Quantum anomalous Hall states on decorated magnetic surfaces

David Vanderbilt
Rutgers University

Kevin Garrity & D.V.
Phys. Rev. Lett.**110**, 116802 (2013)

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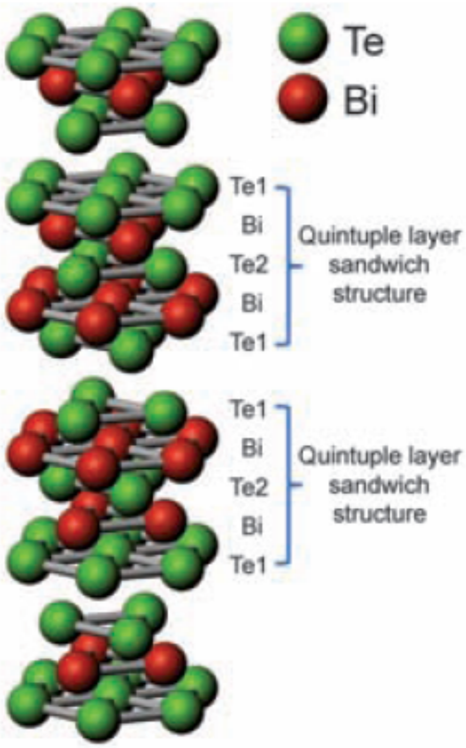
ISSP Theory Seminar, Tokyo, June 7, 2013

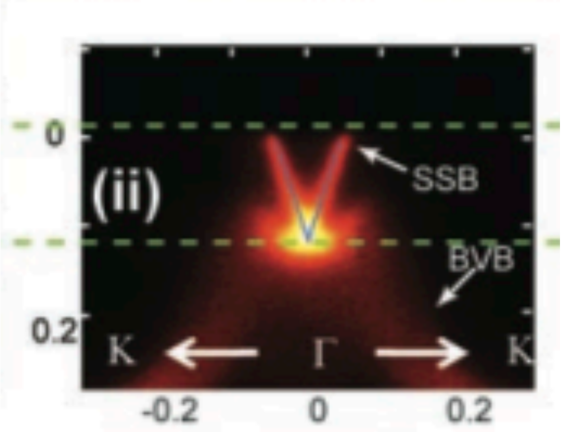
Recently: Topological insulators (TR-invariant)

Experimental Realization of a Three-Dimensional Topological Insulator, Bi 2Te3
Y. L. Chen, *et al.*
Science **325**, 178 (2009);
DOI: 10.1126/science.1173034

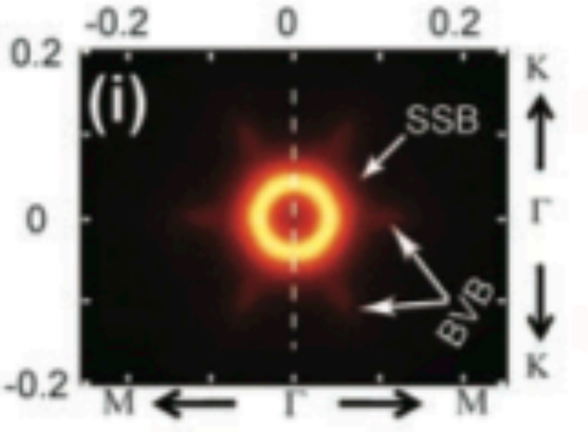


Photoemission

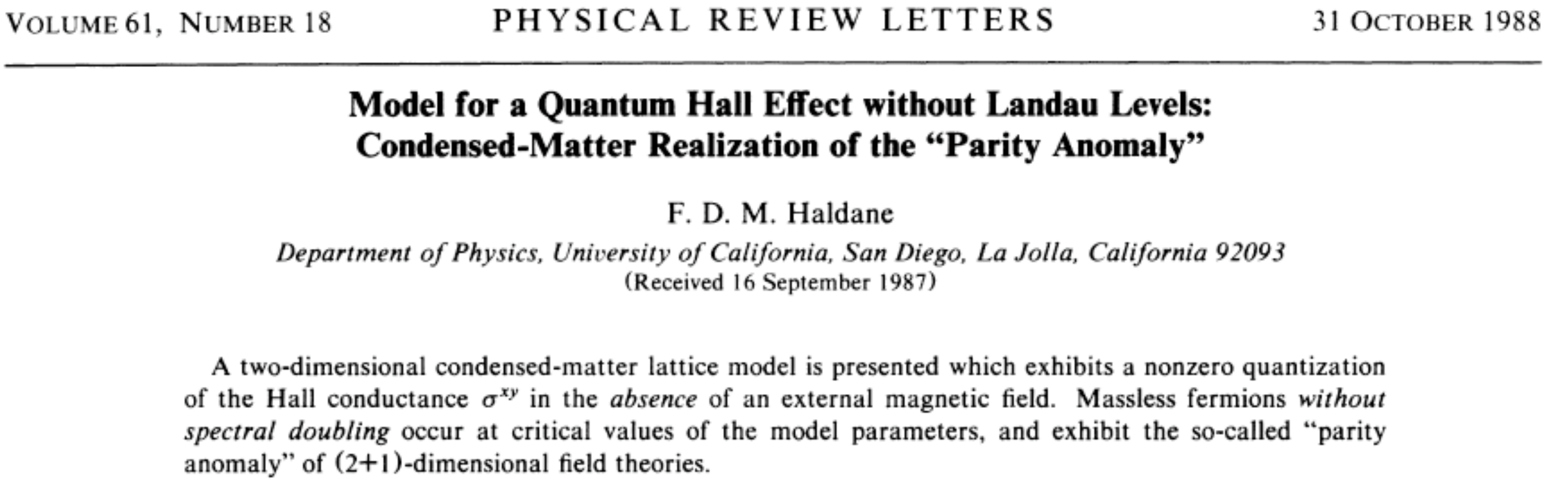
$I(E,k)$



$I(E_F;k_x,k_y)$



1988: QAH insulator (TR-broken)



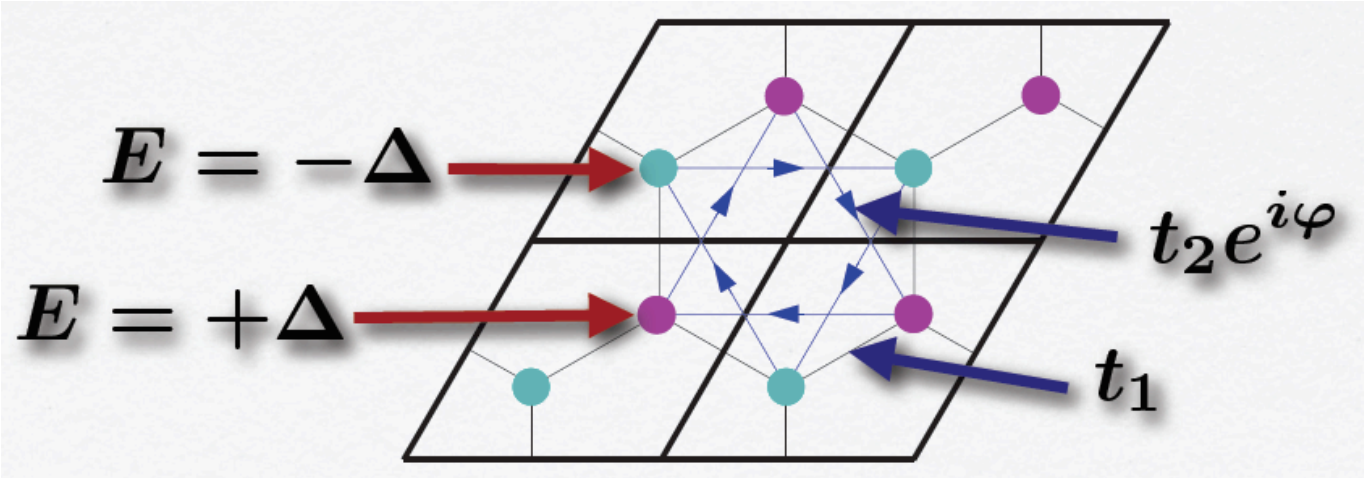
VOLUME 61, NUMBER 18 PHYSICAL REVIEW LETTERS 31 OCTOBER 1988

**Model for a Quantum Hall Effect without Landau Levels:
Condensed-Matter Realization of the "Parity Anomaly"**

F. D. M. Haldane
Department of Physics, University of California, San Diego, La Jolla, California 92093

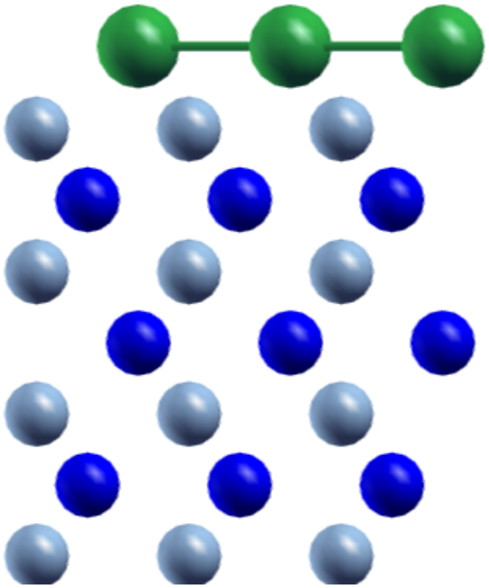
(Received 16 September 1987)

A two-dimensional condensed-matter lattice model is presented which exhibits a nonzero quantization of the Hall conductance σ^{xy} in the *absence* of an external magnetic field. Massless fermions *without spectral doubling* occur at critical values of the model parameters, and exhibit the so-called "parity anomaly" of (2+1)-dimensional field theories.

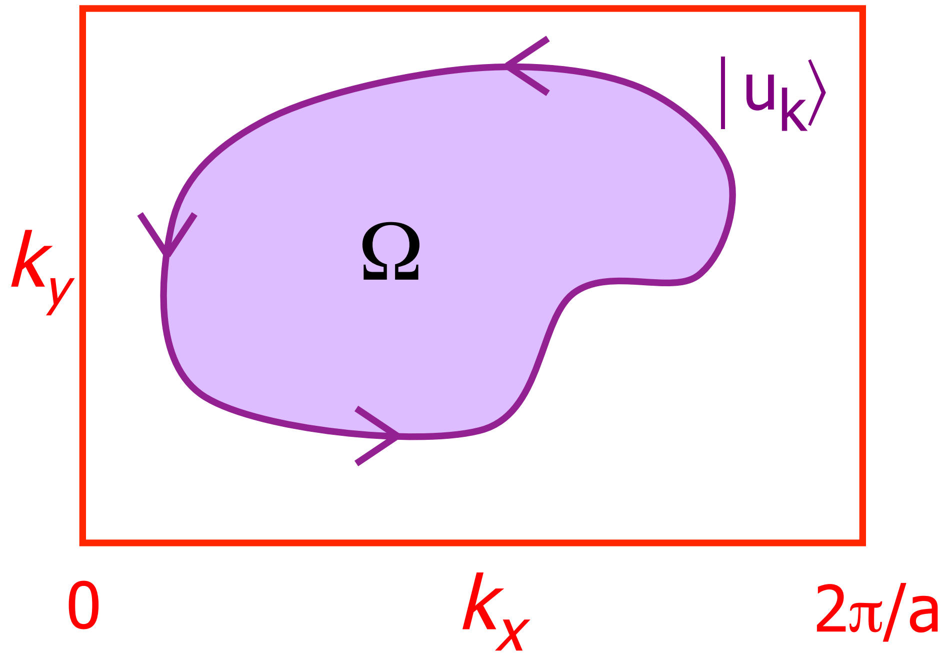


Outline

- Quick review: QAH (Chern) insulators
- Realization on decorated magnetic surfaces?
  - Propose specific realization
  - First-principles calculations
  - Some success
  - Discuss problems and possible solutions



Berry curvature in the Brillouin zone



$$\Omega_z(\mathbf{k}) = -2\,\mathrm{Im}\left\langle \frac{du}{dk_x}\middle|\frac{du}{dk_y}\right\rangle$$

$$\phi = \int_{\mathrm{FS}} \Omega_z(\mathbf{k})\, d^2k$$

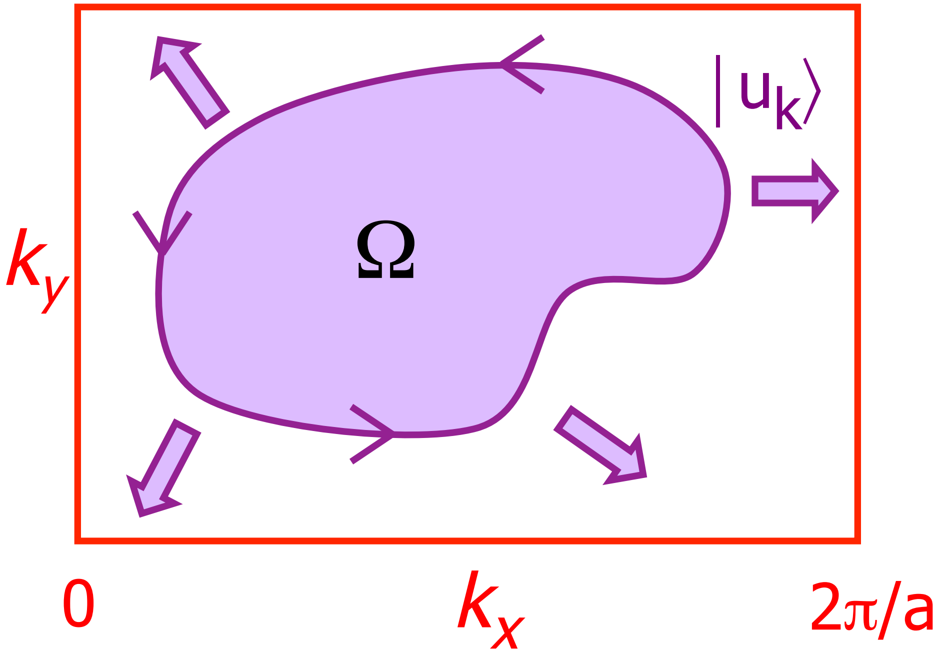
Metal

Anomalous Hall conductivity:

$$\sigma_{xy} = \frac{-e^2}{2\pi h}\,\phi$$

Karplus and Luttinger; Sundaram and Niu

Berry curvature in the Brillouin zone



$$\boxed{\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x}\middle|\frac{du}{dk_y}\right\rangle}$$

$$\phi = \int_{\mathrm{FS}} \Omega_z(\mathbf{k})\, d^2k$$

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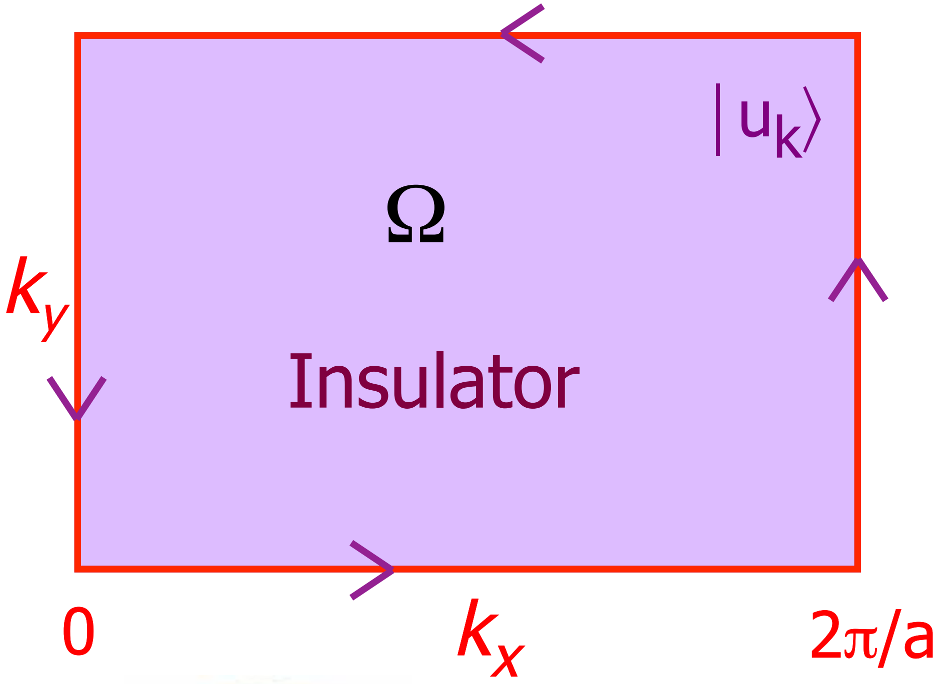
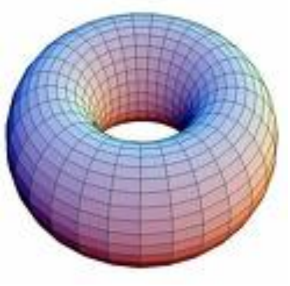


$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x}\middle|\frac{du}{dk_y}\right\rangle$$

$$\phi = \int_{BZ} \Omega_z(\mathbf{k})\, d^2k = 2\pi C$$



Quantum Anomalous Hall: $$\boxed{\sigma_{xy} = \frac{-e^2}{h} C}$$

"Chern number" or "TKNN invariant"

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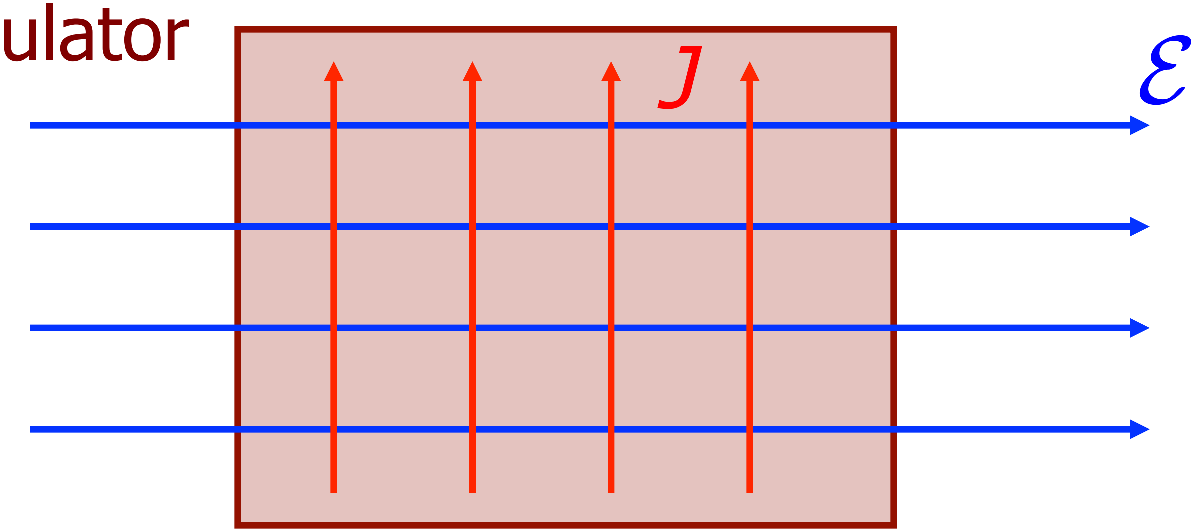
Quantum anomalous Hall effect

Ferromagnetic
insulator

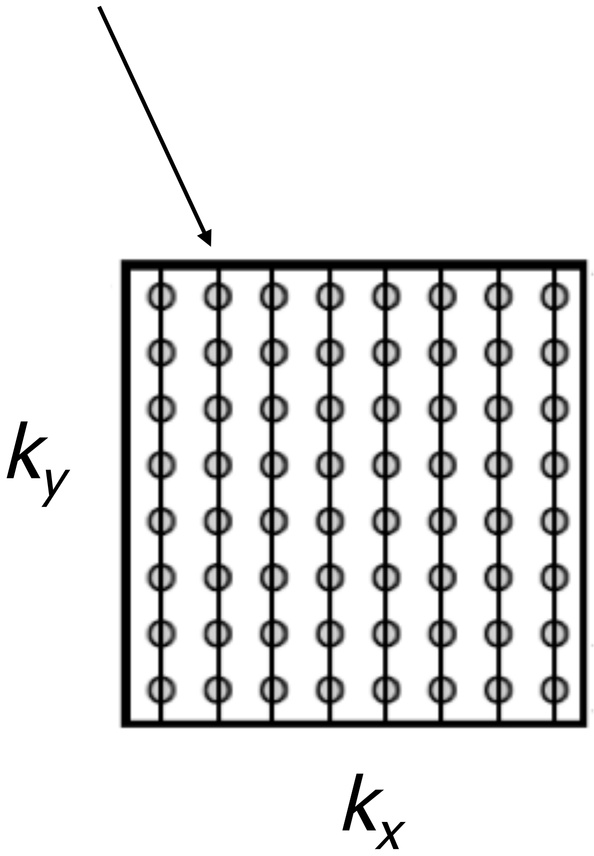


$\sigma_{xy} \neq 0$

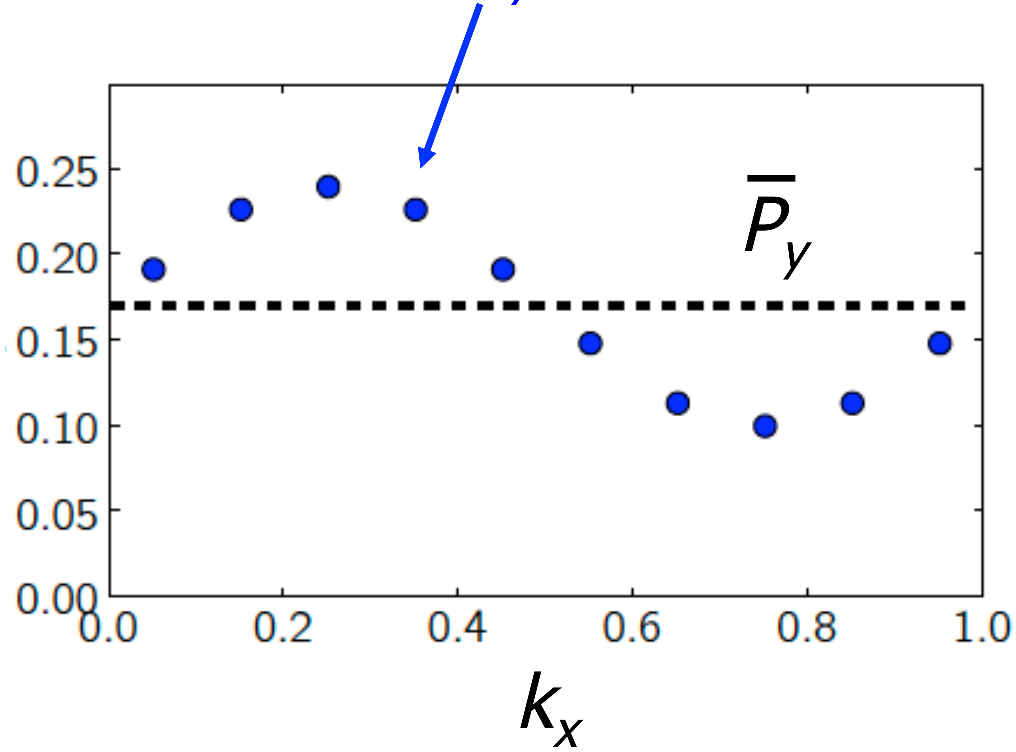
Like integer quantum Hall, but no B_{ext}

String Berry phases for normal band

$$\phi(k_x) = -\mathrm{Im}\ln\left[\langle u_1|u_2\rangle\langle u_2|u_3\rangle\ldots\langle u_{n-1}|u_n\rangle\right]$$

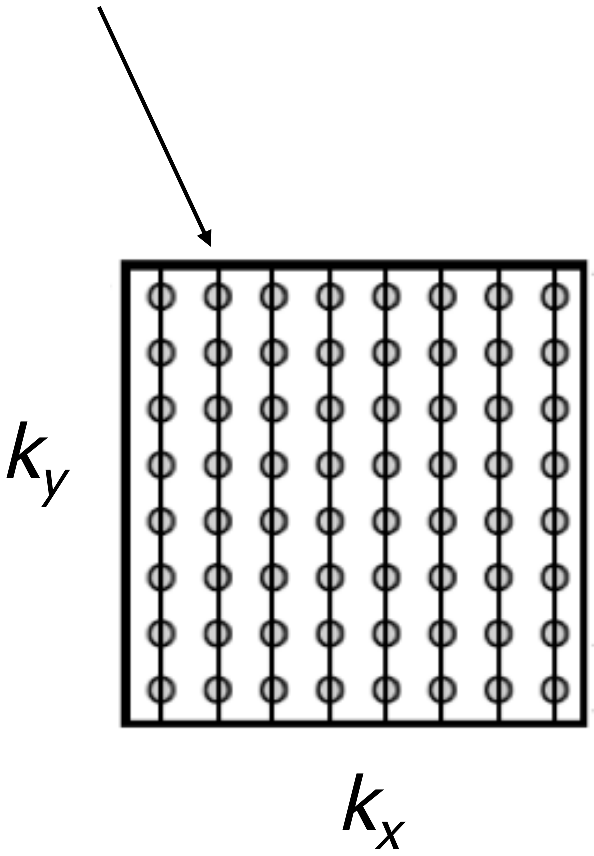


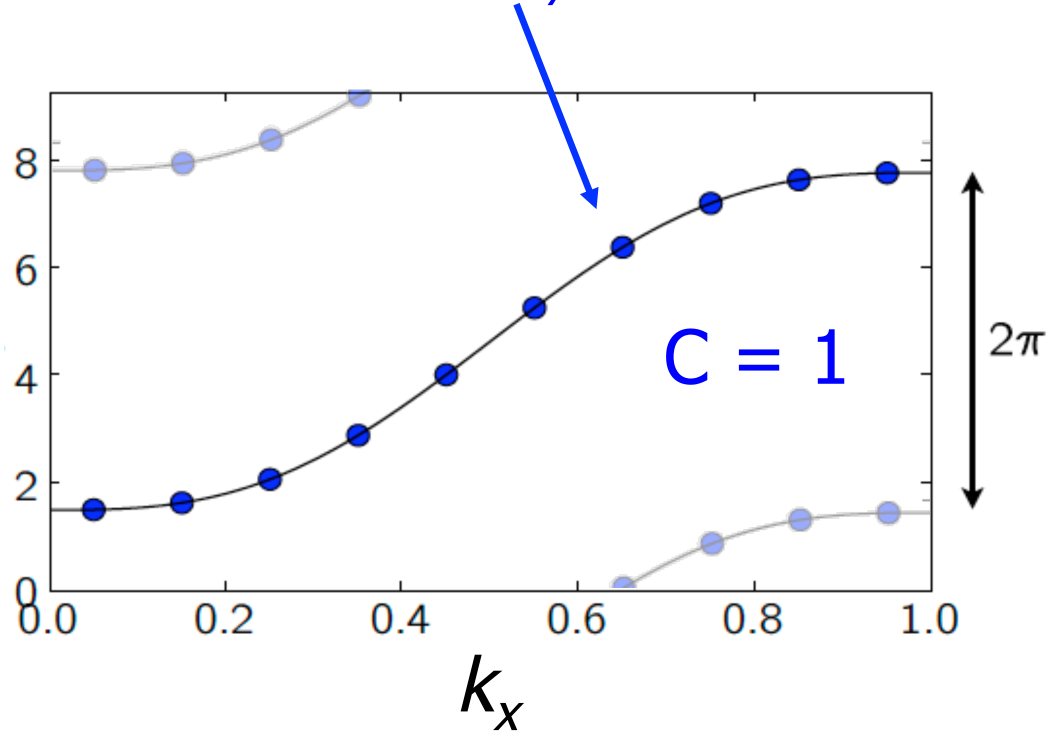
$P_y(k_x) \propto \phi(k_x)$



String Berry phases in QAH band

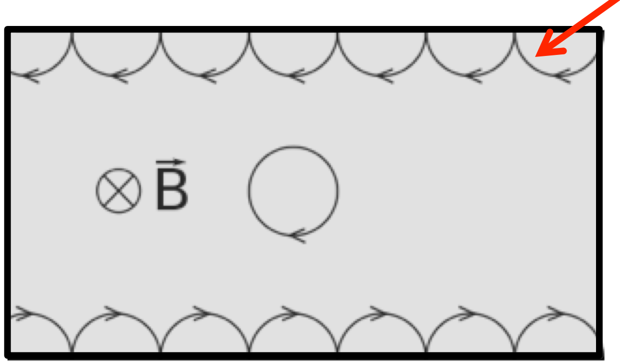
$$\phi(k_x) = -\mathrm{Im}\,\ln\left[\langle u_1|u_2\rangle\langle u_2|u_3\rangle\ldots\langle u_{n-1}|u_n\rangle\right]$$




$P_y(k_x) \propto \phi(k_x)$

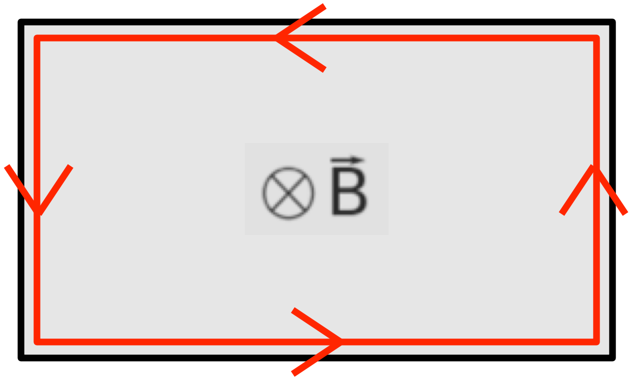
Quantum Hall effect

- Semiclassical picture:



Skipping orbits
(edge states)

- Quantum picture:



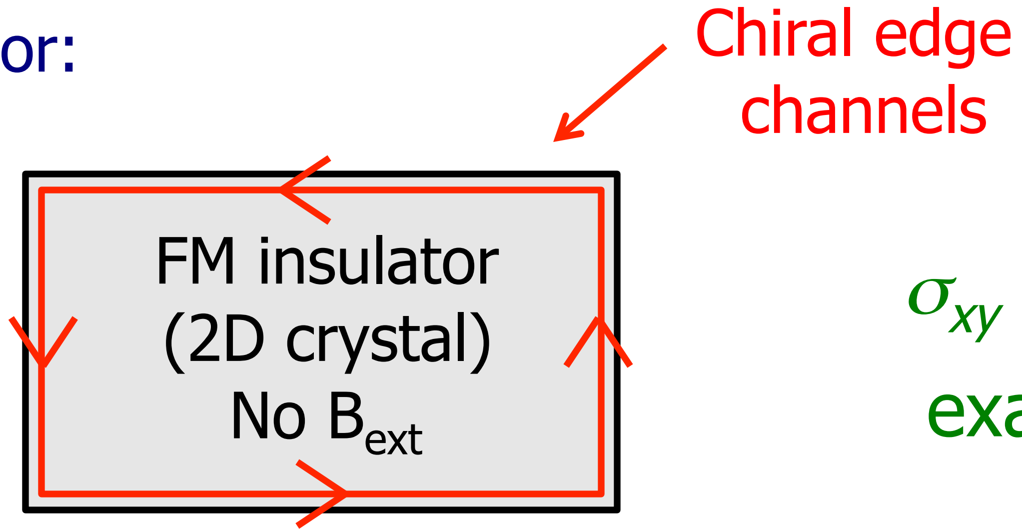
Chiral edge
channels

σ_{xy} = e^2/h

exactly !

Quantum anomalous Hall effect

- QAH insulator:



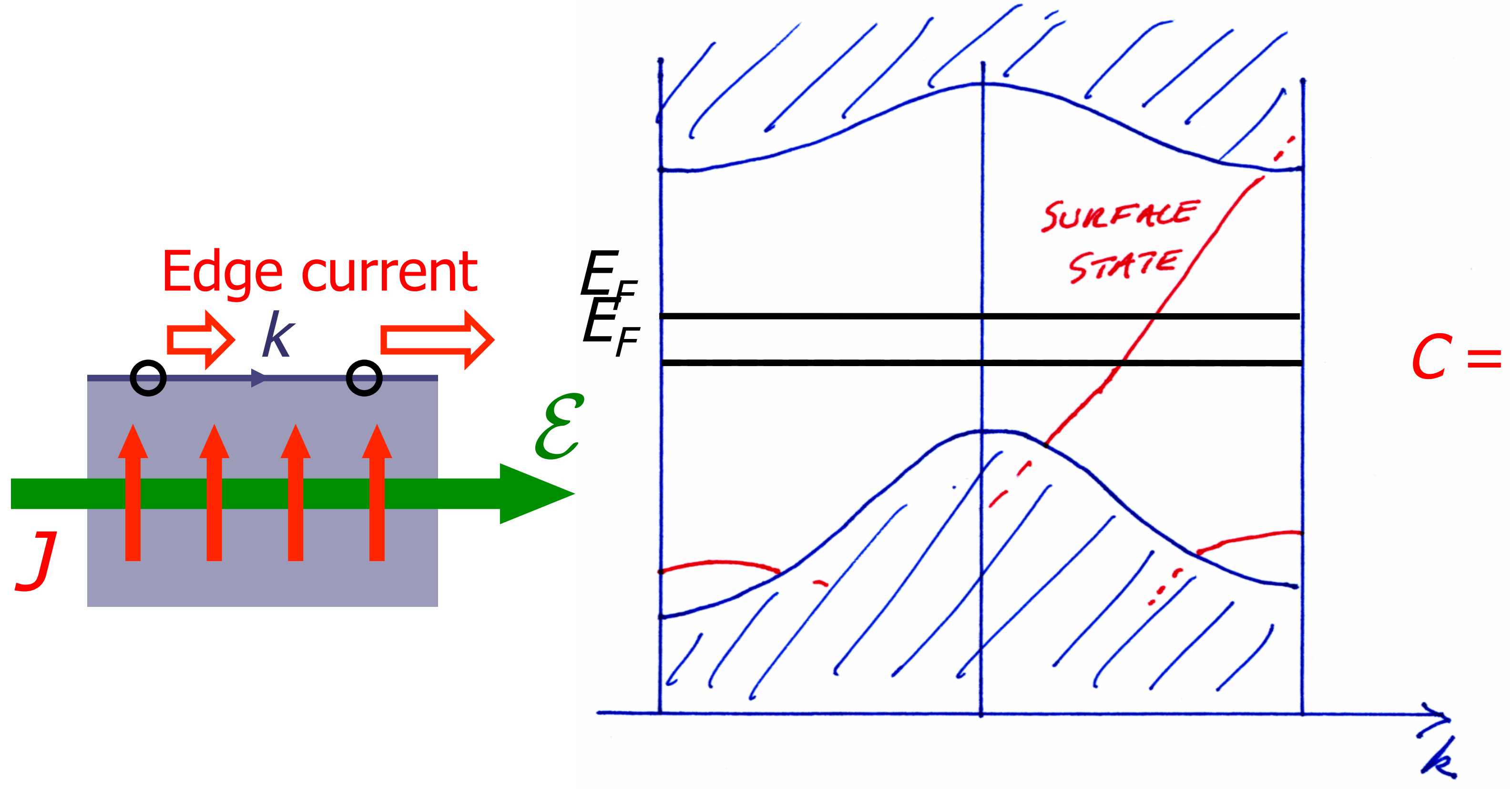
Chiral edge channels

FM insulator
(2D crystal)
No B_{ext}

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

exactly !

Edge states: 2D QAH insulator



$C = +1$

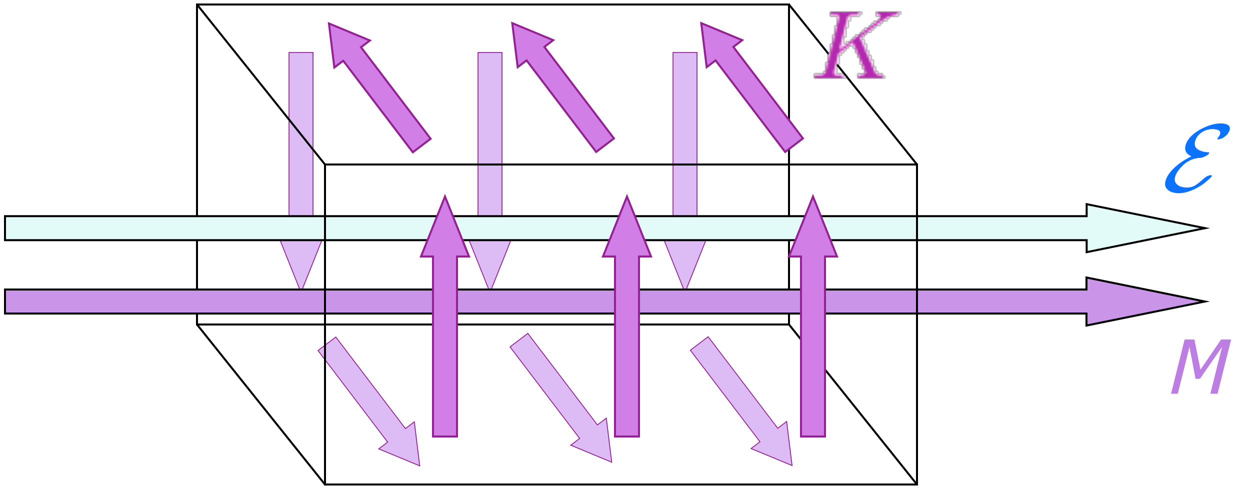
Conservation of charge $\Rightarrow$ chiral surface state

Bulk-boundary correspondence

QAH insulators

- “QAH insulator” = “Chern insulator”
- Quantized Hall conductance even in the absence of macroscopic magnetic fields
- Quite possibly at room temperature
- Usefulness:
  - Precision measurement?
  - Dissipationless “wires” for microelectronics?
  - Magnetoelectric coupling?

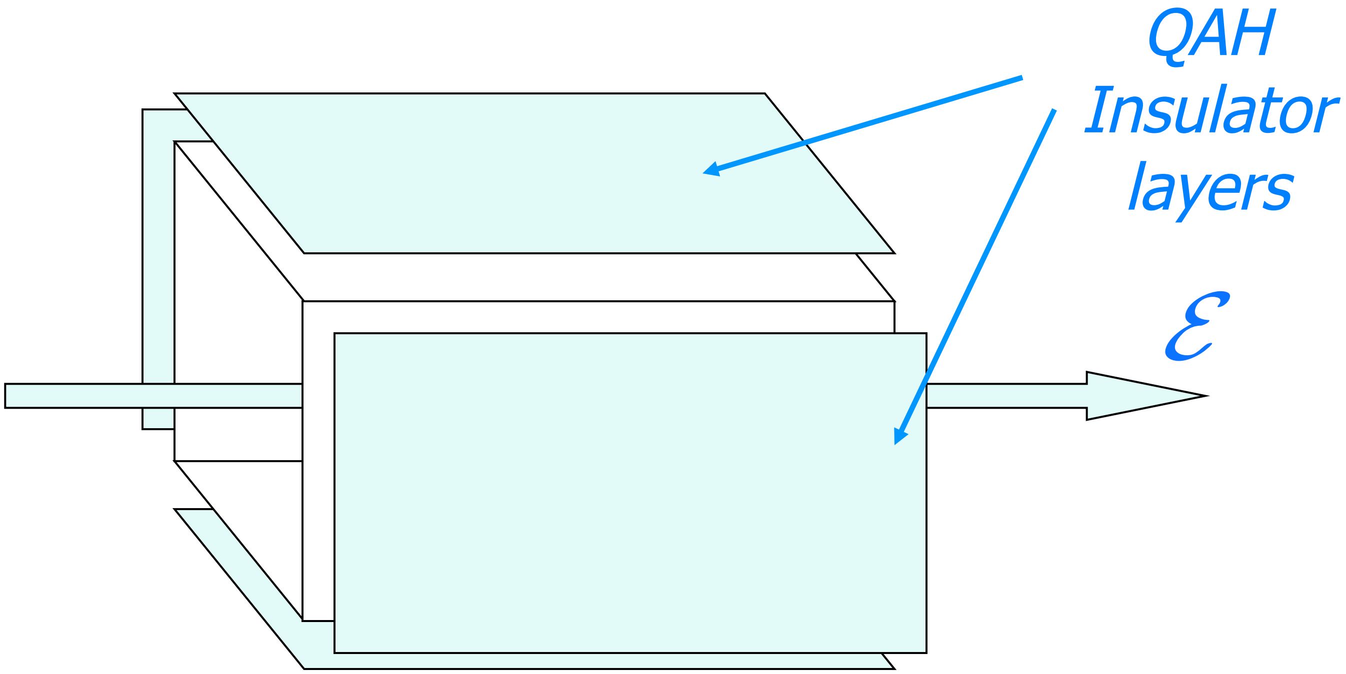
Orbital MEC ↔ Surface dissipationless σ_{xy}



Interpret magnetization $= M = K$

$$\mathbf{K} = \sigma_{\mathbf{xy}} \vec{\mathcal{E}} \times \hat{\mathbf{n}}$$

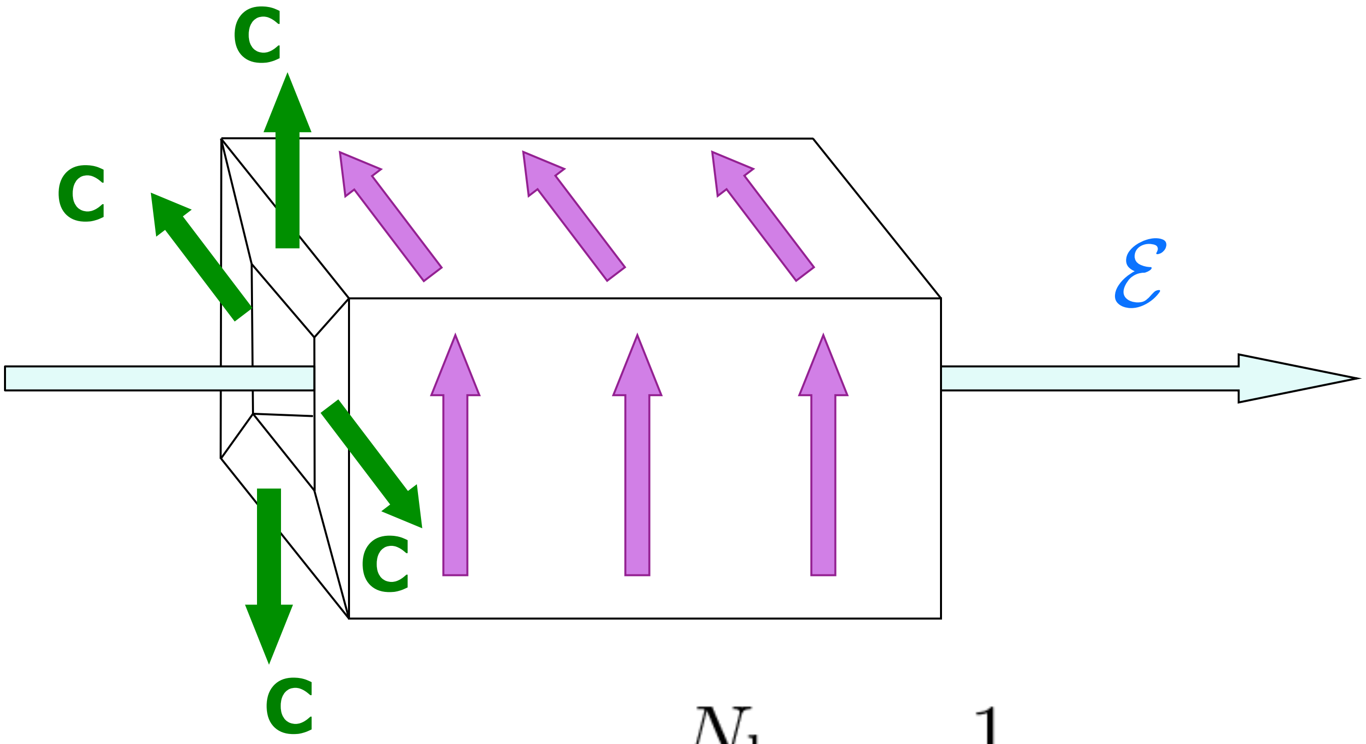
How to build a magnetoelectric coupler



Mag-elec coupling is $\alpha = \dfrac{dP}{dH} = \dfrac{dM}{d\mathcal{E}} = \dfrac{e^2}{h} = \dfrac{1}{2\pi}\dfrac{1}{137}$ g.u.

For comparison, Cr_2O_3 has $\alpha \simeq 10^{-4}$ g.u.

How to build a magnetoelectric coupler



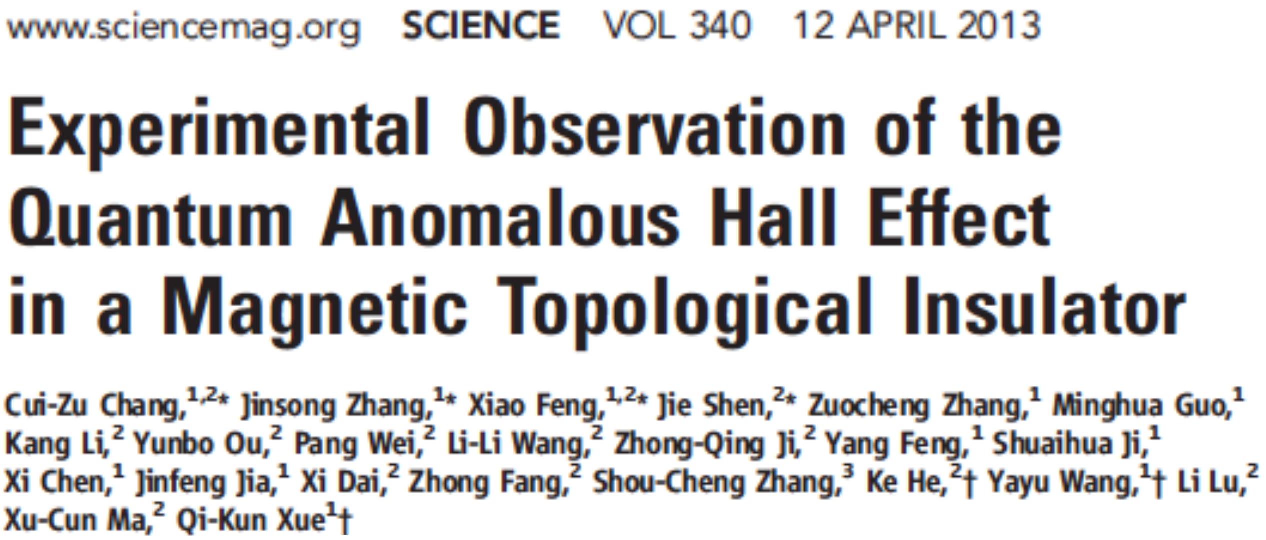
$$\alpha = \frac{N_{\text{layers}}}{2\pi}\frac{1}{137}\ \text{g.u.}$$

This can easily be 10^6 times that of Cr_2O_3 !

Can QAH insulators be found?

- Requirements
  - Spontaneously broken TR (FM or FiM)
  - Insulator
  - Strong spin-orbit splitting
- Prefer gap > 0.2 eV (Q Hall at T_{room})
- Proposals
  - Magnetically doped TR-invariant TI’s
  - Magnetic adatoms on graphene
  - 2D adlayer on a magnetic insulator

Magnetic doping: Claim for QAH



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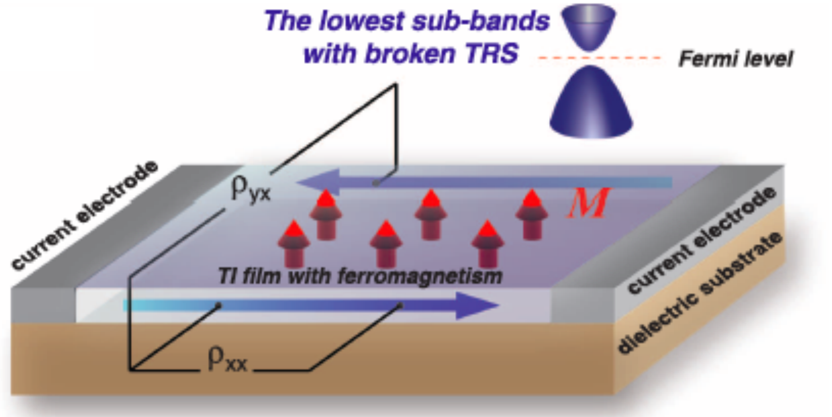
Experimental Observation of the Quantum Anomalous Hall Effect in a Magnetic Topological Insulator

Cui-Zu Chang,[1,2]* Jinsong Zhang,[1]* Xiao Feng,[1,2]* Jie Shen,[2]* Zuocheng Zhang,[1] Minghua Guo,[1]
Kang Li,[2] Yunbo Ou,[2] Pang Wei,[2] Li-Li Wang,[2] Zhong-Qing Ji,[2] Yang Feng,[1] Shuaihua Ji,[1]
Xi Chen,[1] Jinfeng Jia,[1] Xi Dai,[2] Zhong Fang,[2] Shou-Cheng Zhang,[3] Ke He,[2]† Yayu Wang,[1]† Li Lu,[2]
Xu-Cun Ma,[2] Qi-Kun Xue[1]†



Observed below ~1K

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Our strategy

Heavy atoms

-Large spin-orbit

Magnetic insulator

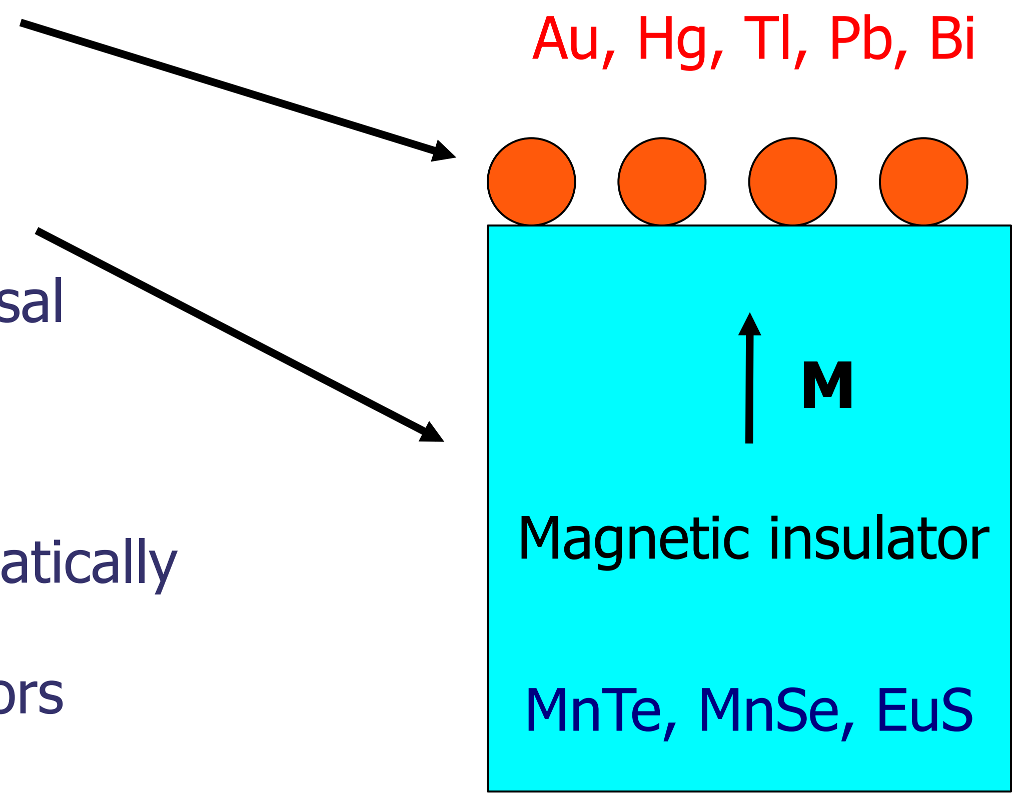
-Breaks time reversal
-FM or A-type AFM

Advantages:

-Spins align automatically
-No doping
-Large gap insulators
-Large spin-orbit

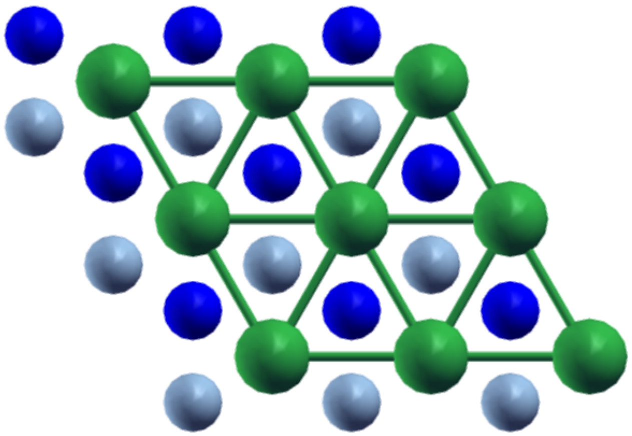
Disadvantages:

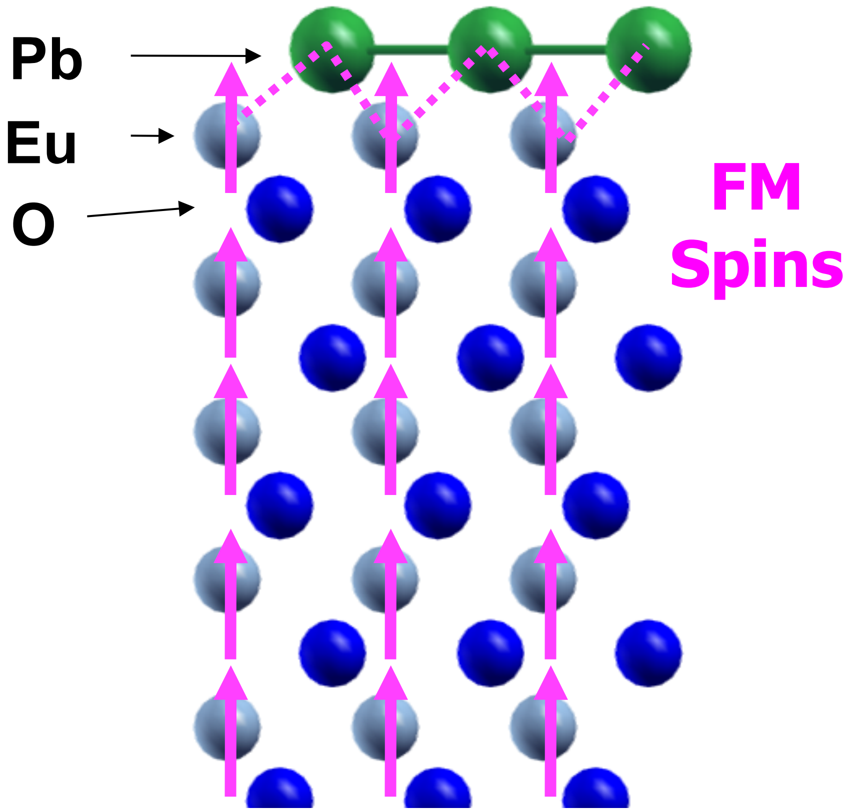
-Preparing surfaces is difficult



Our surface systems

- MnTe or MnSe or EuO
- Monolayer of heavy atoms
- Direct contact with magnetic ions





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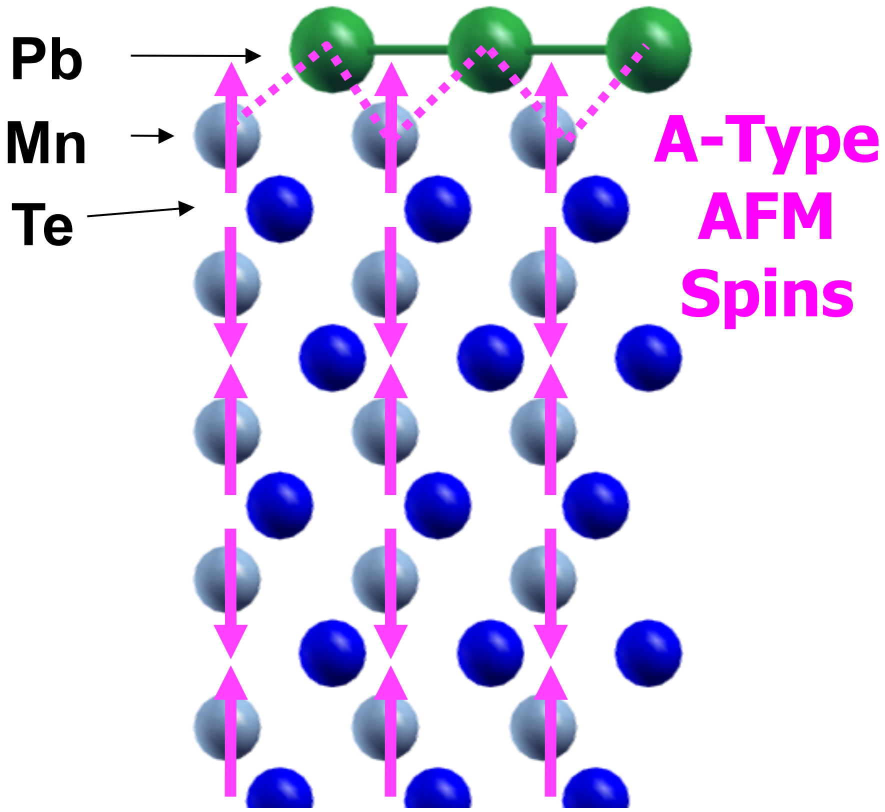

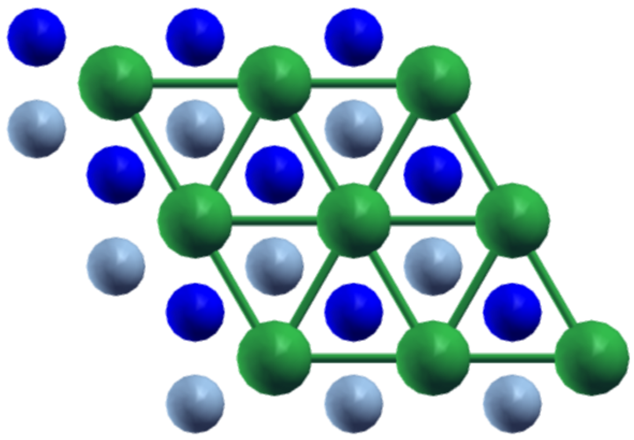

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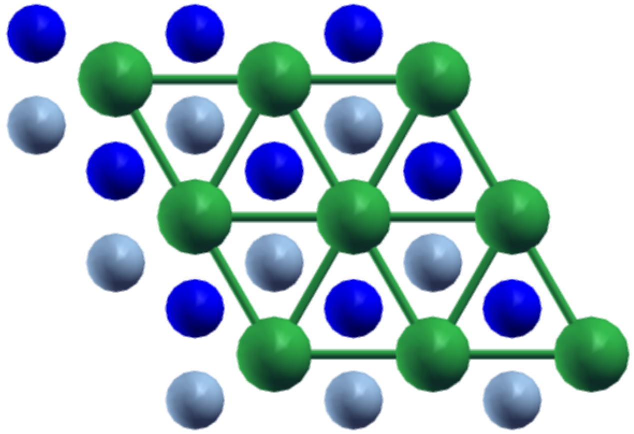
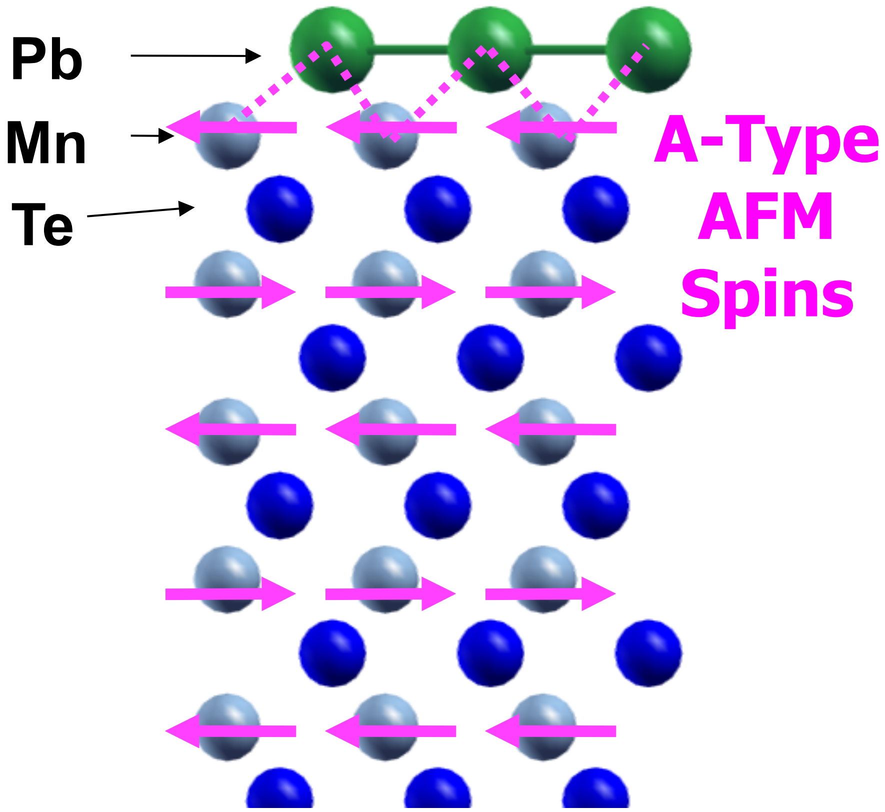




Calculation Details

- Quantum Espresso with OPIUM norm-conserving potentials
- VASP PAW's
- LDA + U
  - U=5 eV for Mn, 6 eV for Eu
- wannier90 → Interpolation to compute Chern numbers

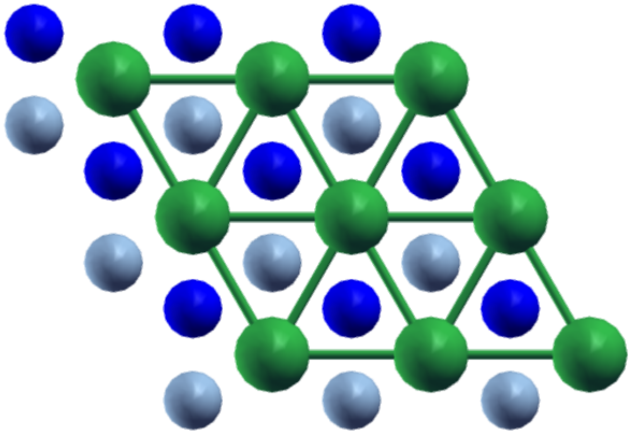
$$C = \frac{1}{2\pi}\int_{\mathrm{BZ}} d\mathbf{k}\,\Omega(\mathbf{k}) = \frac{1}{2\pi}\oint_{\mathrm{BZ}} d\mathbf{k}\cdot\mathbf{A}(\mathbf{k})$$

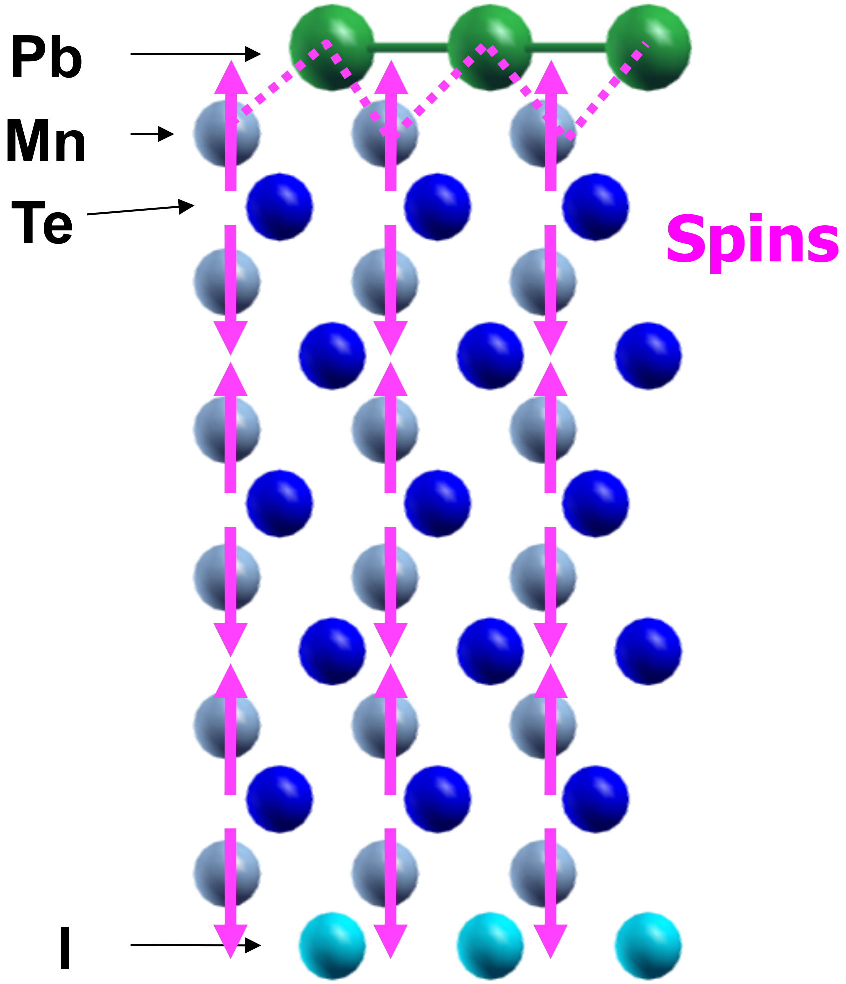
- wannier90 post-processing code AHC[1-2]

[1] Wang *et. al.* PRB 74 195118 (2006)
[2] Wang *et. al.* PRB 76 195109 (2007)

Attempt I: One ML heavy atoms

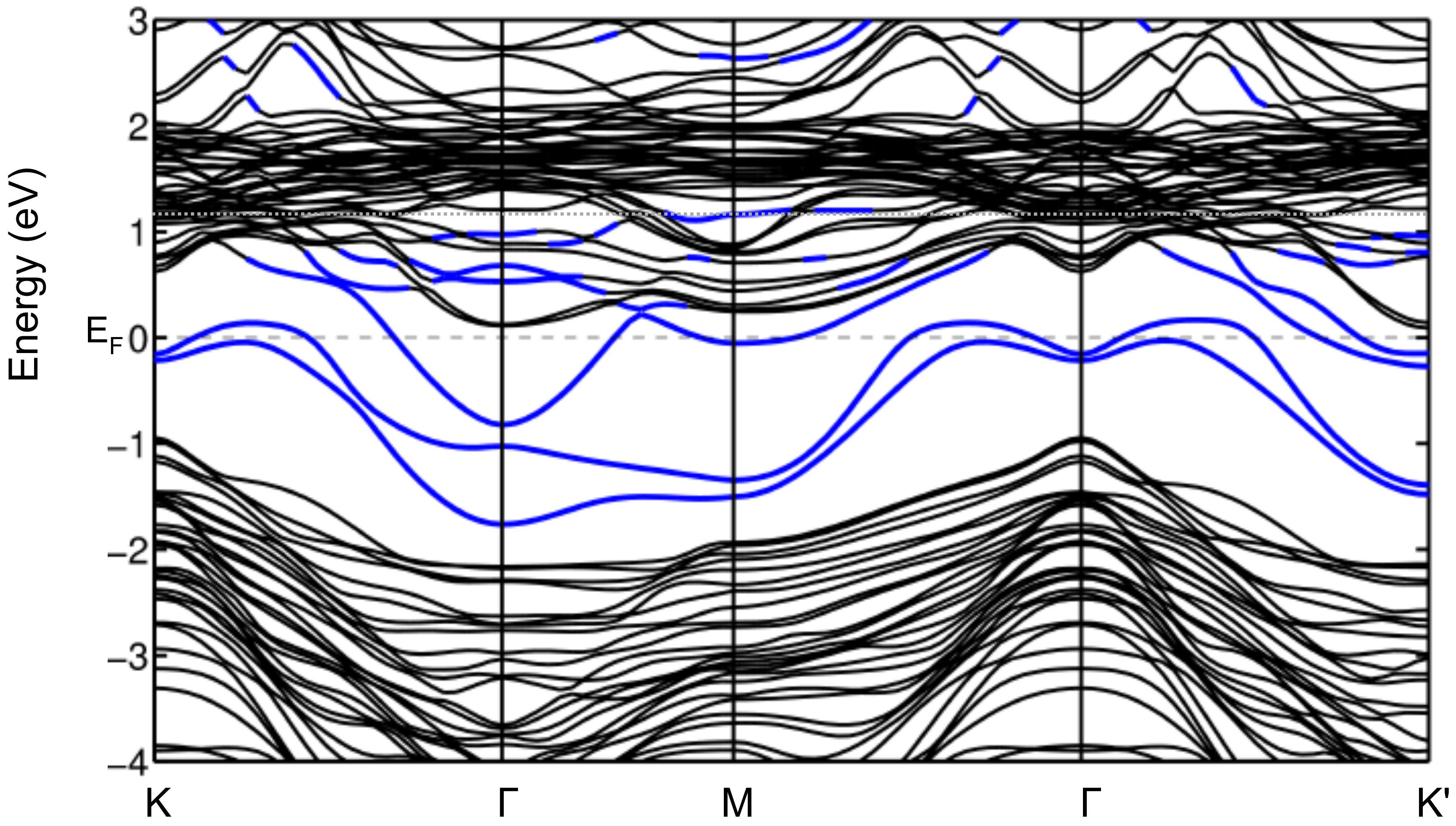
- 6 layers MnTe
- 1 ML heavy atom
  - Directly on Mn
- Polar surface
- (Bottom: 1 ML iodine)





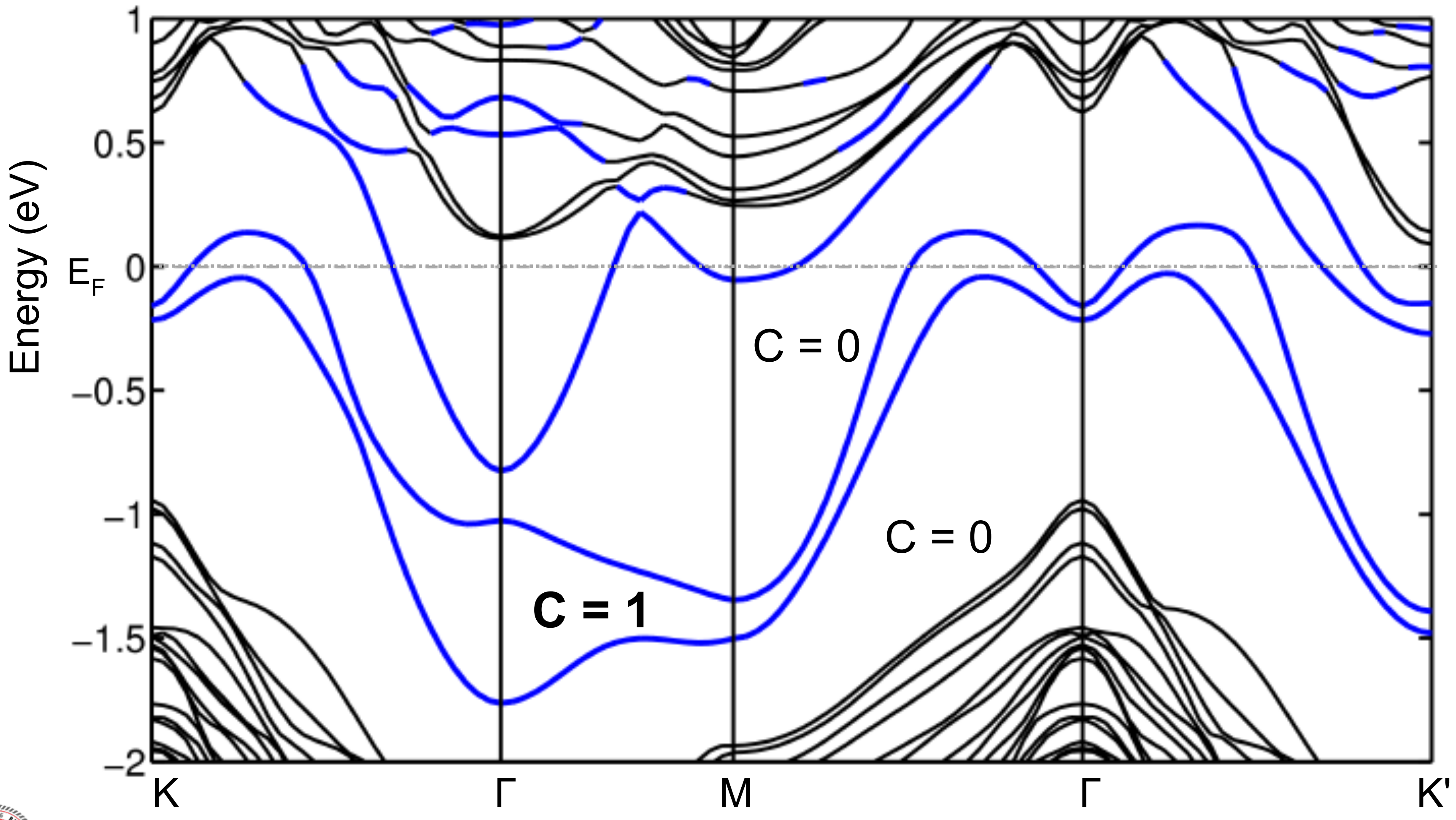
1 ML Tl on MnTe

Surface Band Structure



1 ML Tl on MnTe

Surface Band Structure – Zoomed In



Three observations

- Non-zero Chern numbers are common
  - Provided E_{hop}, E_{SO} and E_{mag} are at similar scale
- Bands are generically isolated in 2D
  - SO + broken TR = no symmetry-induced degeneracies
  - No accidental degeneracies
    - Avoided crossing: $H_{2x2} = f_0 I + f_x \sigma_x + f_y \sigma_y + f_z \sigma_z$
    - Degeneracy requires $f_x = f_y = f_z = 0$ (codim=3)
- However, if E_{hop} is too large, there is no global gap

Attempt II: 1/3 ML heavy atoms

Result:

- Bands tend to be flatter
- Global band gaps are easier to find
- But Chern numbers are typically all zero

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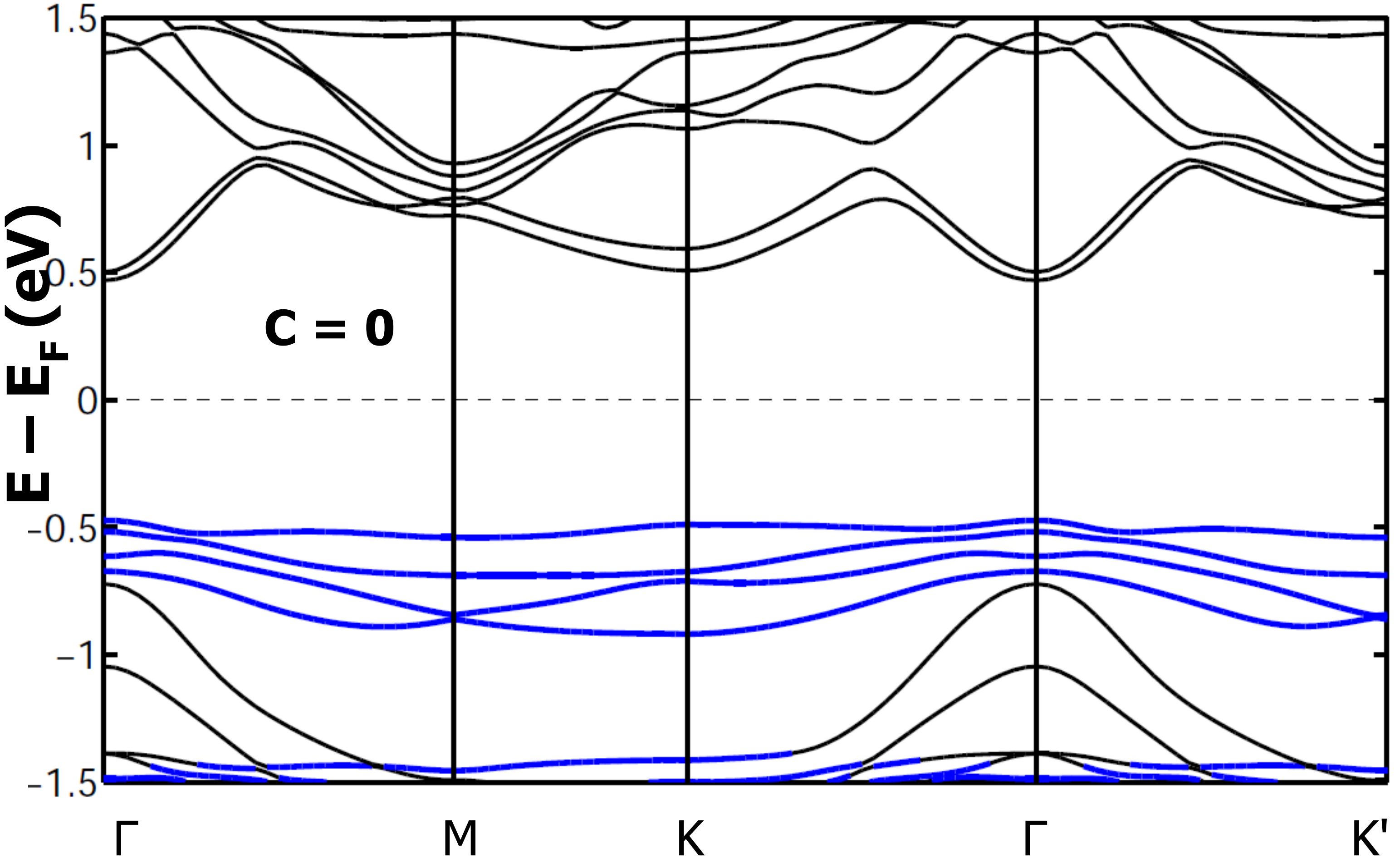
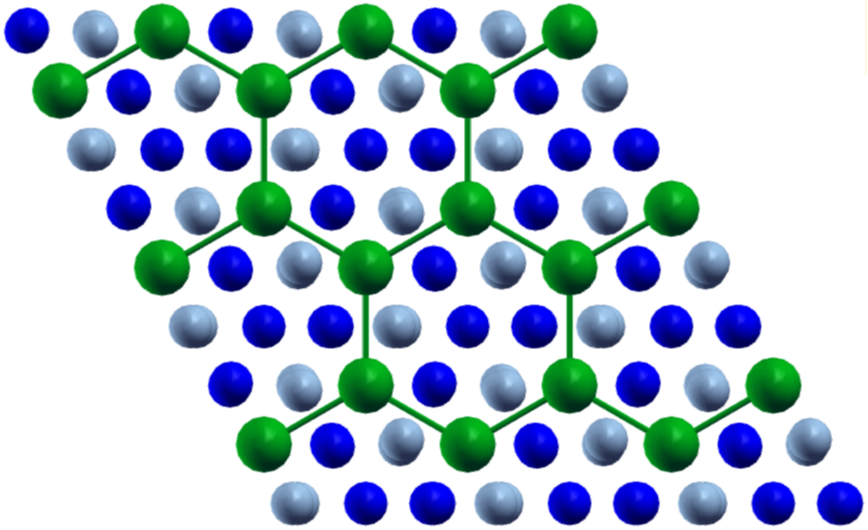
Attempt II: 1/3 ML heavy atoms

1/3 ML Bi on MnSe

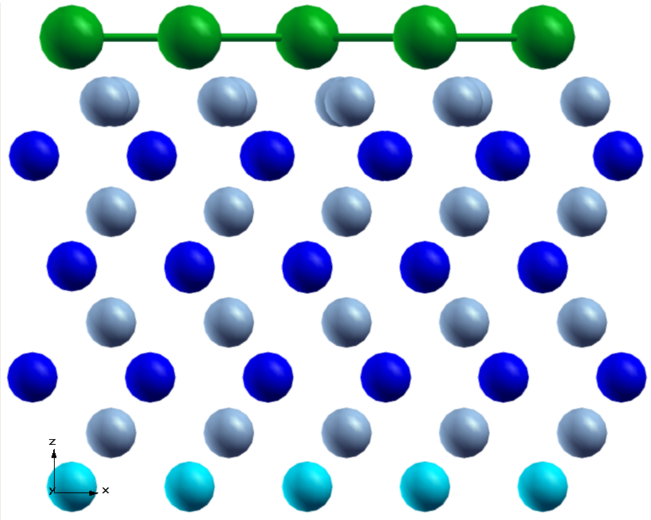


Attempt III: 2/3 ML honeycomb

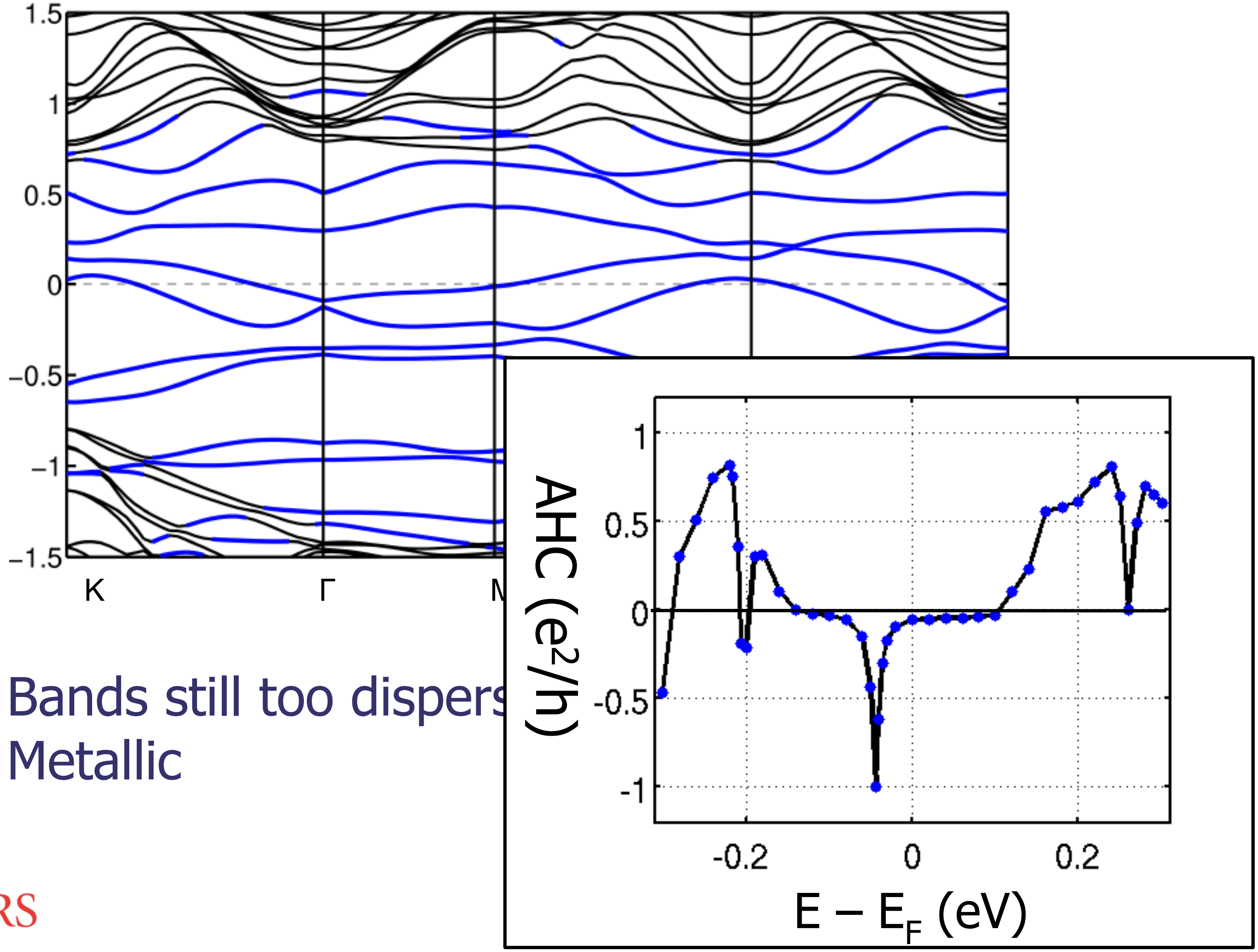
Top view



Side view

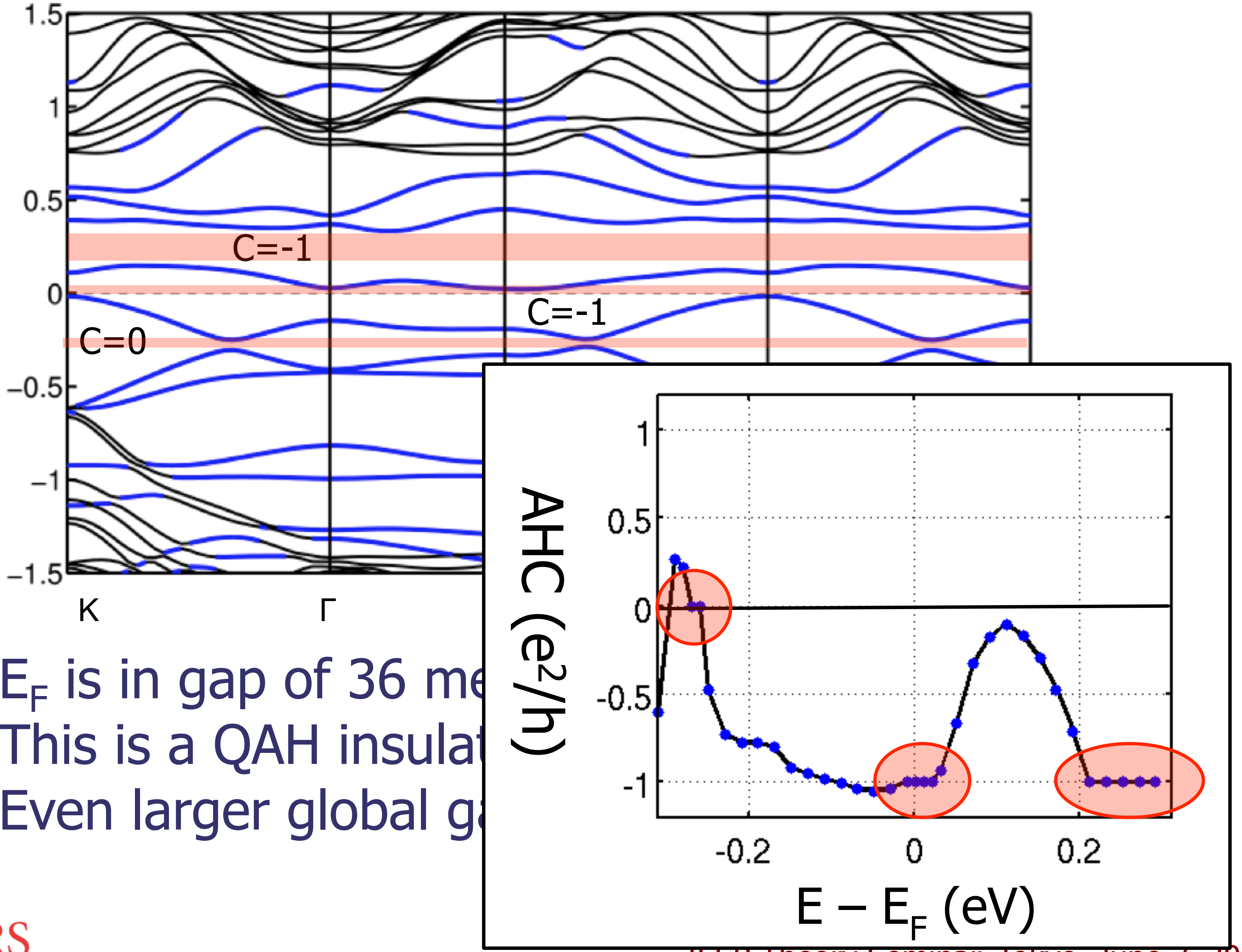


2/3 ML of Pb on MnTe – spins along *x*



- Bands still too dispers
- Metallic

2/3 ML of Pb on MnTe – spins along *z*



- E_F is in gap of 36 me
- This is a QAH insulat
- Even larger global ga

Can we align spins along z?

EuO (FM)

- Rocksalt structure
- Our surface is a (111) surface
- Spins prefer (111) directions
- Anisotropy is weak

Possible approach:

- Apply a weak Bext to fix spin direction?
- But not very satisfying…

Can we align spins along z?

MnTe (A-type AFM)

- NiAs structure
- Our surface is (0001)
- Spins prefer to lie in-plane!

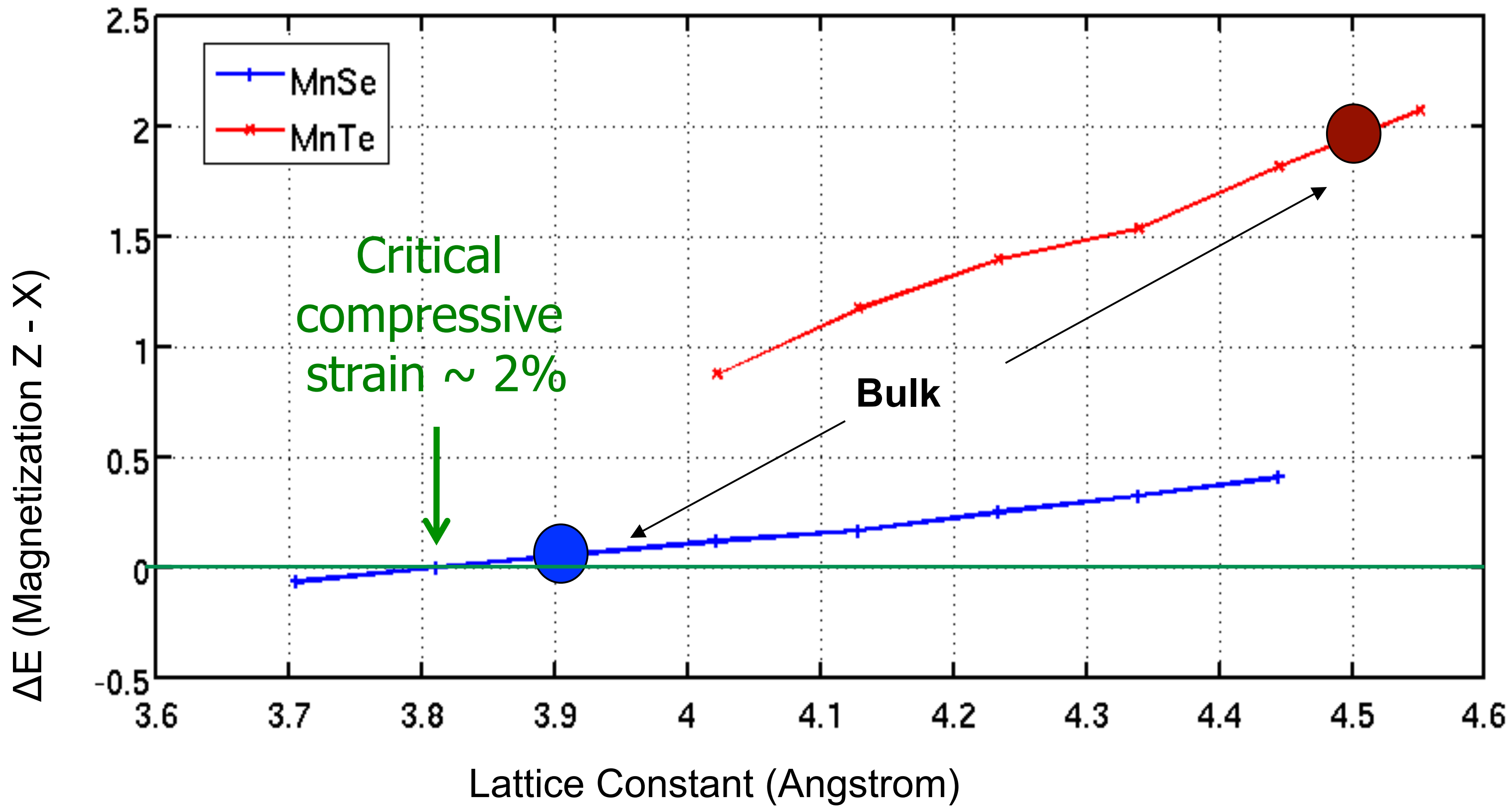
“That’s a bummer”

Can we align spins along z?

MnSe (A-type AFM)

- NiAs structure
- Our surface is (0001)
- Spins prefer to lie in-plane at equilibrium strain conditions
- But lie out-of-plane if…

Can we align spins along z?



Critical compressive strain ~ 2%

Bulk

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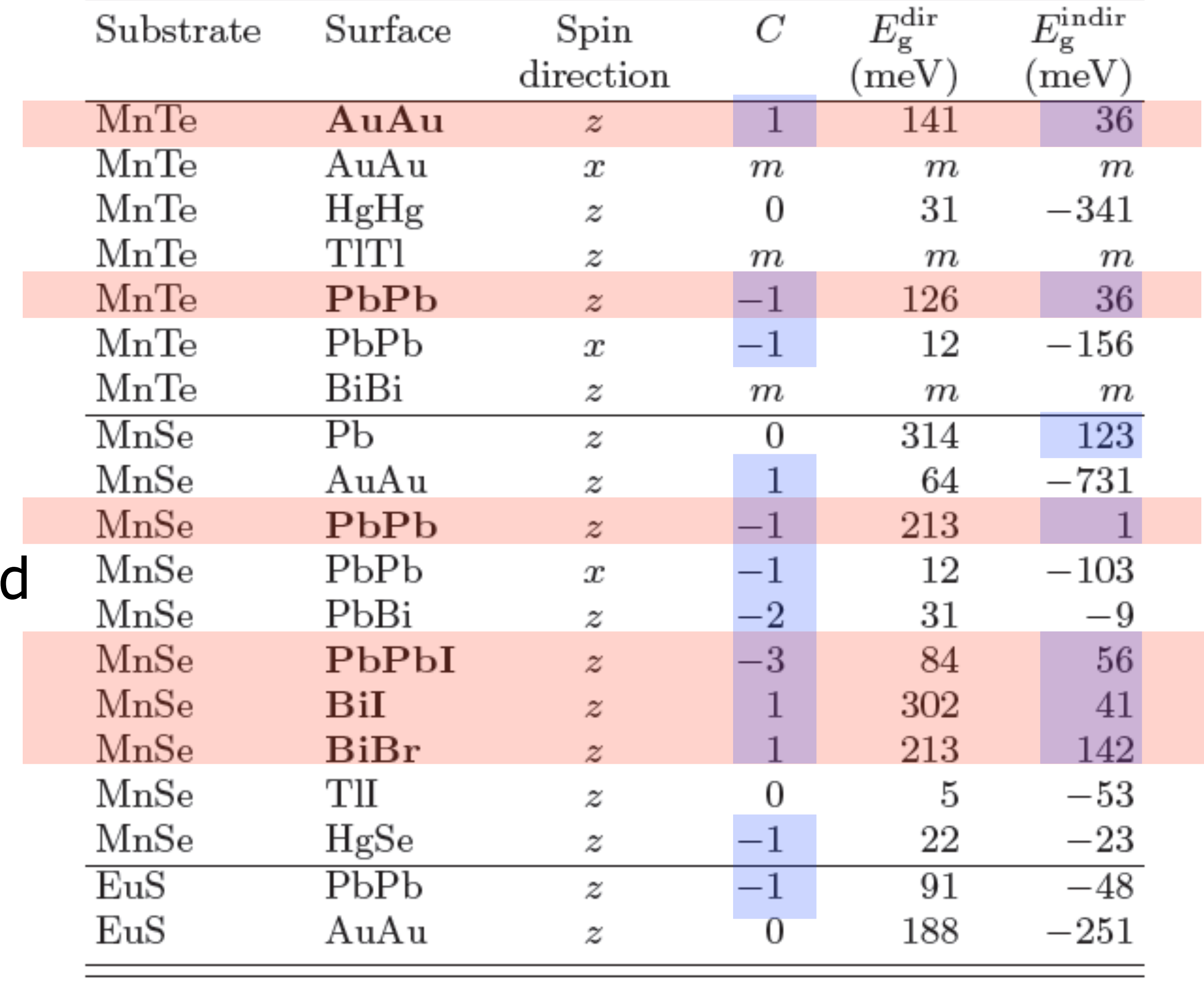
Search for Chern Insulators



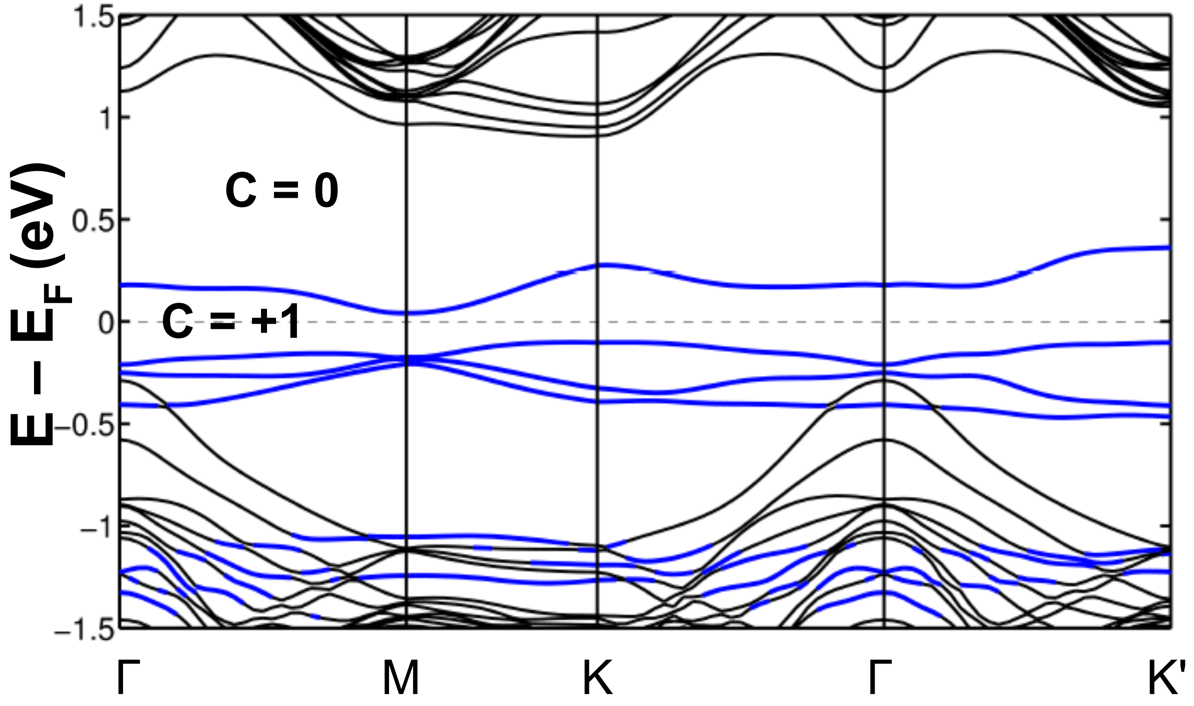
Substrate	Surface	Spin direction	C	E_g^{dir} (meV)	E_g^{indir} (meV)
MnTe	**AuAu**	z	1	141	36
MnTe	AuAu	x	m	m	m
MnTe	HgHg	z	0	31	−341
MnTe	TlTl	z	m	m	m
MnTe	**PbPb**	z	−1	126	36
MnTe	PbPb	x	−1	12	−156
MnTe	BiBi	z	m	m	m
MnSe	Pb	z	0	314	123
MnSe	AuAu	z	1	64	−731
MnSe	**PbPb**	z	−1	213	1
MnSe	PbPb	x	−1	12	−103
MnSe	PbBi	z	−2	31	−9
MnSe	**PbPbI**	z	−3	84	56
MnSe	**BiI**	z	1	302	41
MnSe	**BiBr**	z	1	213	142
MnSe	TlI	z	0	5	−53
MnSe	HgSe	z	−1	22	−23
EuS	PbPb	z	−1	91	−48
EuS	AuAu	z	0	188	−251

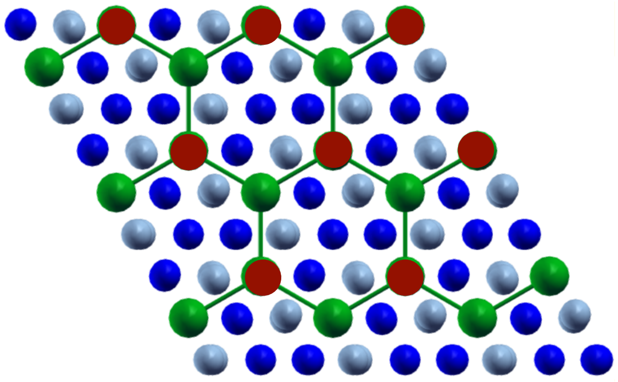
Strained -2%

For spins along z

Our champion to date

Bi/Br on MnSe: 142 meV gap





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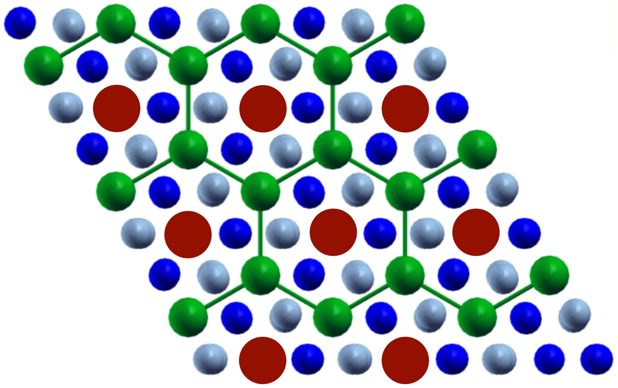
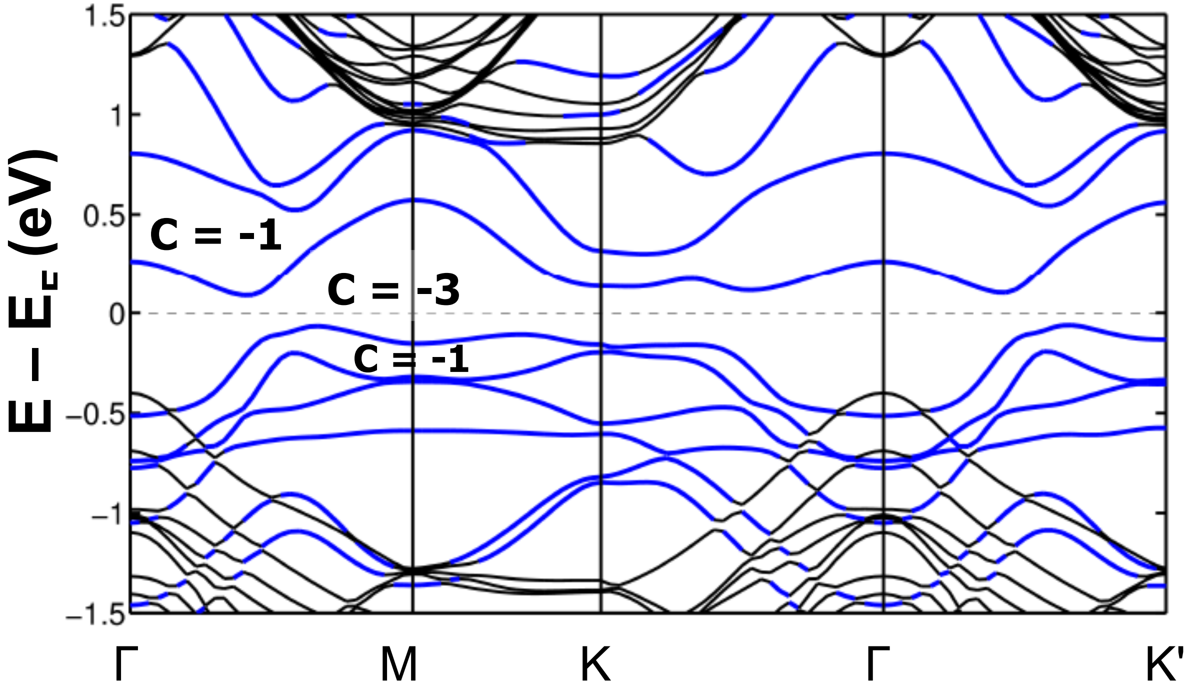
Another good candidate

PbPb/I on MnSe: 56 meV gap





Summary of strategy

- Heavy atoms + magnetic substrates
  - Isolated bands
  - Typically have Chern numbers
  - Problem is to find global gap
- First principles verification
  - For model structures, gaps of at least 0.14 eV are possible

Problems with our surfaces

- We prefer magnetic easy axis normal to surface
  - See earlier discussion
- Surfaces studied in current work have not been checked for thermodynamic instability
  - Atoms are relaxed etc.
  - But does metal layer wet?
  - Does desired coverage lie on convex hull?
  - Do surface reactions occur?
- Low-T growth might result in metastable structures…

Problems with our surfaces

- Adatoms (Pb, Bi) prefer (+) oxidation states
  - We are putting them in contact with magnetic cations (Mn or Eu), also in (+) oxidation states
  - This may not be realistic for thermodynamic stability

  Possible solution:
  - Coadsorption of anions (I, Br, …)

Surface search strategy?

- Find other surface systems?
  - Prefer spins normal to surface
  - FM, or AFM with uniform surface spins
  - Thermodynamically consistent with heavy-atom overlayers
- Experiment
  - Confirm ordered overlayer structure
  - Metallic? Measure σ_{xx}, σ_{xy} …
  - Insulating? Measure σ_{xy}!
- Work hand-in-hand with theory…

Summary and conclusions

- QAH insulator state
  - Predicted in 1988
  - Possible discovery in 2013
  - Seek large-gap examples for robust T_{room} operation
- Proposal for experimental realization
  - Heavy adatom layers on magnetic insulators
  - Proof-of-concept from first-principles calculations
  - Experimental realization still challenging