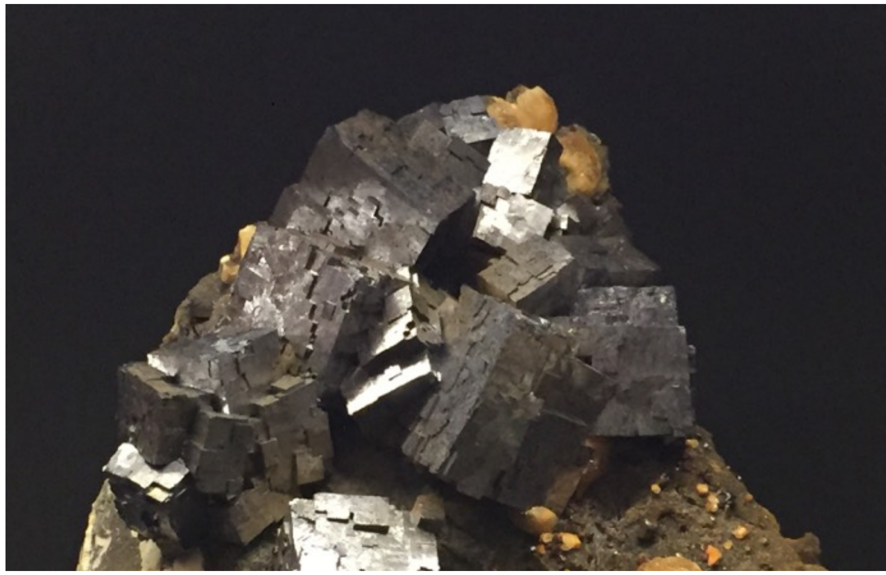
University of Zurich[UZH]

Titus Neupert

Yukawa Institute, Kyoto,
November 03, 2017





Higher order topological insulators

A paradigm for topological states of matter

$$\partial(\partial M) = \varnothing$$

(the boundary of a boundary is empty)

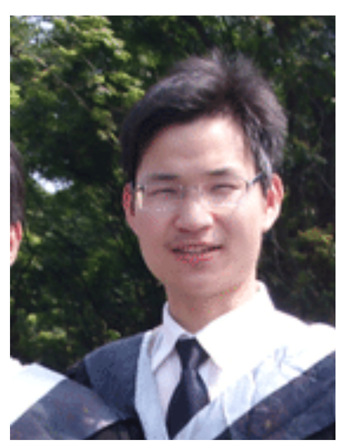
… works when things are sufficiently smooth.

Crystals have no smooth surface!

arXiv:1708.03636

Frank Schindler
(U Zurich)

Maia Vergniory
(Donostia)



Zhijun Wang
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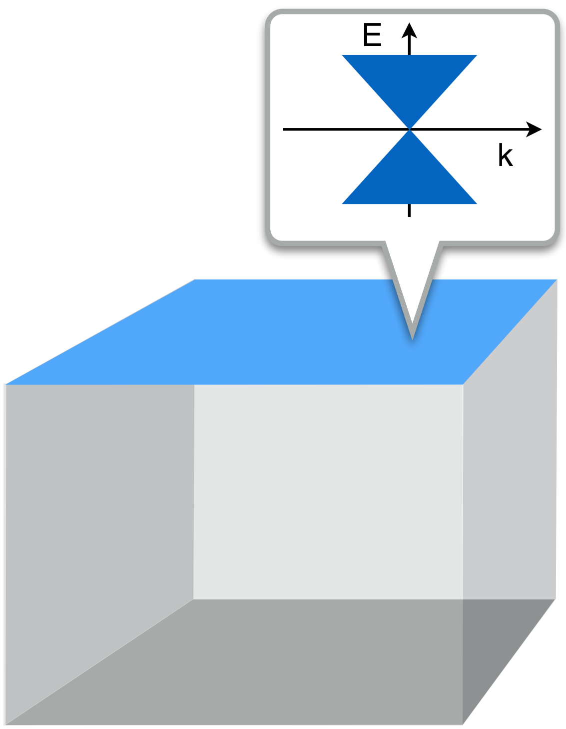
Ashley Cook
(U Zurich)

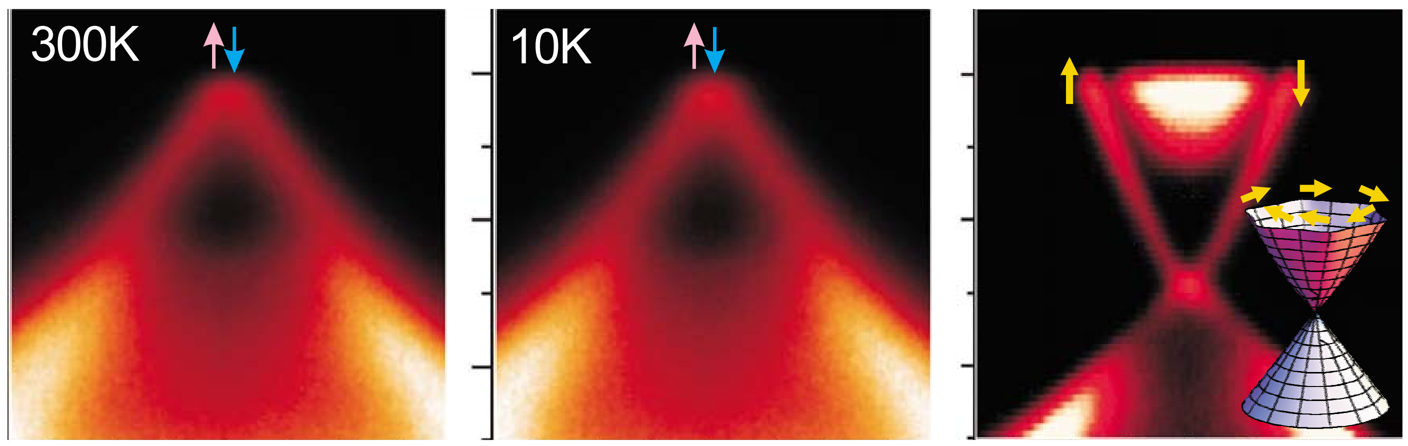
Stuart Parkin
(Max Planck Halle)

Andrei Bernevig
(Princeton U)

Topological Insulators



Bulk-boundary correspondence:
gapless Dirac cones, gapped bulk band structure



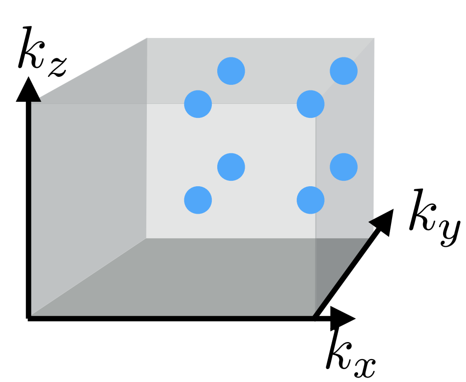
Topological invariant: $$\theta = -\epsilon_{abc} \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3} \mathrm{tr} \left[\mathcal{A}_a \partial_b \mathcal{A}_c + \mathrm{i}\frac{2}{3} \mathcal{A}_a \mathcal{A}_b \mathcal{A}_c \right]$$

$$\mathcal{A}_{a;n,n'} = -\mathrm{i} \langle u_n | \partial_a | u_{n'} \rangle$$

$\theta = 0, \pi$ with time-reversal symmetry

Topological invariant with inversion:

$$\prod_{k \in \mathrm{TRIM}} \xi_k = (-1)^\nu$$ product over inversion eigenvalues at time-reversal invariant momenta



Superconducting and magnetic TI surface

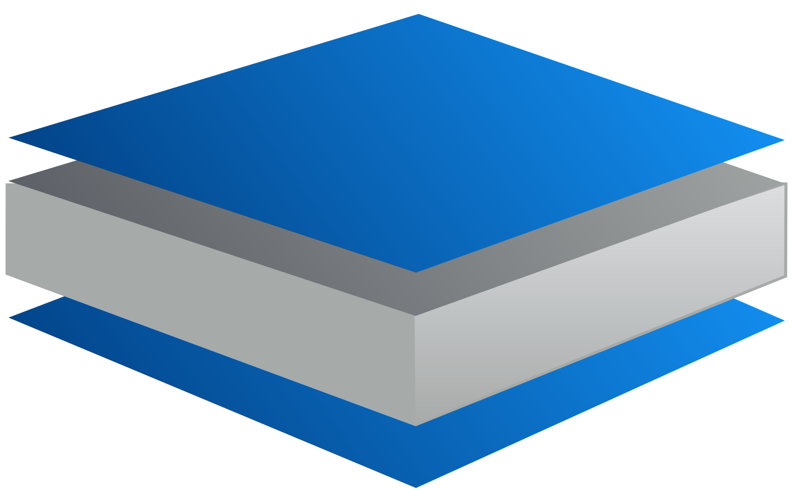
non-interacting SPT phase: $G = U(1) \rtimes Z_2^T$

Dirac cone + s-wave pairing:

U(1) breaking: TRS SC with Majorana in vortex

Fu Kane PRL 08

TI

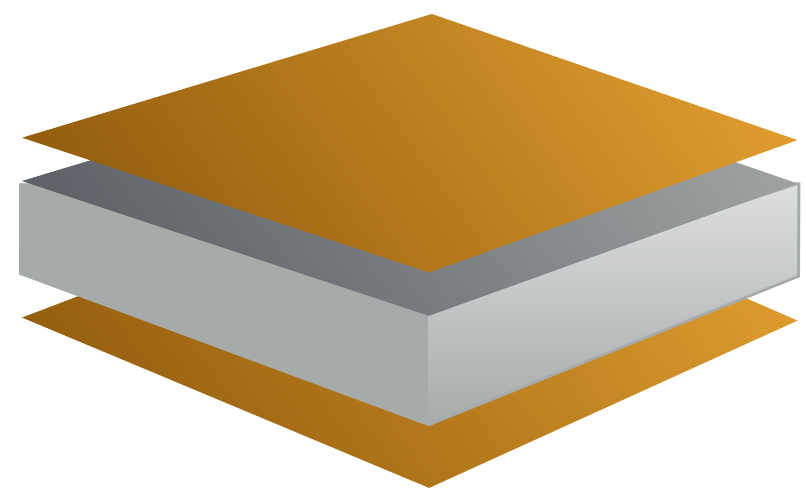


TR breaking: anomalous QHE

fractional conductivity without fractionalization

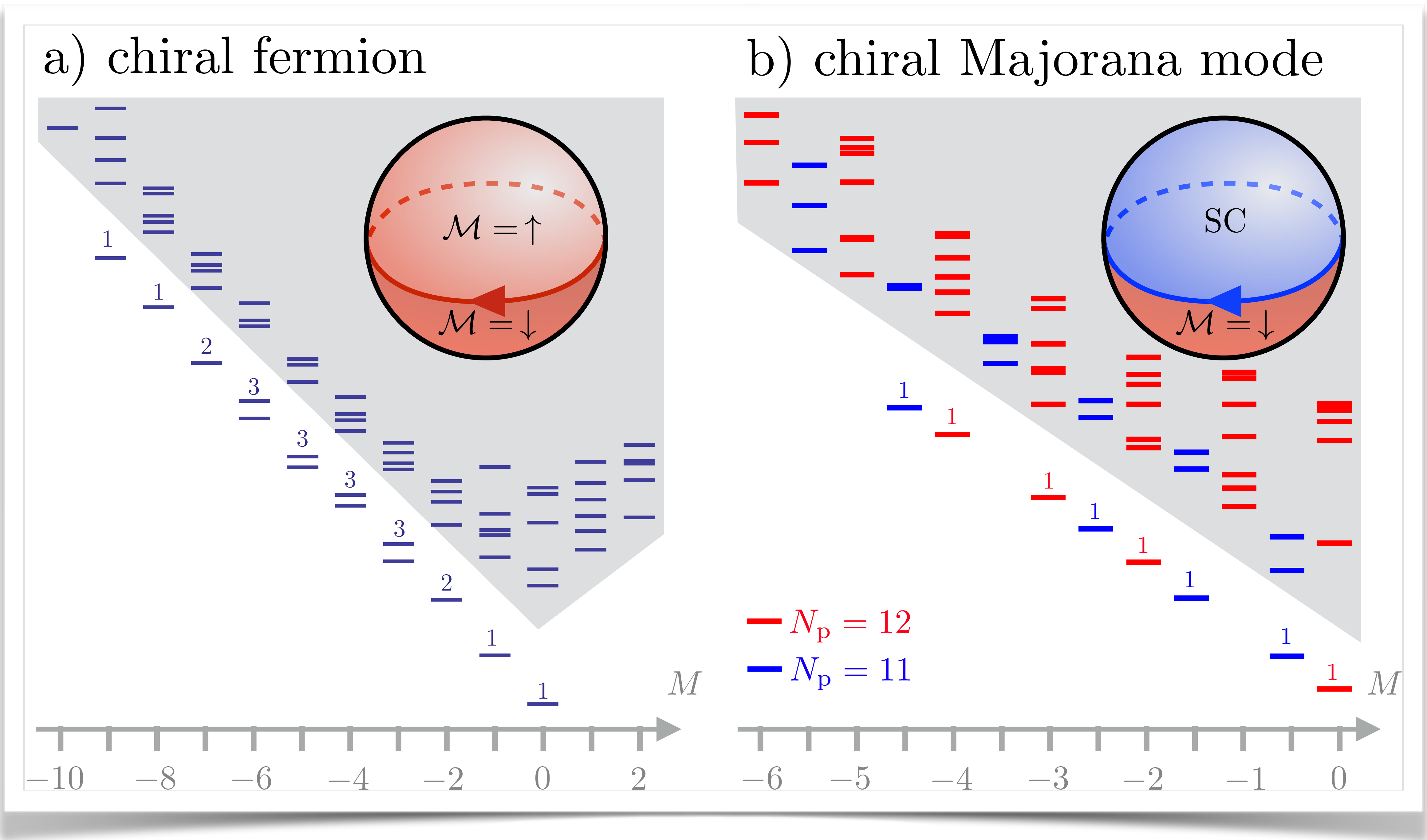
$\sigma_{xy} = 1/2$

Fu Kane Mele PRL 07



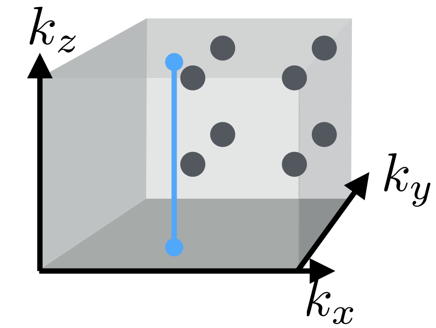
TI

Domain wall modes



Topology from Wilson loops

$$W_{nm}(k_x, k_y) = \overline{\exp}\left[\int_0^{2\pi} \mathrm{d}k_z \langle u_m(\vec{k})|\partial_{k_z}|u_n(\vec{k})\rangle\right]$$



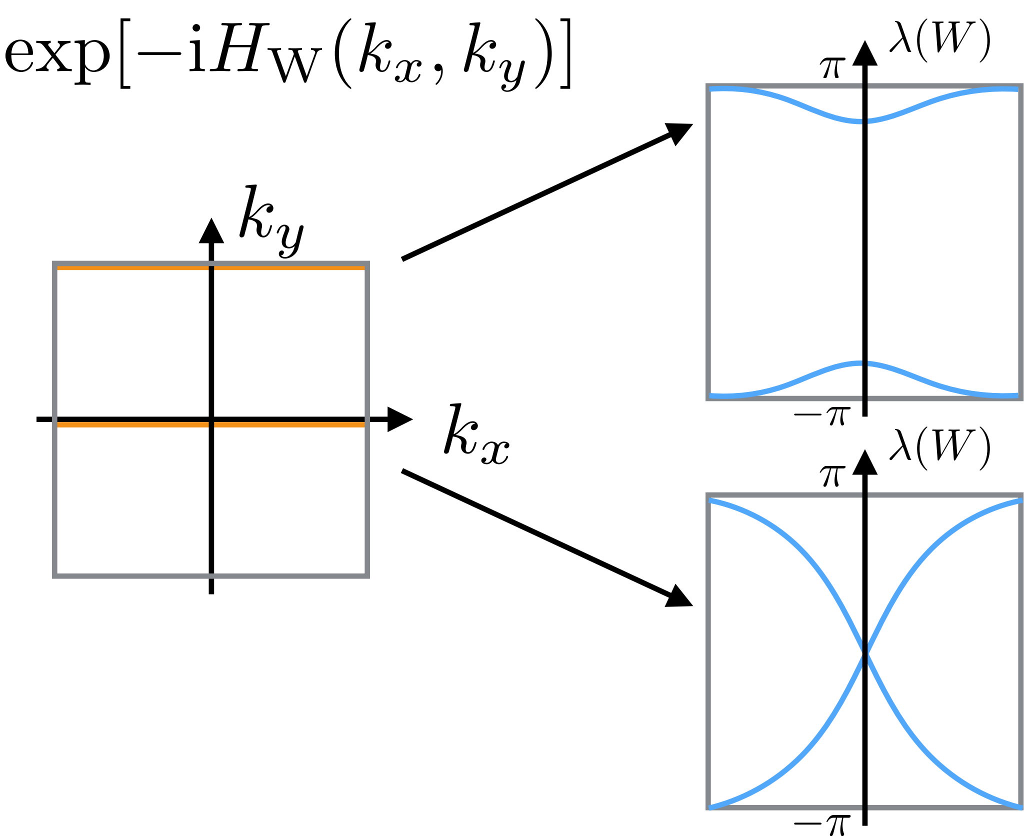
unitary operator in filled band subspace

occupied band eigenstates

Define 'Wilson loop Hamiltonian' $W(k_x, k_y) = \exp[-\mathrm{i}H_{\mathrm{W}}(k_x, k_y)]$

Resembles surface Hamiltonian with qualitatively identical gapless spectrum (single Dirac cone)

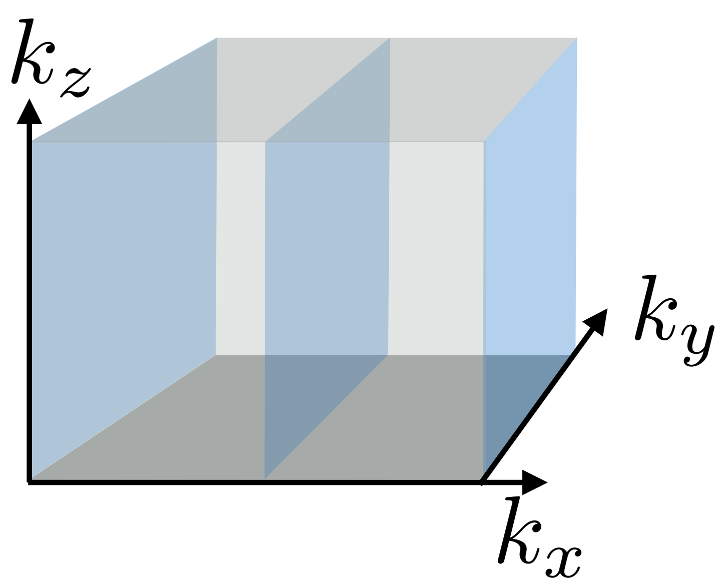
Equivalence: eigenvalues of Wilson loop and projected position operator $\hat{P}\hat{x}\hat{P}$



Topological crystalline insulators

Stabilize more than one Dirac cone by adding crystalline symmetries

Mirror symmetry:
eigenvalues +i and -i in spinful system
eigenstates on the mirror invariant planes in momentum space

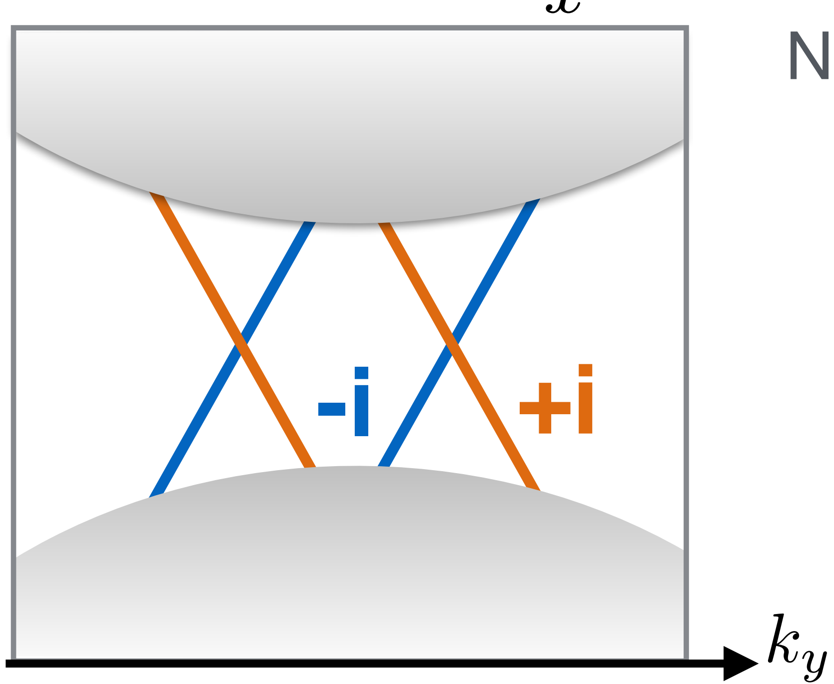


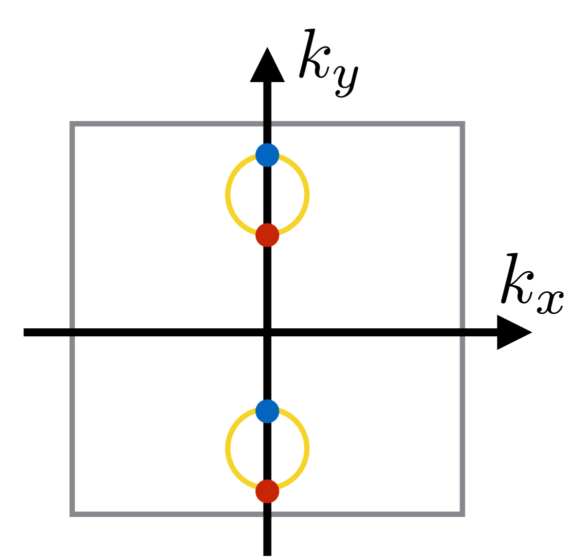
Mirror Chern number:
Chern number in +i/-i subspace on the plane

$$C_{\pm} = \frac{1}{2\pi} \int \mathrm{d}^2\boldsymbol{k}\, \mathrm{tr}\left[\partial_{k_y} \mathcal{A}_z^{\pm} - \partial_{k_z} \mathcal{A}_y^{\pm}\right]_{k_x = 0/\pi}$$

$\in \mathbb{Z}$ Time-reversal symmetry: $C_+ = -C_-$

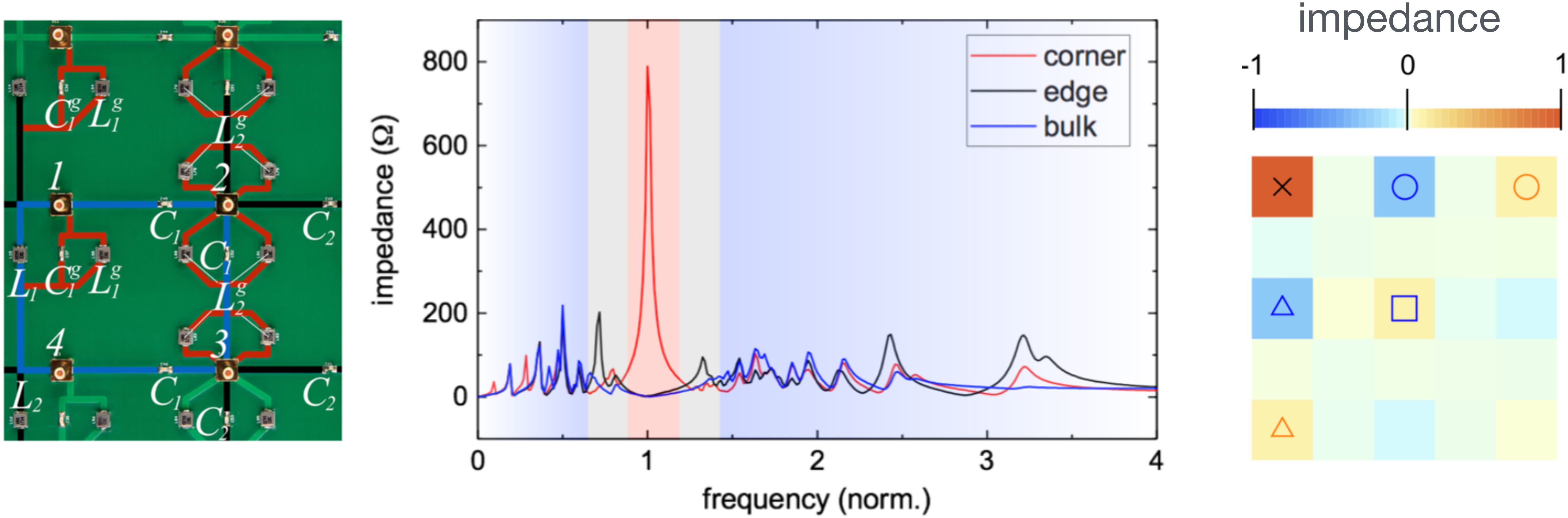
Number of Dirac cones crossing line in surface BZ



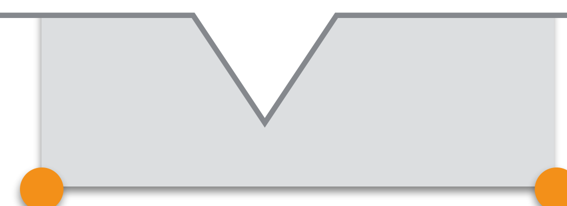


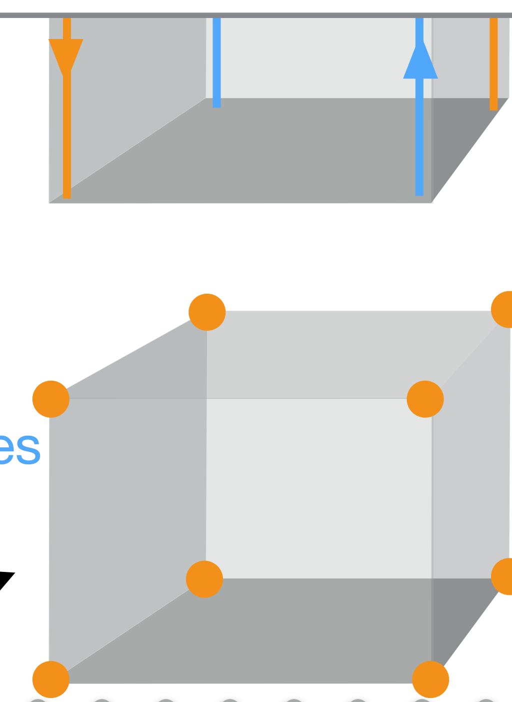
[L. Fu, Phys. Rev. Lett., 2011]

Electric circuit realization arXiv:1708.03647



Mechanical realization, Huber group arXiv:1708.05015





order

3

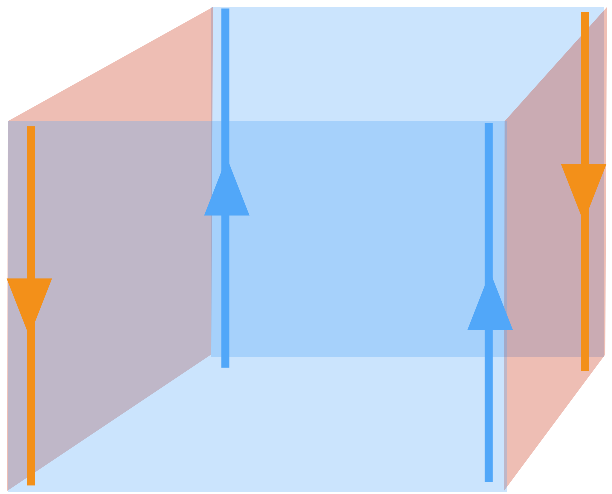
Can only happen with spatial symmetries: **generalizations of TCIs**

[Benalcazar, Bernevig, Hughes Science 357, 61-66 (2017)]

Construction of a 2nd order 3D TI

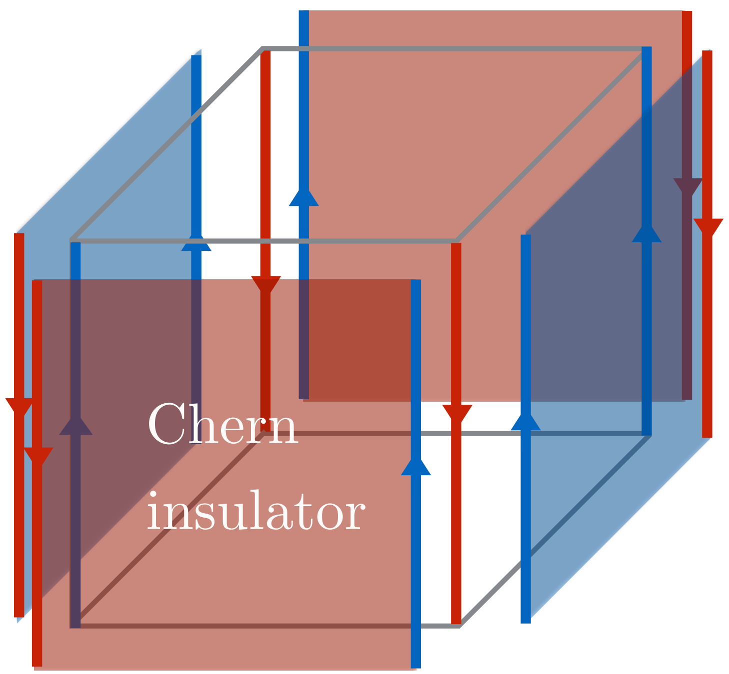
Protecting symmetry: **C_4T** (breaks T, C_4 individually)

surface construction from 3D TI:
decorate surfaces alternatingly with outward and inward pointing magnetization, gives chiral 1D channels at hinges



Adding C_4T respecting IQHE layers on surface can **change number of hinge modes by multiples of 2**

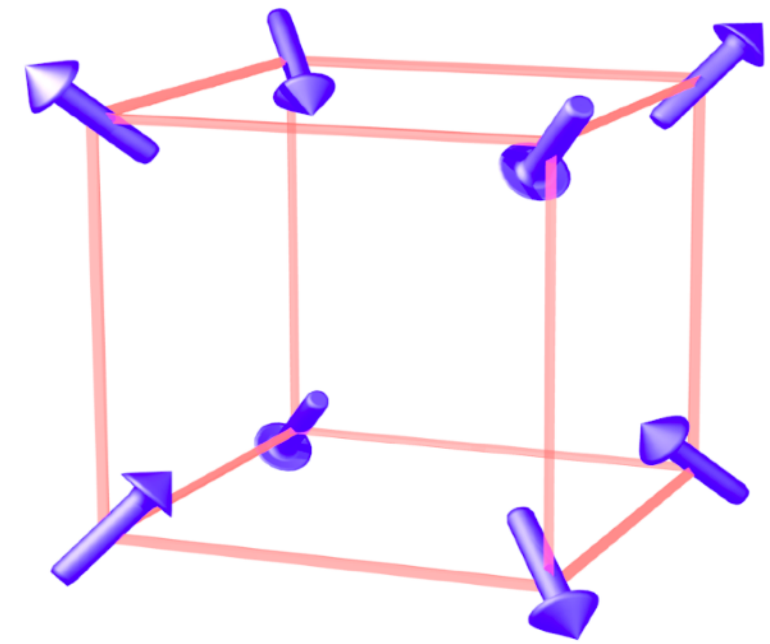
Odd number of hinge modes **stable** against any C_4T respecting surface manipulation



Bulk $\mathbb{Z}_2$ topological property

Construction of a 2nd order 3D TI

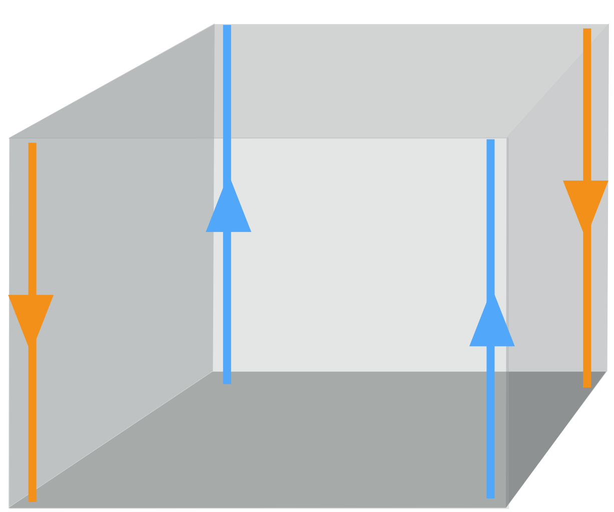
Protecting symmetry: **C_4T**
(breaks T, C_4 individually)



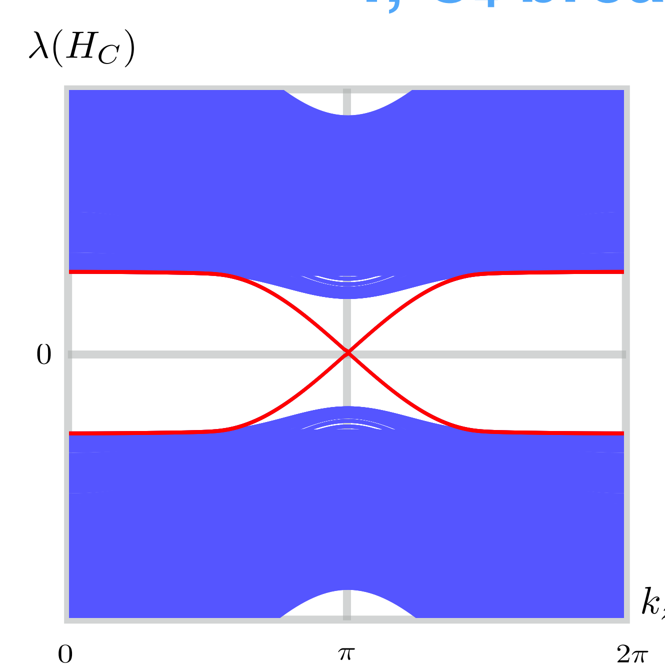
Bulk construction
TI band structure plus (sufficiently weak) triple-q (π,π,π) magnetic order

Toy model with only C_4T in z-direction

$$H_4(\vec{k}) = \underbrace{\left(M + \sum_i \cos k_i\right) \tau_z\sigma_0 + \Delta_1 \sum_i \sin k_i \, \tau_y\sigma_i}_{\text{3D TI}} + \underbrace{\Delta_2(\cos k_x - \cos k_y)\, \tau_x\sigma_0}_{\text{T, } C_4 \text{ breaking term}}$$



Spectrum of column geometry



Topological invariant of a 2nd order 3D TI

Same quantization with C_4T as with T alone:

$\boxed{\theta = 0, \pi \quad \text{is topological invariant}}$

$$Z_{\rm top} = e^{\mathrm{i}\frac{\theta}{8\pi^2}\int \mathrm{d}^4x\, \boldsymbol{E}\cdot\boldsymbol{B}}$$

Different from existing indices, because $\boxed{(C_4T)^4 = -1}$

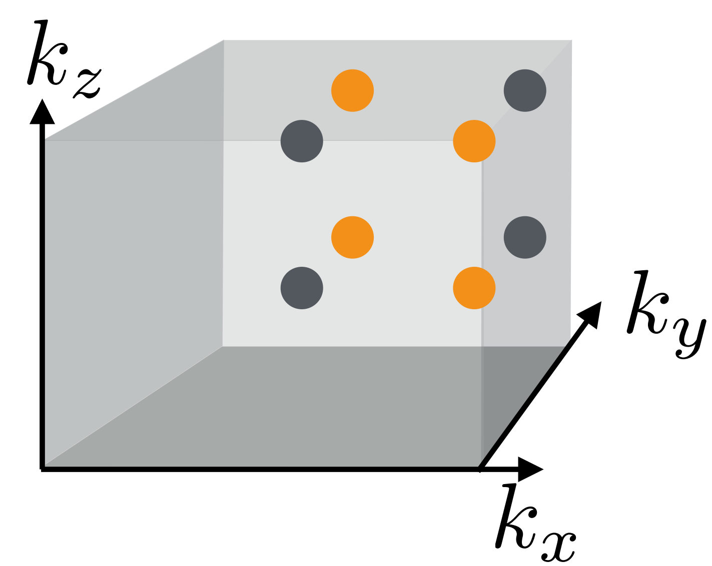
Case of additional **inversion times TRS**, IT, symmetry:
use $(IC_4)^4 = -1$ with eigenvalues $\xi_{\vec{k}}\{e^{i\pi/4}, e^{-i\pi/4}\}$ $\xi_{\vec{k}} = \pm 1$

Due to $[IC_4, IT] = 0$ ‘Kramers’ pairs with same $\xi_{\vec{k}} = \pm 1$ are degenerate.

Band inversion formula for topological index à la Fu Kane for C_4T invariant momenta

$$\boxed{(-1)^\nu = \prod_{\vec{k}\in\mathcal{I}_{\hat{C}_4^z\hat{T}}} \xi_{\vec{k}}}$$

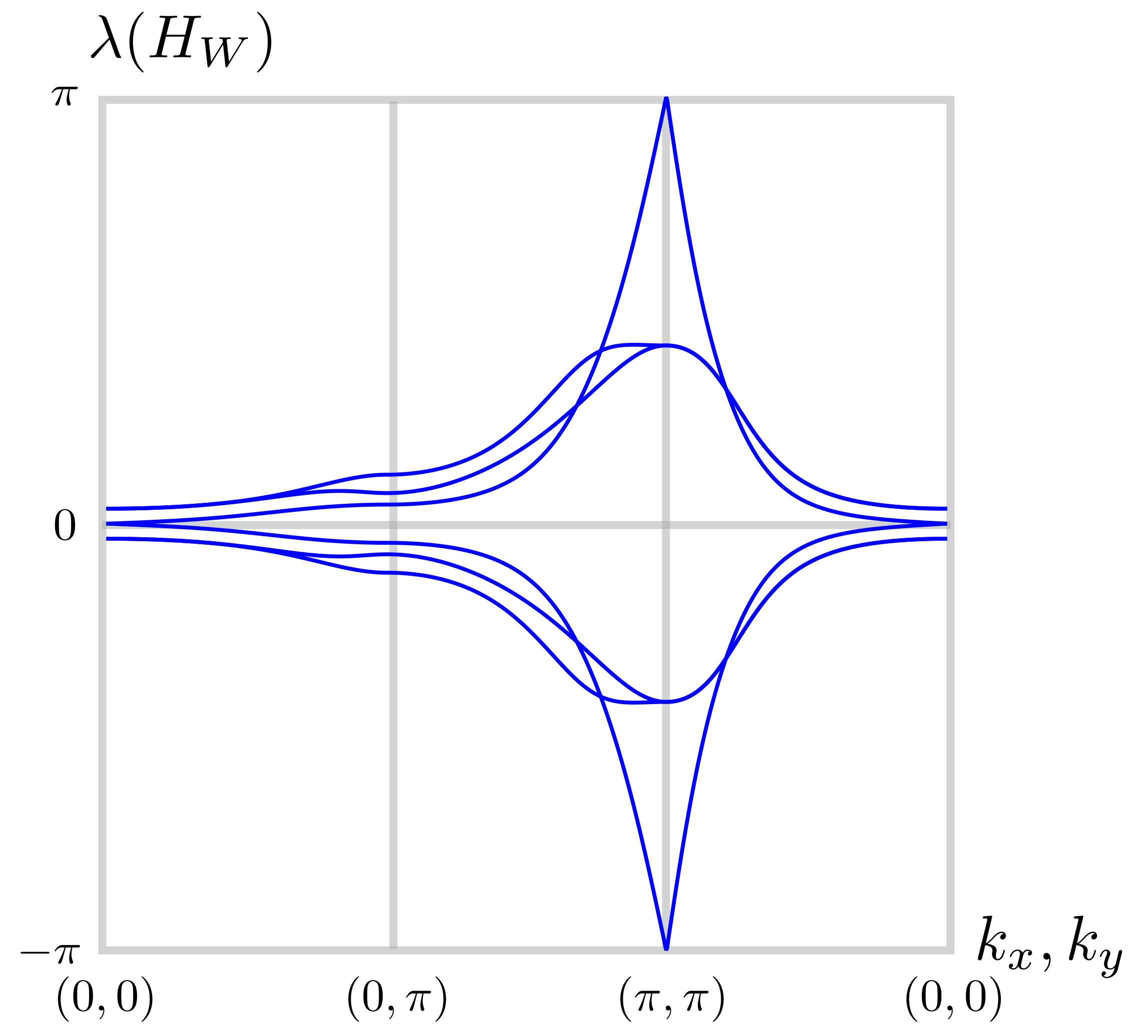
$$\mathcal{I}_{\hat{C}_4^z\hat{T}} = \{(0,0,0), (\pi,\pi,0), (0,0,\pi), (\pi,\pi,\pi)\}$$



Wilson loop topology of a 2nd order 3D TI

Wilson-loop based bulk topological characterization

$$W_{nm}(k_x,k_y) = \overline{\exp}\left[\int_0^{2\pi} \mathrm{d}k_z \langle u_m(\vec{k})|\partial_{k_z}|u_n(\vec{k})\rangle\right]$$



C_4T implies Kramers-like degeneracies in Wilson loop spectrum at C_4T invariant momenta

$$(k_x,k_y) \in \{(0,0),(\pi,\pi)\}$$

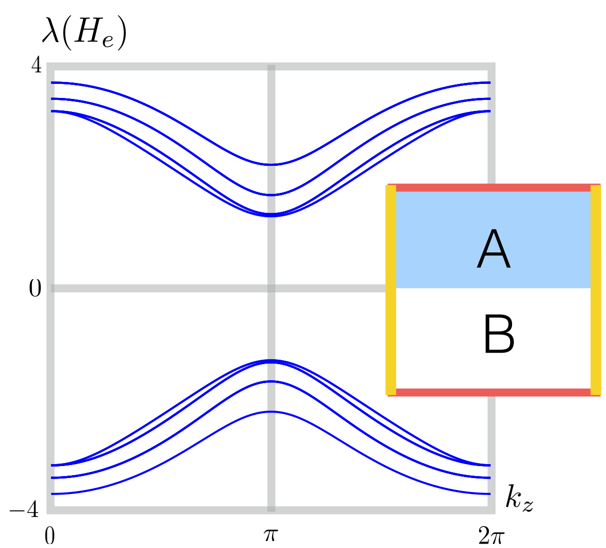
Z_2 Wilson loop winding between these momenta is topological invariant

$$\nu = \frac{1}{2\pi}\sum_l \left(\int_{(0,0)}^{(\pi,\pi)} \mathrm{d}\vec{k}\cdot\partial_{\vec{k}}\lambda_l(\vec{k}) - \lambda_l(\pi,\pi) + \lambda_i(0,0)\right) \mod 2$$

Boundary topology of a 2nd order 3D TI

Nested entanglement spectrum

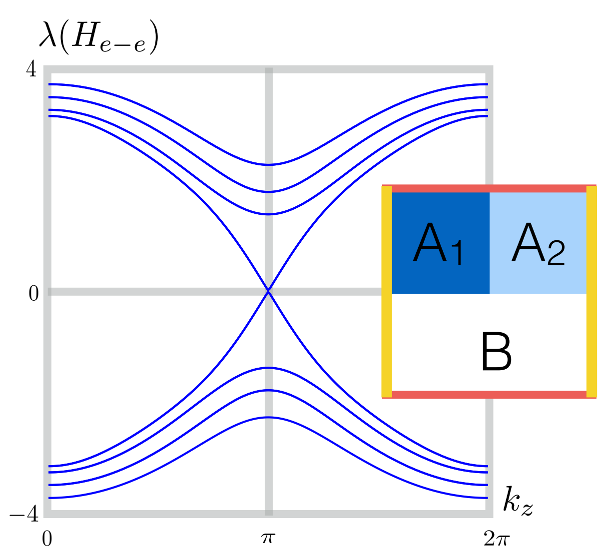
$$\rho_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi| \equiv \frac{1}{Z_\mathrm{e}} e^{-H_\mathrm{e}}$$



entanglement spectrum is gapped

Define: entanglement spectrum of entanglement Hamiltonian

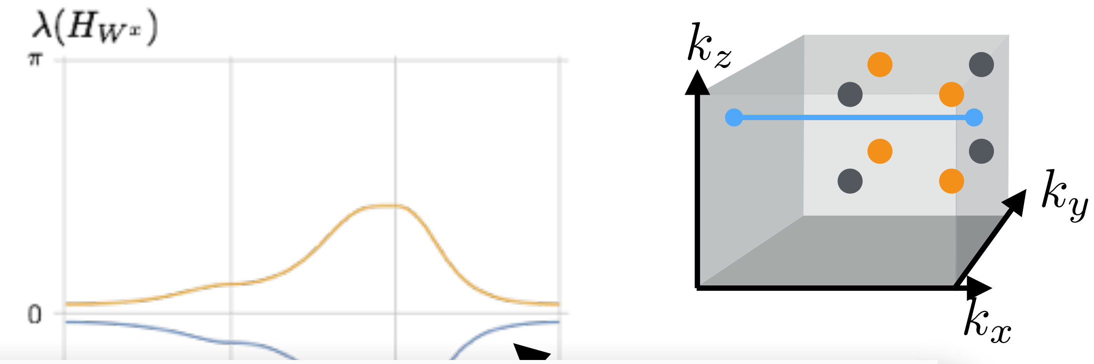
$$\rho_{\mathrm{e};A_1} = \mathrm{Tr}_{A_2} |\Psi_\mathrm{e}\rangle\langle\Psi_\mathrm{e}| \equiv \frac{1}{Z_{\mathrm{e-e}}} e^{-H_{\mathrm{e}-}}$$



gapless chiral hinge modes

Nested Wilson loop spectrum

x-direction Wilson loop spectrum gapped



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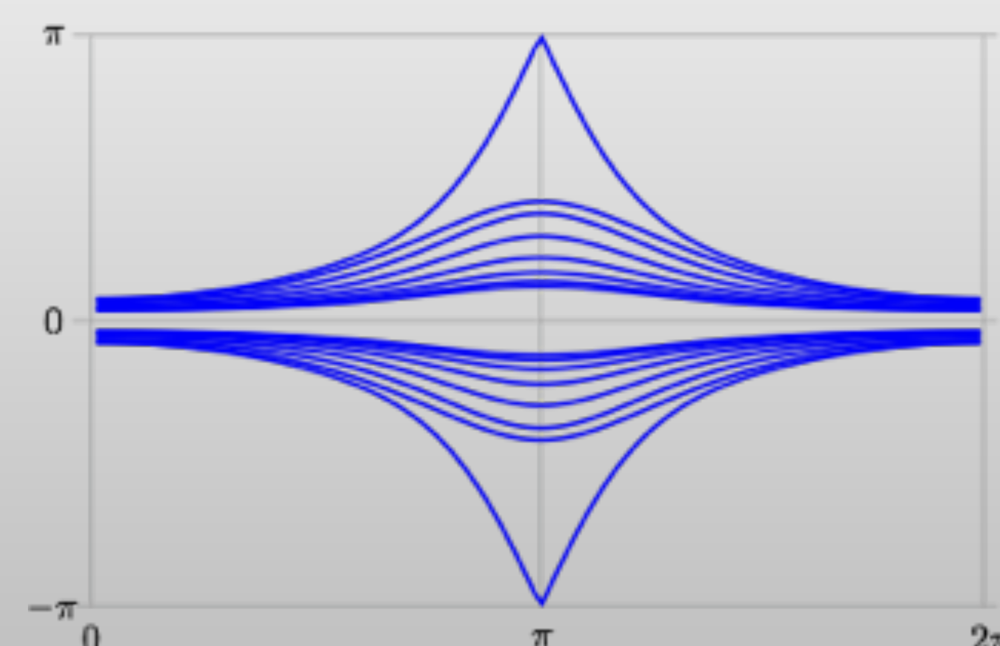
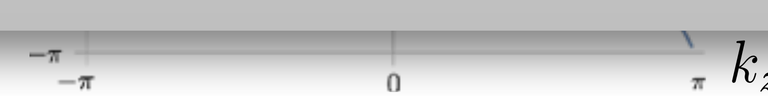
ss chiral

...one more:

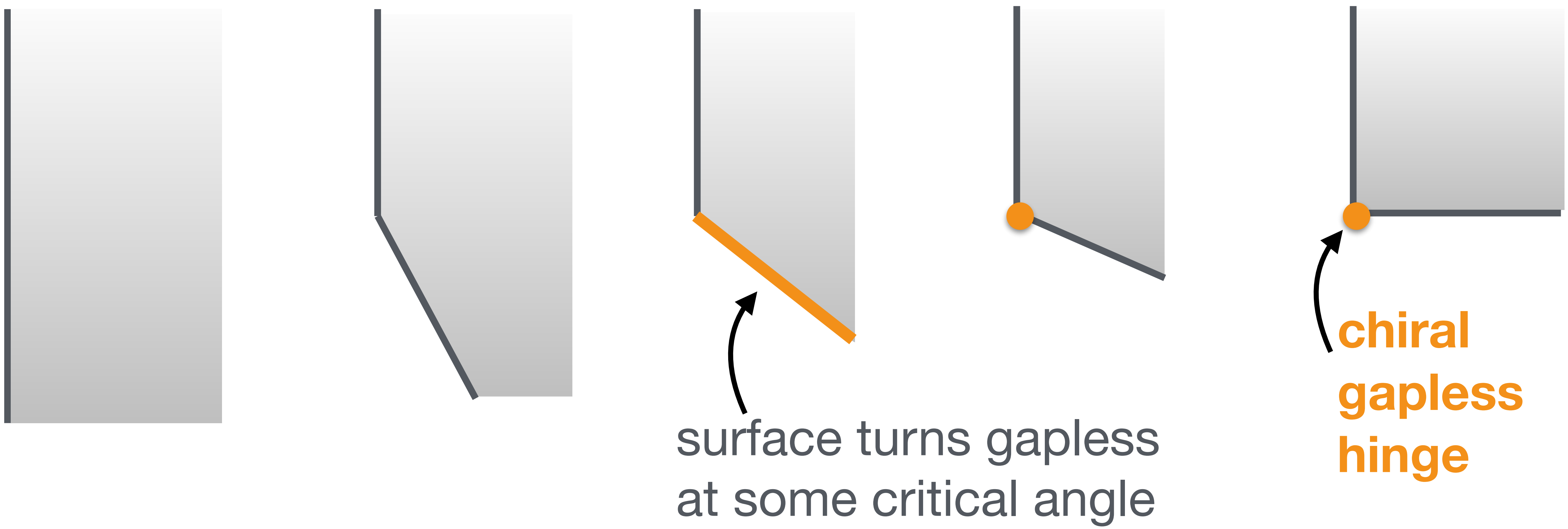
Wilson loop of gapped slab spectrum: **gapless modes**





Gapless surfaces?

consider adiabatically inserting a hinge



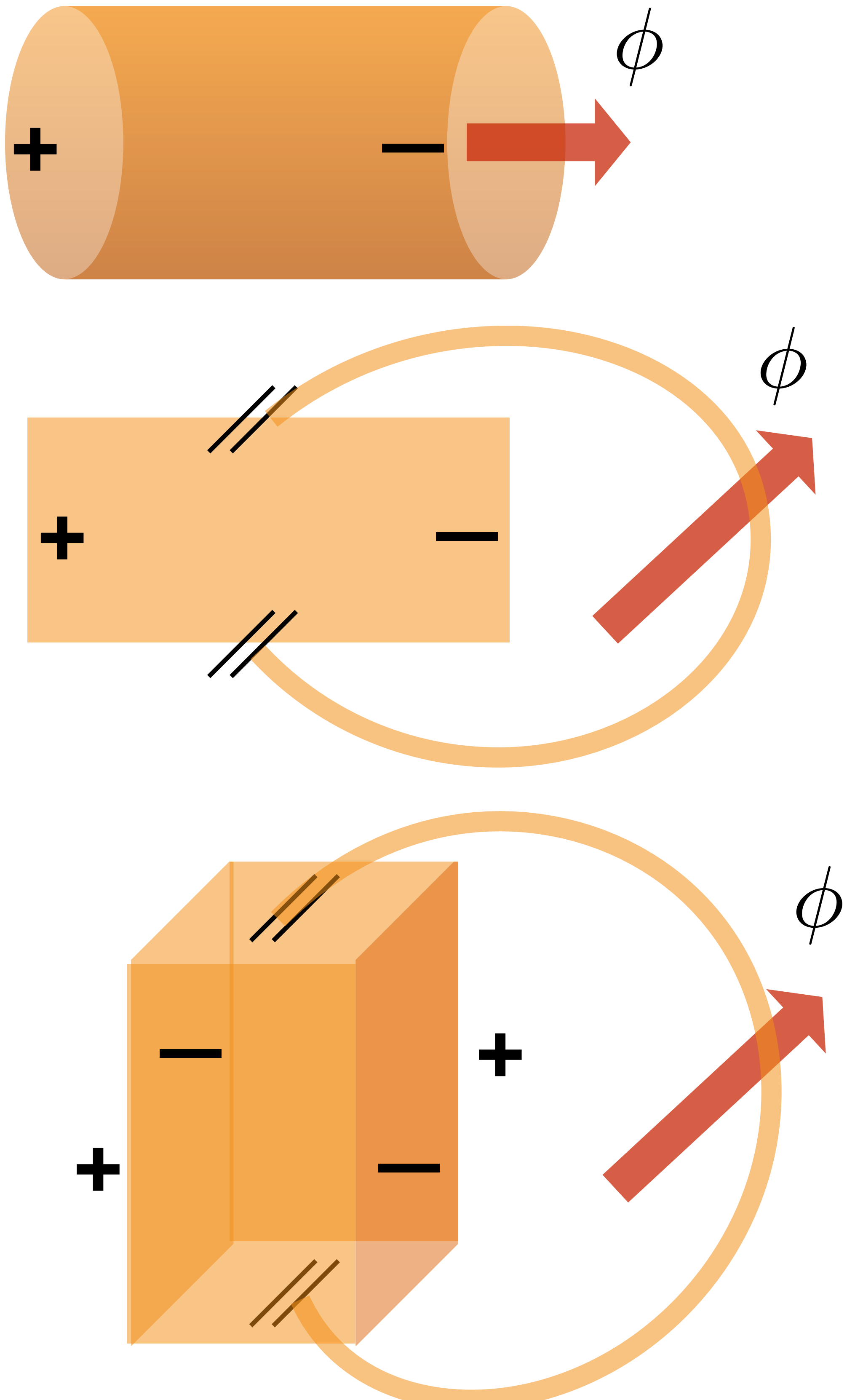
$$H_4(\vec{k}) = \left(M + \sum_i \cos k_i\right) \tau_z\sigma_0 + \Delta_1 \sum_i \sin k_i\, \tau_y\sigma_i + \Delta_2(\cos k_x - \cos k_y + \boxed{r} \sin k_x \sin k_y)\, \tau_x\sigma_0$$

Critical angle **nonuniversal**, not fixed to particular crystallographic direction. Different from gapless surfaces of TCIs.

Electromagnetic response

Flux insertion in quantum Hall system creates quantized **dipole**

Flux insertion in chiral higher-order TI creates quantized **quadrupole**



2nd order 3D topological superconductor

$$H_4(\vec{k}) = \left(M + \sum_i \cos k_i\right) \tau_z\sigma_0 + \Delta_1 \sum_i \sin k_i \, \tau_y\sigma_i + \Delta_2(\cos k_x - \cos k_y)\, \tau_x\sigma_0$$

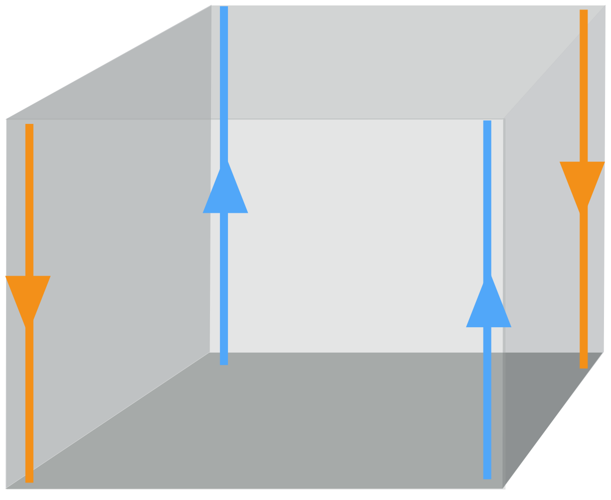
has a **particle hole symmetry** $P = \tau_y\sigma_y K$

Interpretation: Superconductor with generic dispersion and superposition of two order parameters

Δ_1 spin triplet, p-wave $d_{\vec{k},i} = \mathrm{i}\Delta_1 \sin k_i$
Balian-Werthamer state in superfluid Helium-3-B

Δ_2 spin singlet $d_{x^2-y^2}$-wave

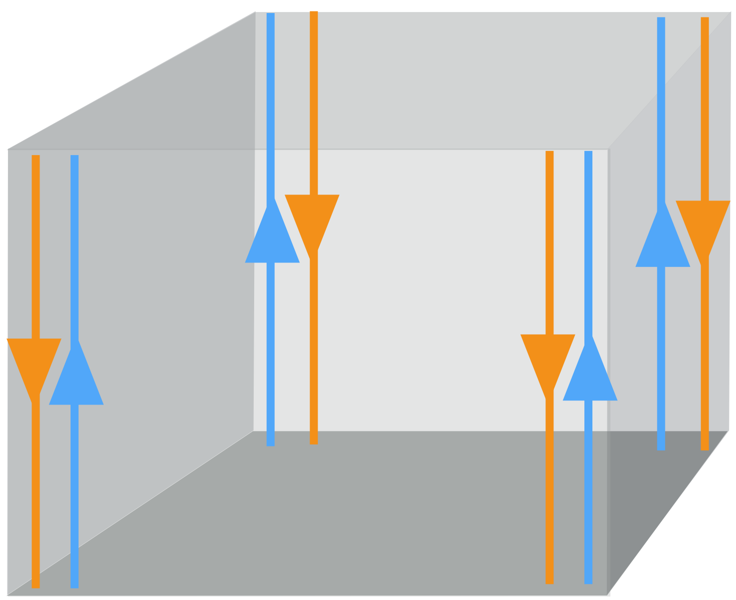
$p + \mathrm{i}d$ superconductor with chiral Majorana hinge modes



Time-reversal symmetric 2nd order 3D TI

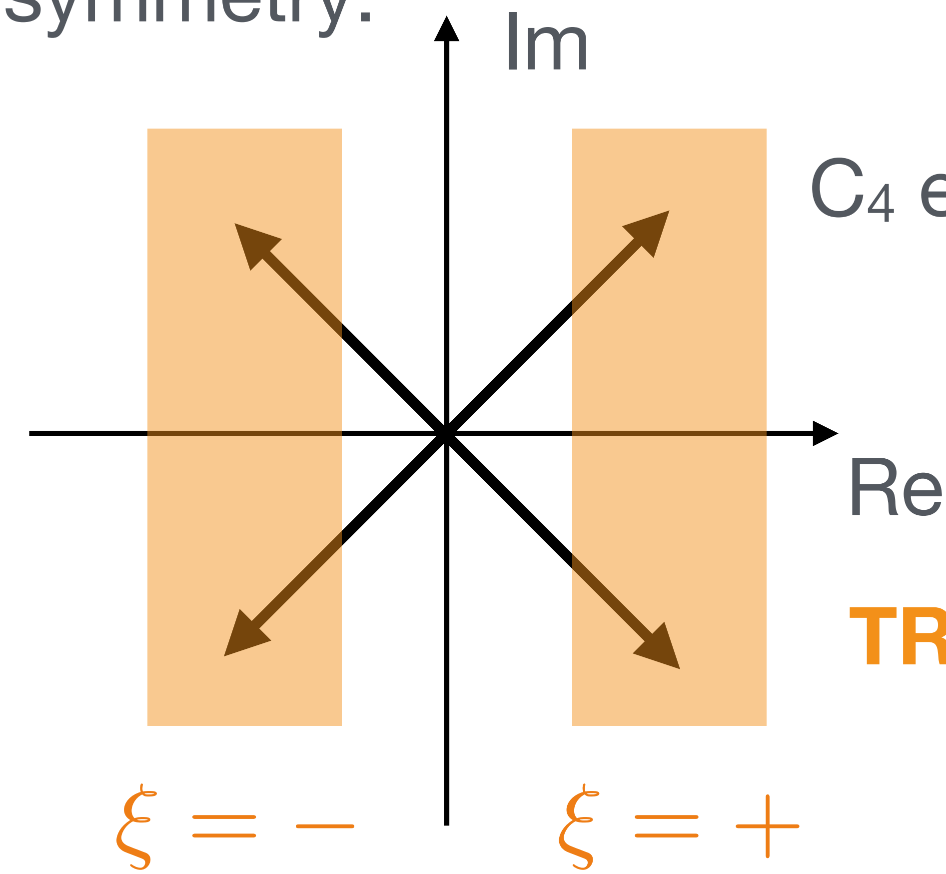
Stabilized by mirror symmetries and TRS

One Kramers pair of modes on each hinge,
like quantum spin Hall edge



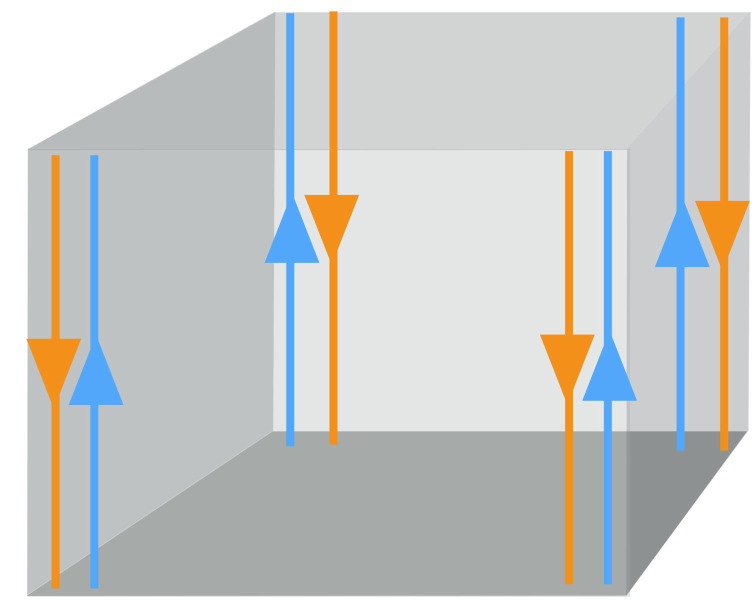
Time-reversal symmetric 2nd order 3D TI

Can also be defined with C_4 and time-reversal symmetry:



C_4 eigenvalues

TRS Kramers pairs



Define **3D Z_2 index** independently in each ξ subspace.

One nontrivial: 3D Z_2 TI, surfaces are gapless

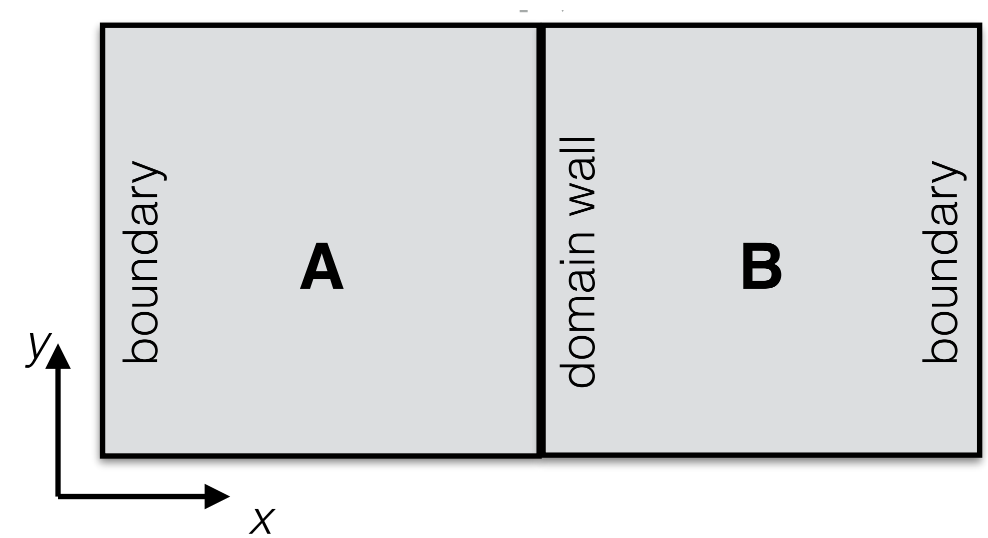
Both nontrivial: 3D higher-order TI, surfaces gapped, edges gapless

Both trivial: trivial insulator

Time-reversal symmetric 2nd order 3D TI

Surface perturbations:

No mirror chiral modes allowed in **2D**

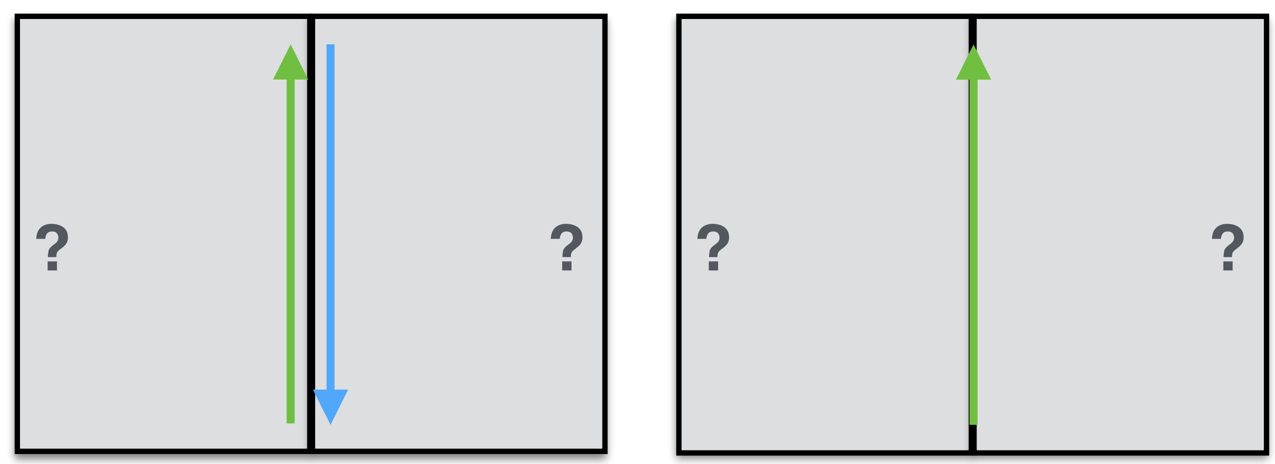


Mirror x → −x, leaves domain wall invariant

eigenvalue +i

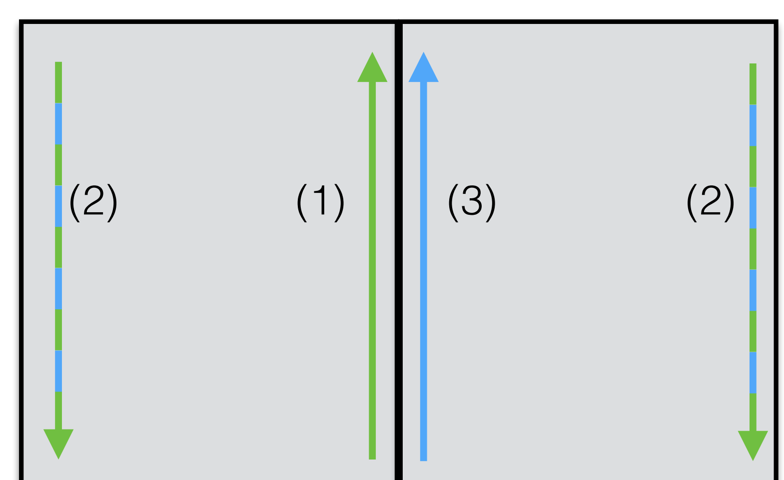
eigenvalue −i

Not allowed:



Allowed 2D surface perturbations:

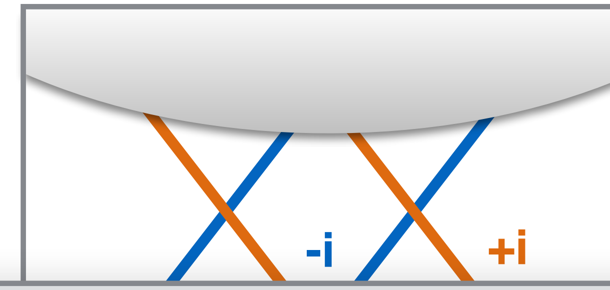
Number of upmovers of both mirror eigenvalues are equal

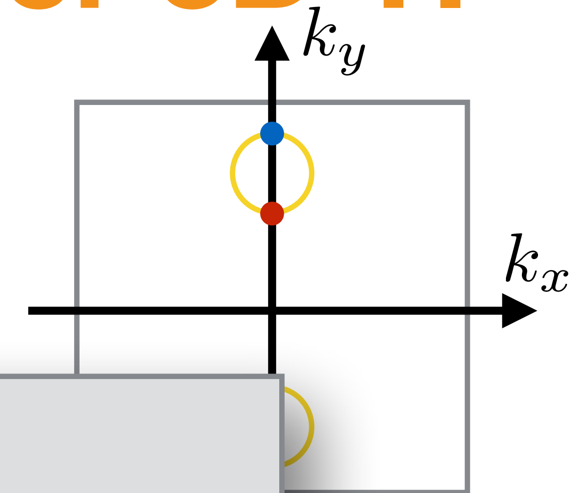


Time-reversal symmetric 2nd order 3D TI

Bending the surface of a topological crystalline insulator

mirror Chern number = 2





$\mathbb{Z}$ (upmovers − downmovers) with mirror eigenvalue −i

= with time-reversal $\mathbb{Z}$

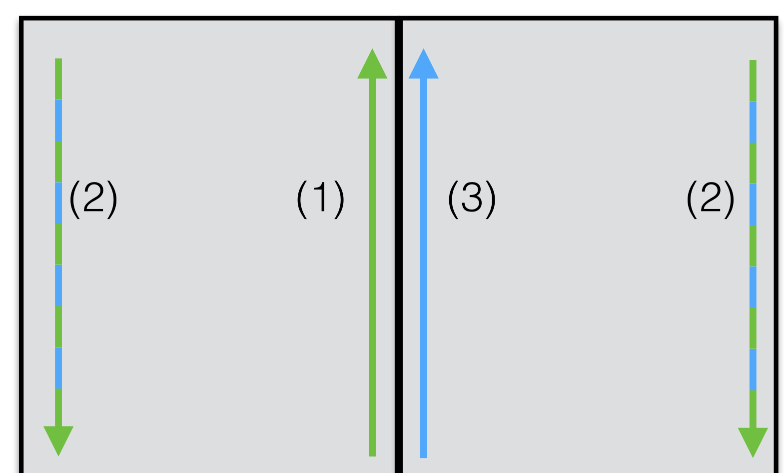
$\mathbb{Z}$ (upmovers − downmovers) with mirror eigenvalue + i

One upmover with mirror eigenvalue +i (=mirror Chern number/2)

Requires 3D bulk.

Allowed 2D surface perturbations:

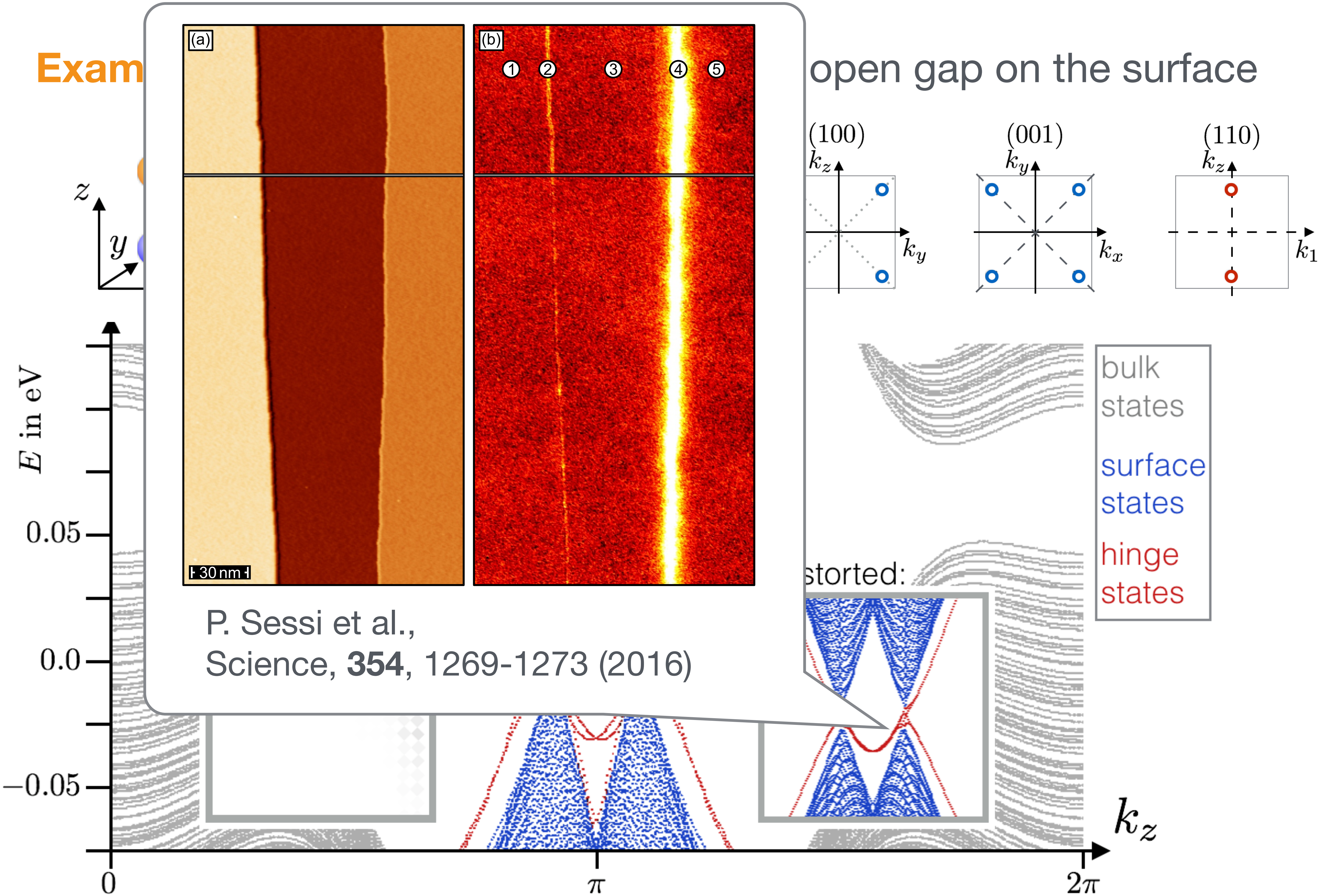
Number of upmovers of both mirror eigenvalues are equal



Time-reversal symmetric 2nd order 3D TI

Exam

open gap on the surface



P. Sessi et al.,
Science, **354**, 1269-1273 (2016)

Summary: **Higher-order topological insulators**

No TRS:

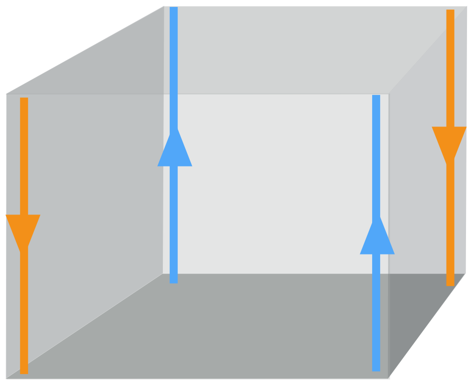
C_4T symmetry: Z_2 classification

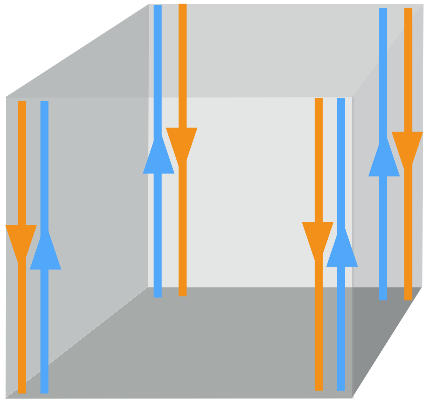
mirror symmetry: ZxZ classification

TRS:

C_4 symmetry: Z_2 classification

mirror symmetry: Z classification

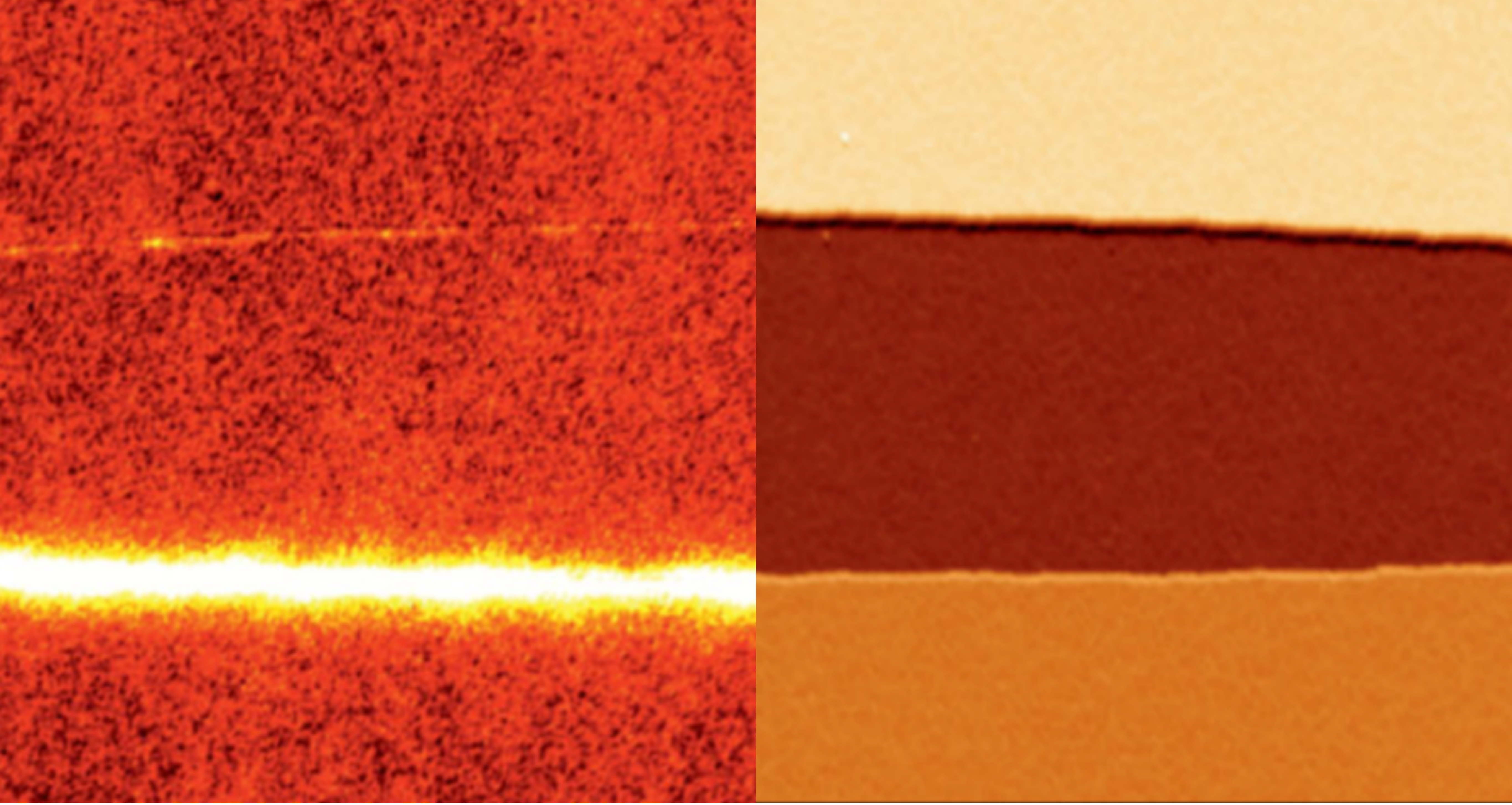




new paradigm for topological phases protected by spatial symmetries

- mirror or rotational symmetries
- hinge modes protected by 3D bulk invariant
- single hinge has same properties as that of QHE/QSHE
- feature nested entanglement spectrum or nested Wilson loop spectrum
- realizations in AFM spin-orbit coupled semiconductors, TCIs (strained SnTe)

arXiv:1708.03636

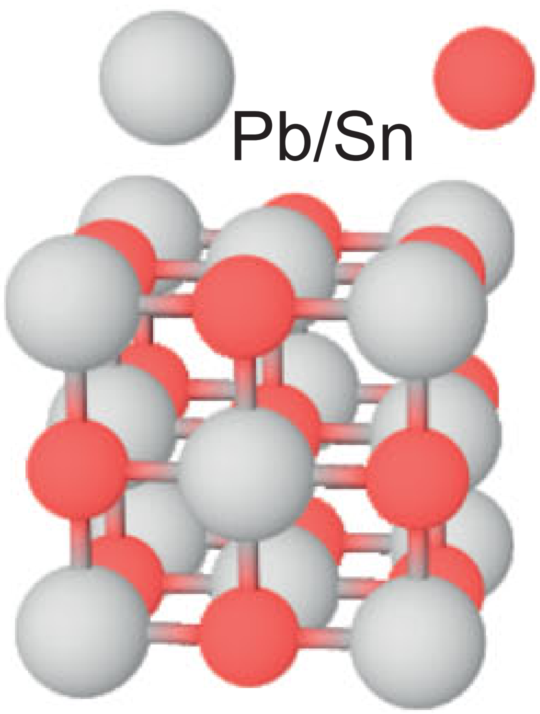


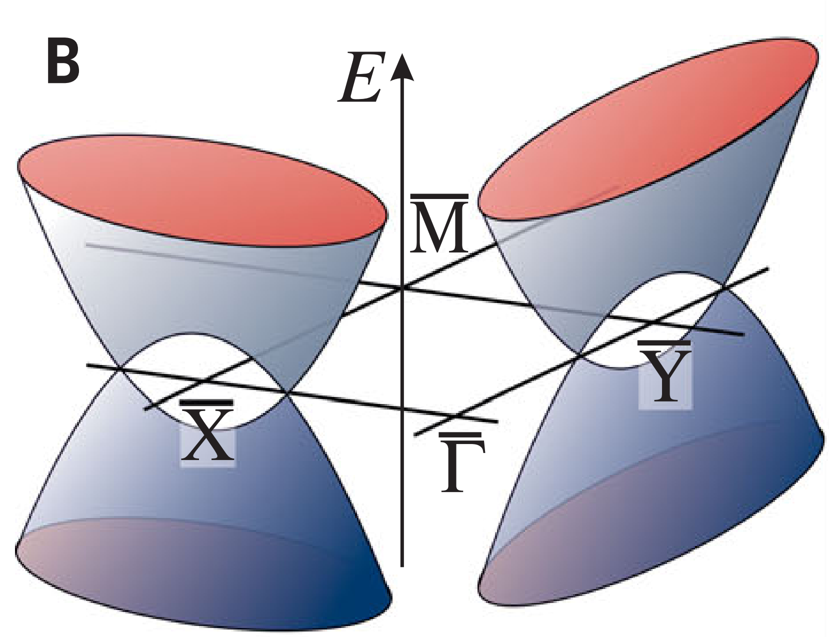
Bonus material

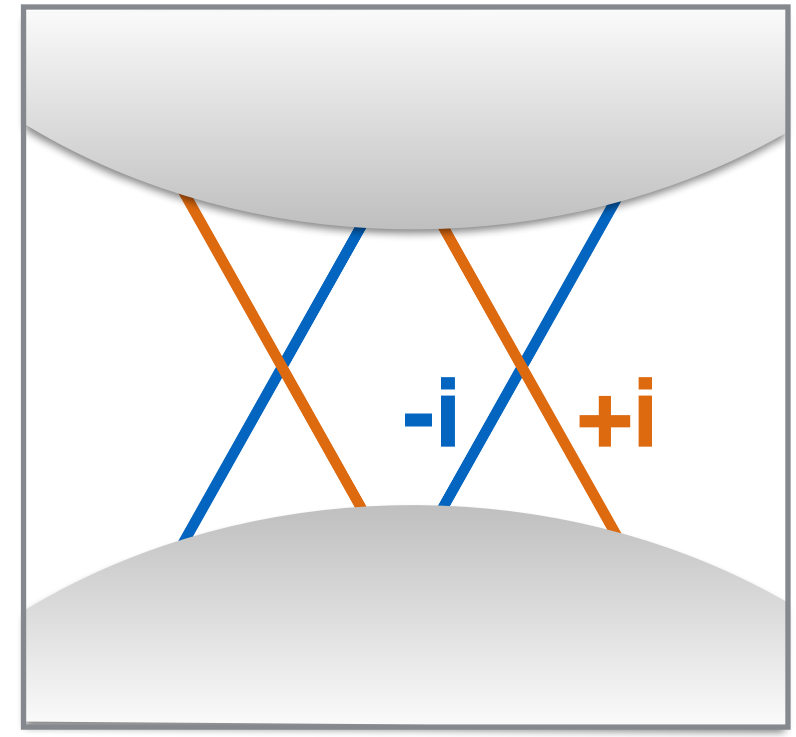
Edge modes at TCI surface steps

P. Sessi et al.,
Robust spin-polarized midgap states at step edges of topological crystalline insulators
Science, **354**, 1269-1273 (2016)

Step edges on topological crystalline insulators

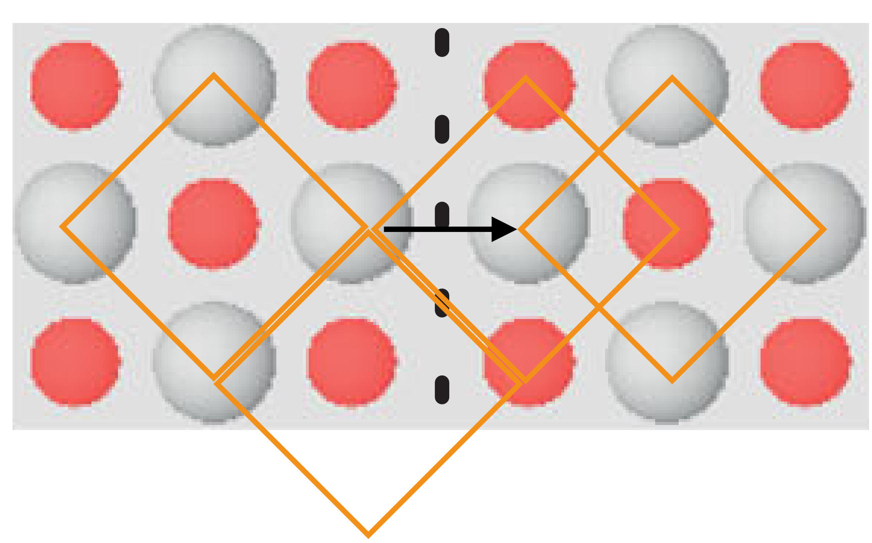






(Pb,Sn)Se: TCI with two pairs of Dirac cones, protected by mirror Chern numbers

Two surface terminations related by half lattice translation

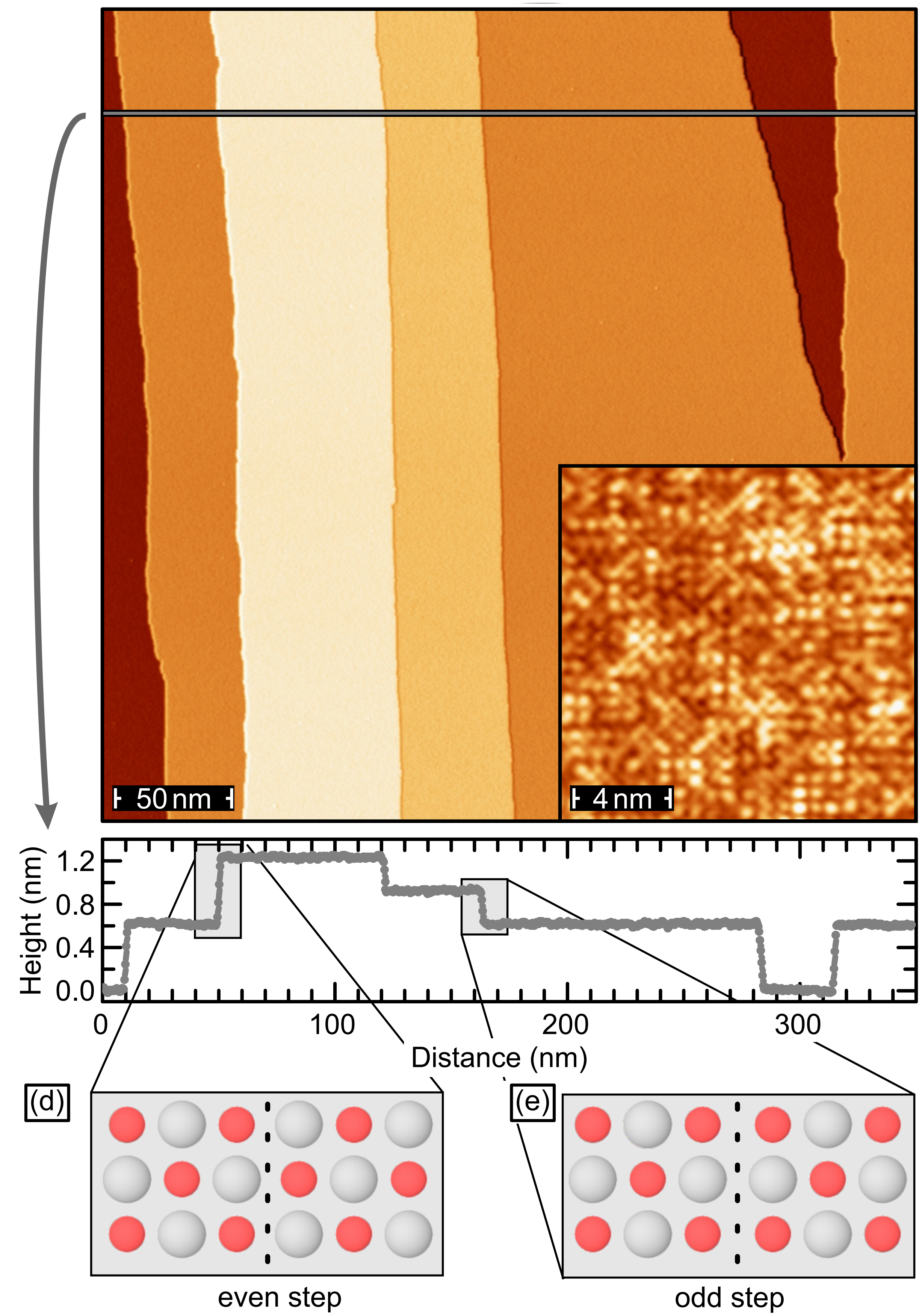


[Hsieh et al., Nature Comm., 2012]

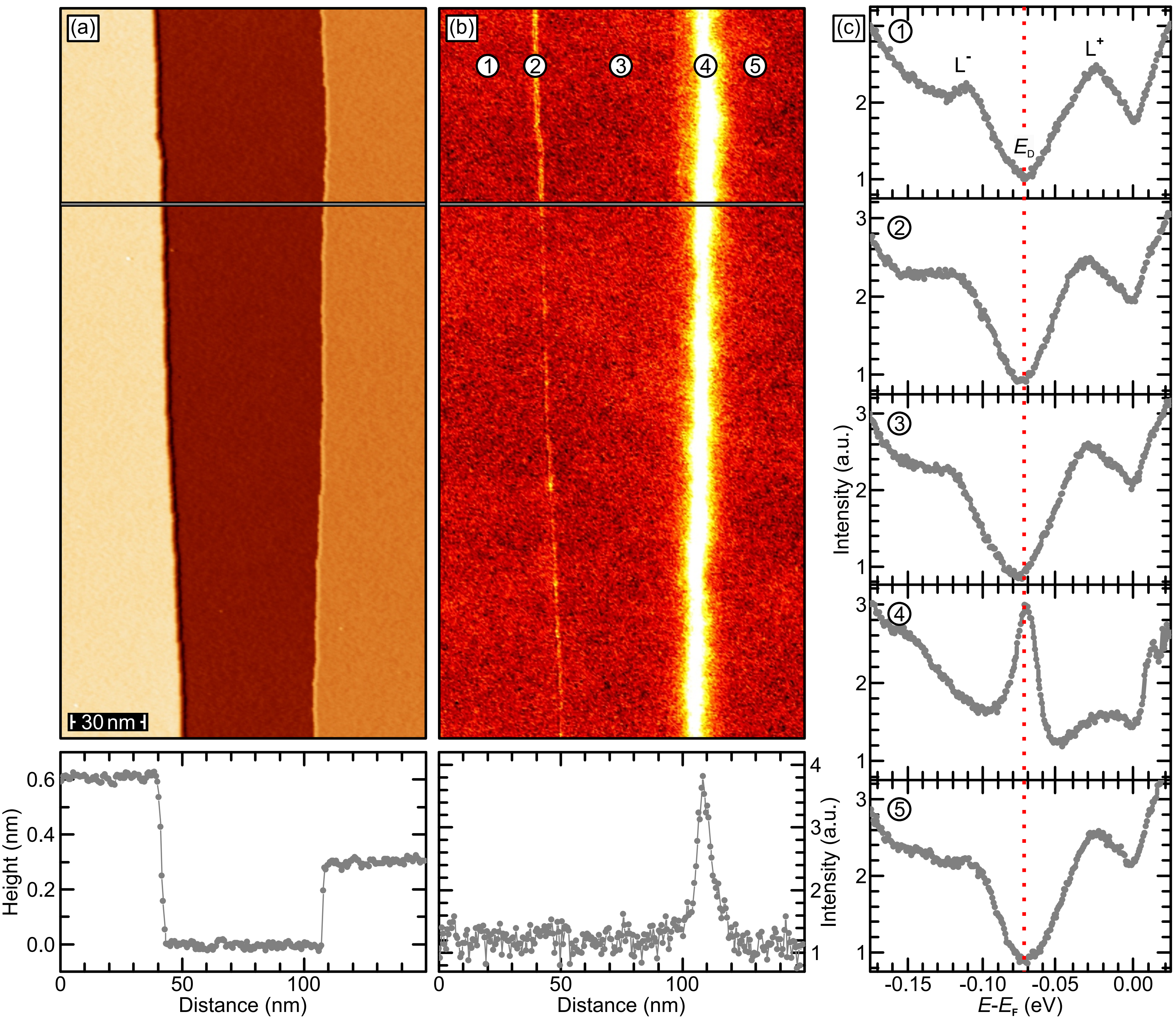
Step edges on topological crystalline insulators

Study step edges on the surface with STM

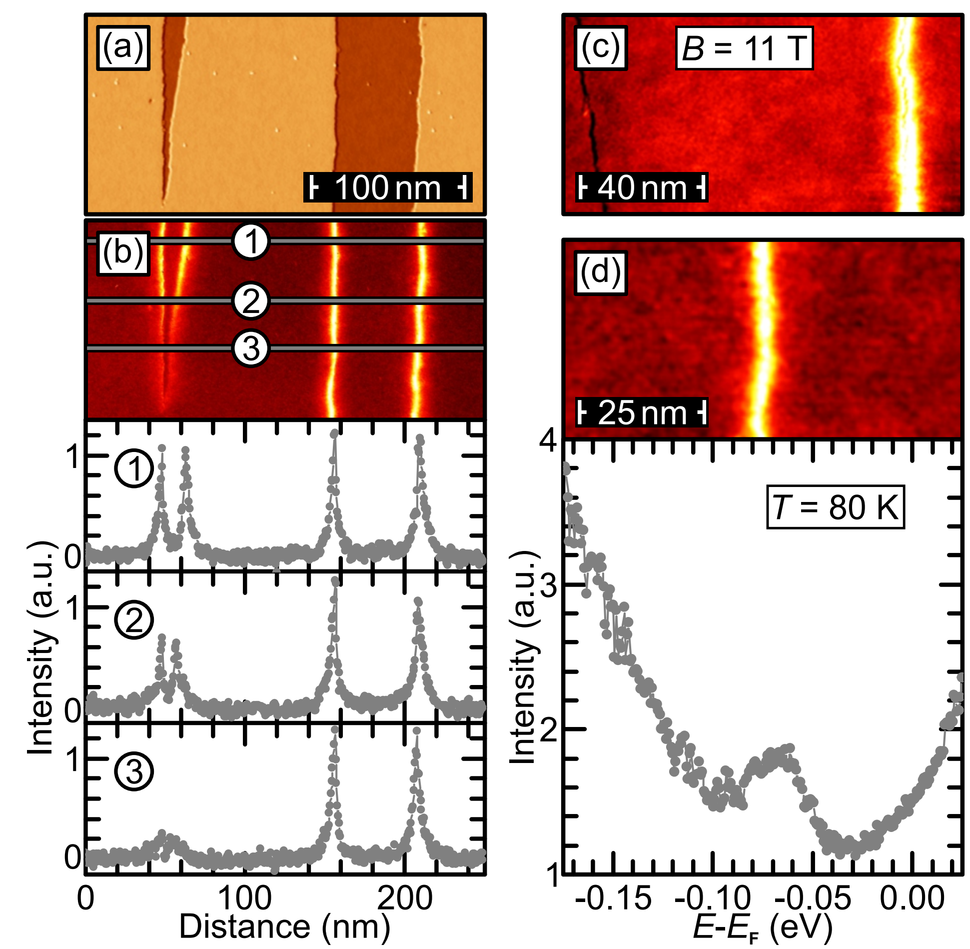
Pick (0,1) step edge orientation and distinguish **even and odd** steps



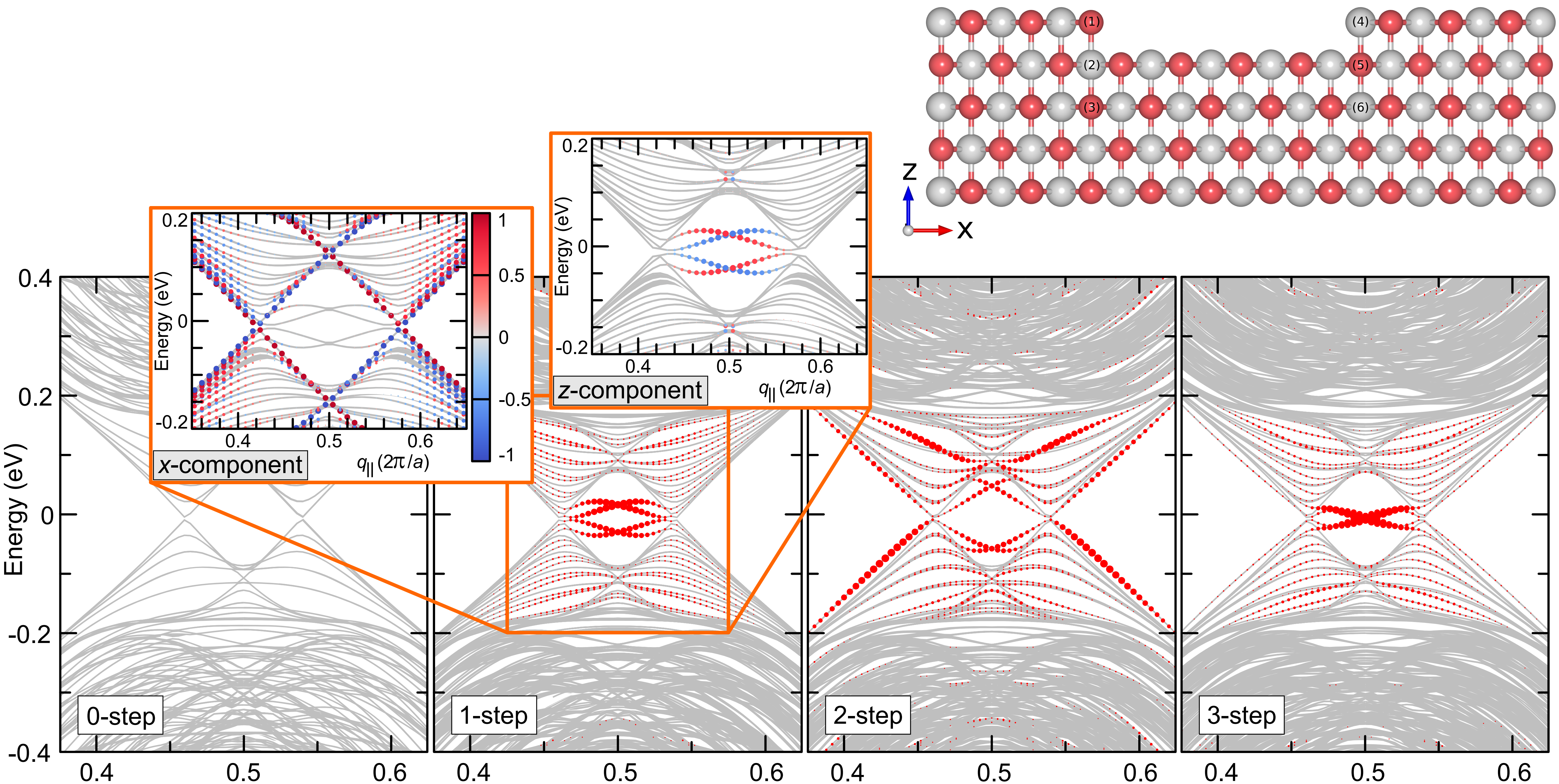
Large 1D DOS at odd steps only



Merging of step edges



Atomistic approach: DFT



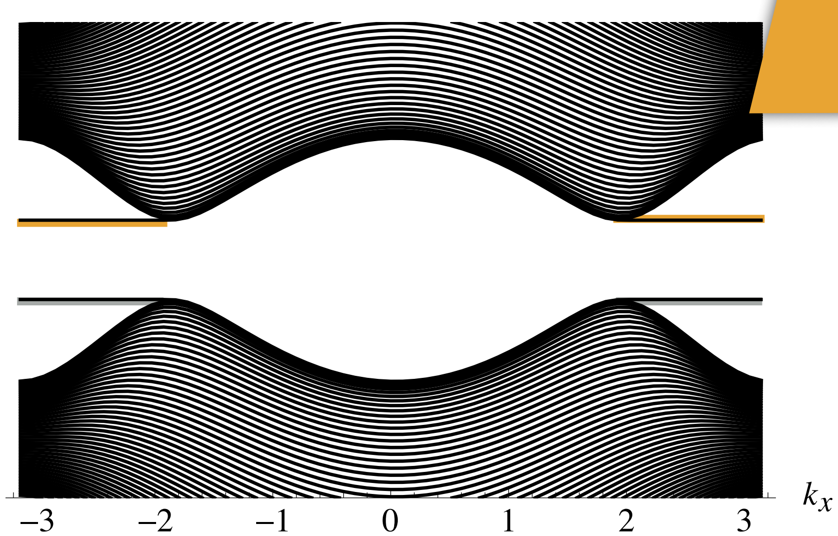
empirical confirmation: **1D DoS only at odd step edges**

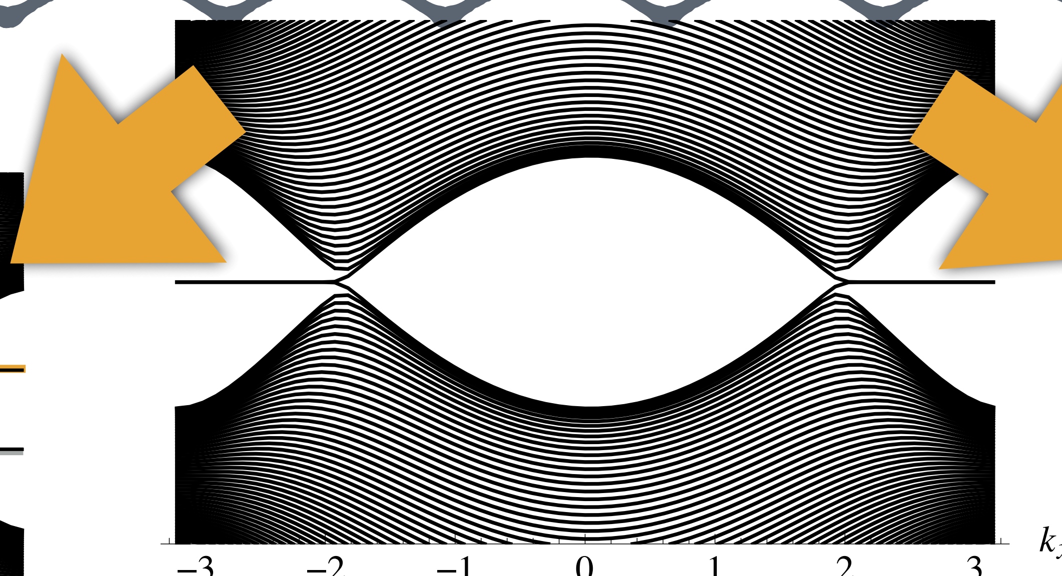
other dispersive features likely stem from finite size

Qualitative explanation:
Flat edge bands in graphene

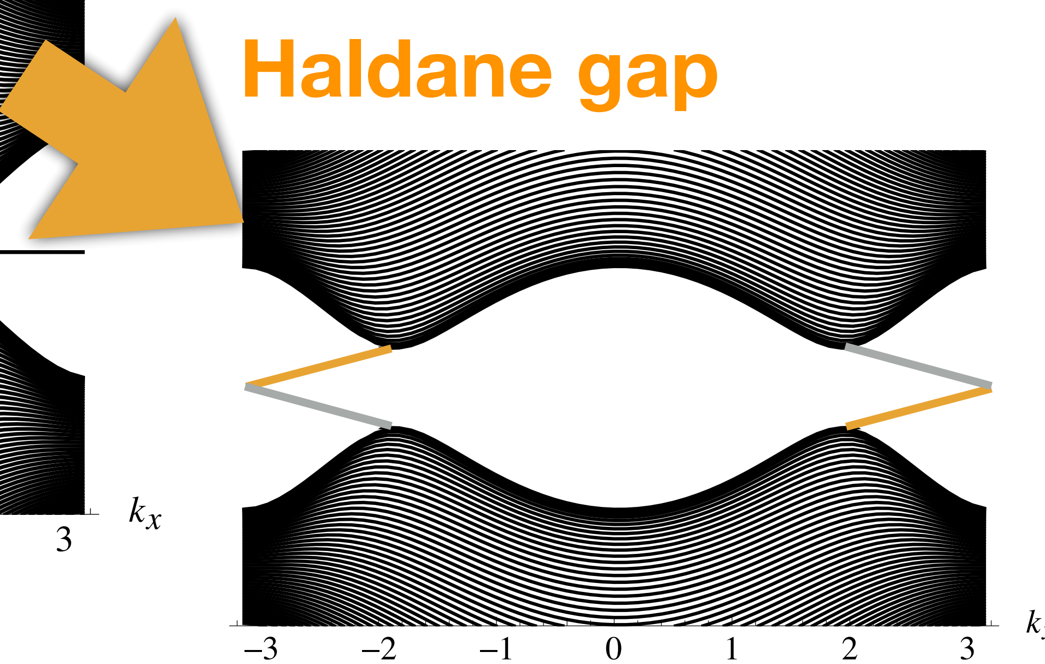
Honeycomb lattice (with spinless fermions), nearest neighbor hopping

trivial gap



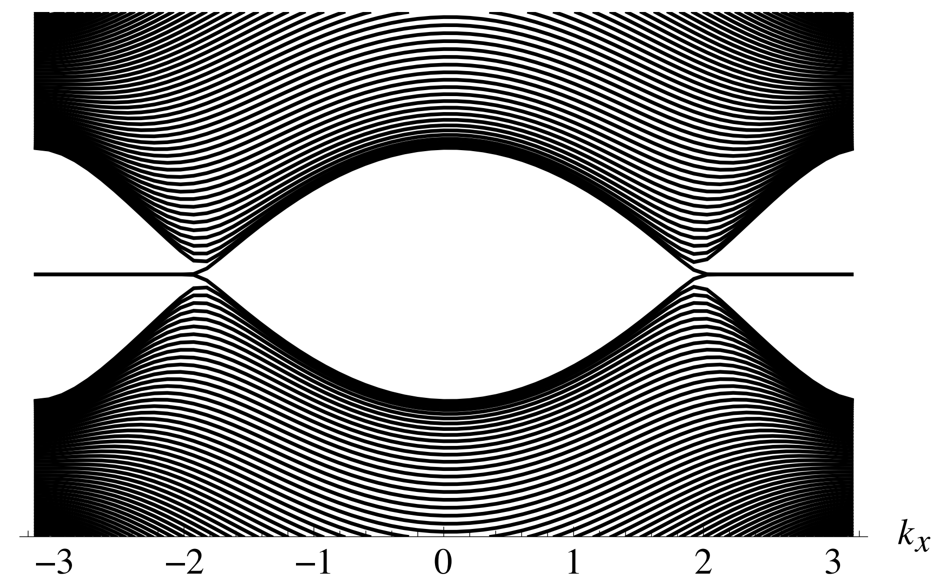


Haldane gap



Qualitative explanation: **Flat edge bands** in graphene

Appearance of edge states dictated by Wilson loop/Berry phase invariant.

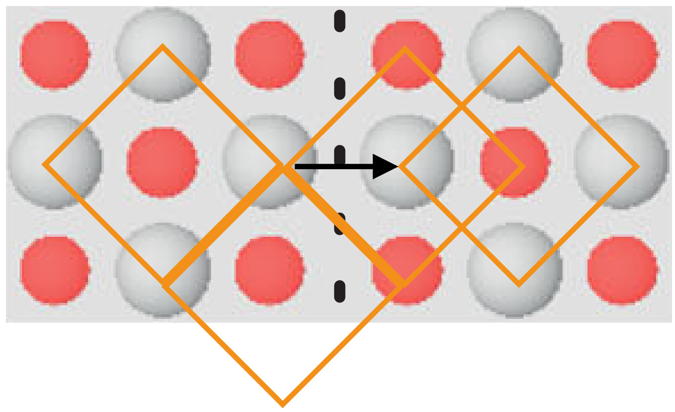


$$W = \exp\left[\int_0^{2\pi} \mathrm{d}k \langle\psi|\partial_k\psi\rangle\right]$$

$$W = \pm 1$$

Half a lattice translation: $$|\psi\rangle \rightarrow e^{\mathrm{i}\pi k}|\psi\rangle \qquad W \rightarrow -W$$

“Bulk-boundary” correspondence is exactly reversed between the two twin domains: depends on **choice of bulk unit cell vs. boundary termination**



Bonus Summary

Edge modes at TCI surface steps

1D edge states at step edges due to Berry phase mismatch between surface Dirac cones

ROBUST:

- 200 meV bulk gap
- no backscattering observable in QPI
- temperature: almost unaltered at T = 80K
- TRS breaking: almost unaltered at B = 11T
- only 10 nm wide