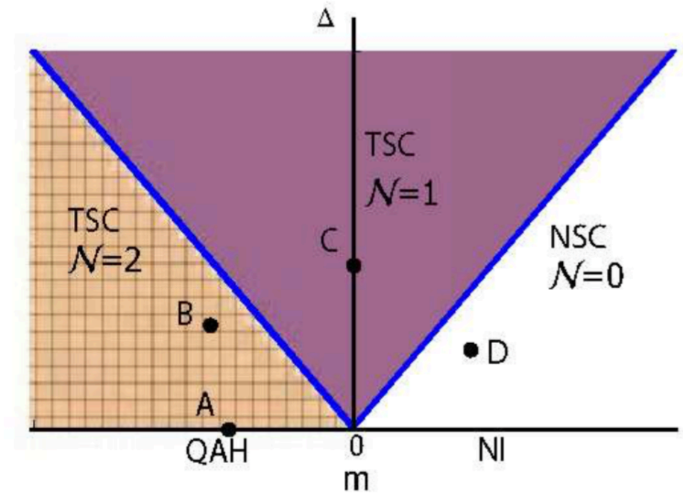
AFM: need C_{2x} symmetry breaking

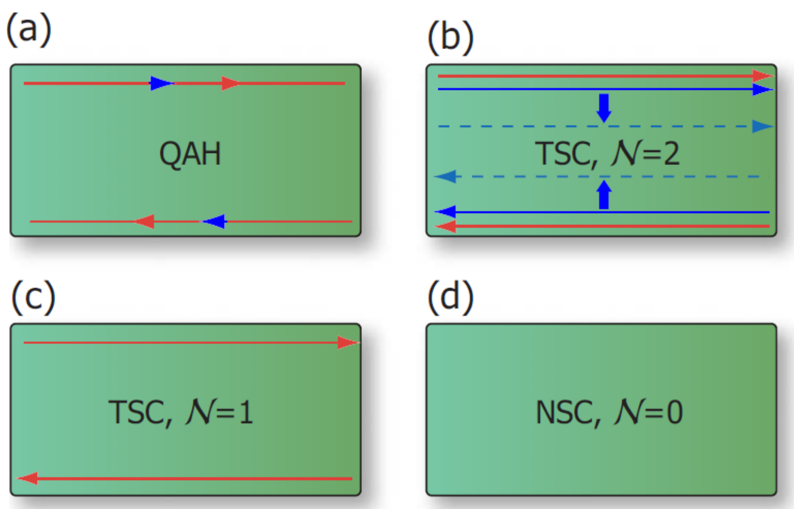
Staggered layer potential

Chiral topological superconductivity from QAH

X L Qi *et al*, PRB **82**, 184516 (2010); J Wang *et al*, PRB **92**, 064520 (2015)







$$h_{\mathrm{QAH}}(\mathbf{p}) = \begin{pmatrix} m(p) & A(p_x - ip_y) \\ A(p_x + ip_y) & -m(p) \end{pmatrix}$$

$$H_{\mathrm{BdG}} = \frac{1}{2}\sum_{\mathbf{p}} \Psi_{\mathbf{p}}^{\dagger} \begin{pmatrix} h_{\mathrm{QAH}}(\mathbf{p}) - \mu & i\Delta\sigma^{y} \\ -i\Delta^{*}\sigma^{y} & -h_{\mathrm{QAH}}^{*}(-\mathbf{p}) + \mu \end{pmatrix} \Psi_{\mathbf{p}}$$

As one sweep the magnetic field, there is NECESSARY an intermediate phase with chiral topological superconductivity!

Outlook

1. Zero-field QAH at higher temperature.
2. TME and axion electrodyanmics from even SL MnBi2Te4.
3. Flat Chern bands in twisted bilayer MnBi2Te4, promising for fractionalized QAH.
4. QAH/SC heterostructure for chiral Majorana fermion.

Bulk (AFM)	Bulk (FM)	Odd layer film	Even layer film
AFM TI	Minimal Weyl semimetal	QAH effect	axion insulator, zero Hall plateau
gapped Dirac SS (T dependent)	Fermi arc	chiral edge states	TME, image monopole

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	Yijun Yu		Shou-Cheng Zhang
	Yujun Deng		

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National Key Research Program of China

应用表面物理国家重点实验室

STATE KEY LABORATORY OF SURFACE PHYSICS

Thank you for your attention!