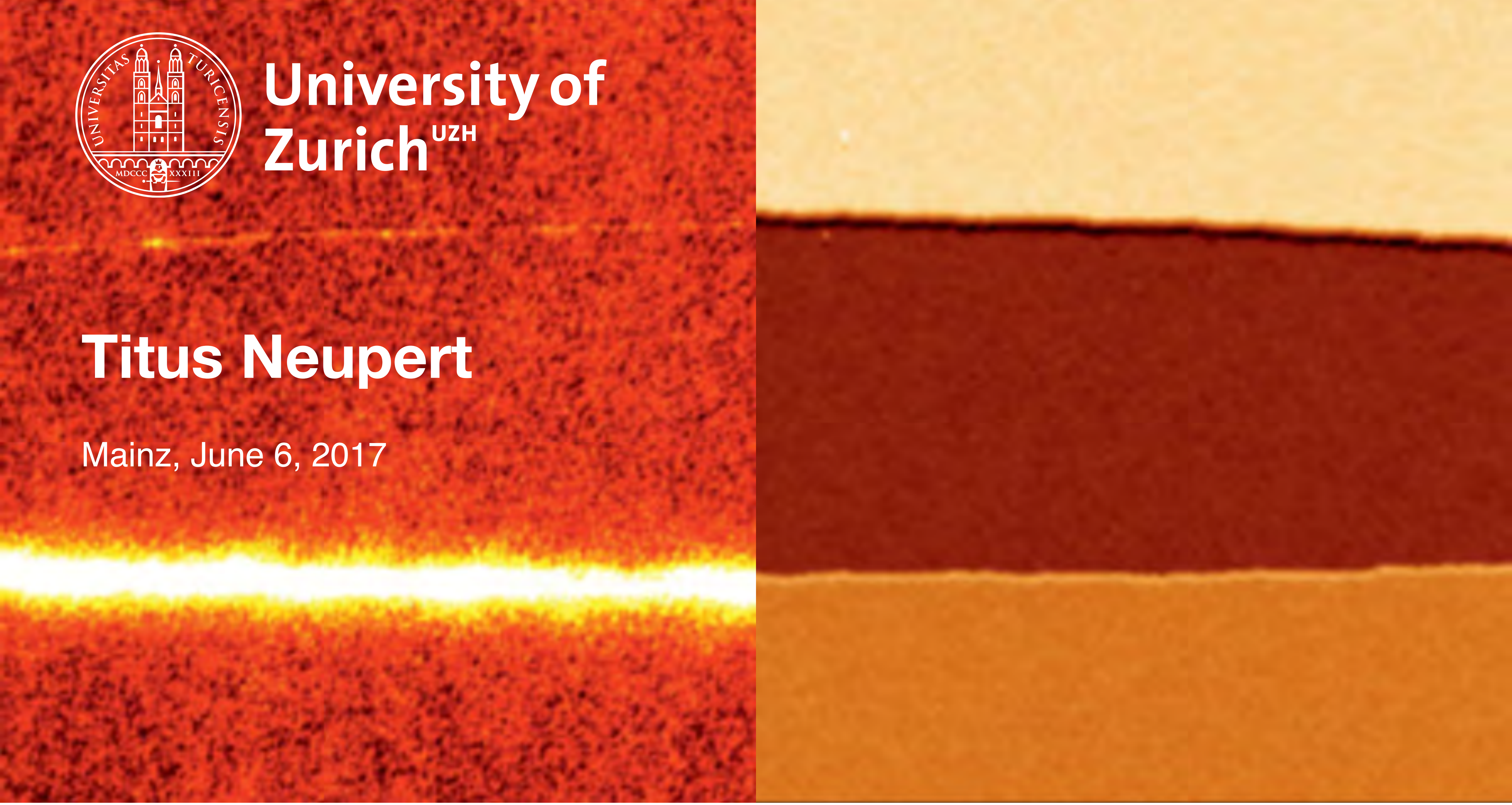


University of
Zurich UZH

Titus Neupert

Mainz, June 6, 2017

1D edge modes of 3D 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!

Outline

1. Edge modes at surface steps

Matthias Bode group
(U Wurzburg)

Tomasz Story group
(IoP Warsaw)

Ronny Thomale group
(U Wurzburg)

2. Higher-order topological insulators

Frank Schindler
(U Zurich)

Maia Vergniory
(Donostia)

Zhijun Wang
(Princeton U)

Ashley Cook
(U Zurich)

Stuart Parkin
(Max Planck Halle)

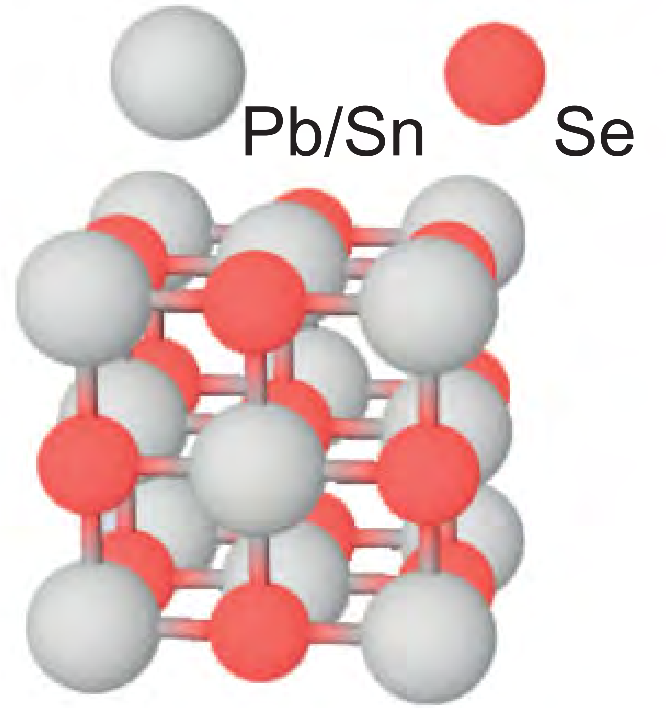
Andrei Bernevig
(Princeton U)

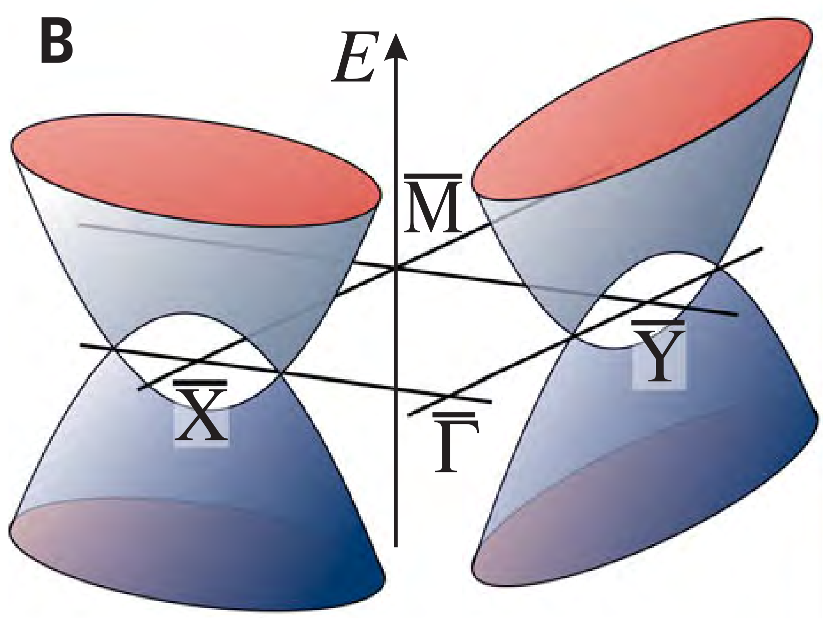
1.

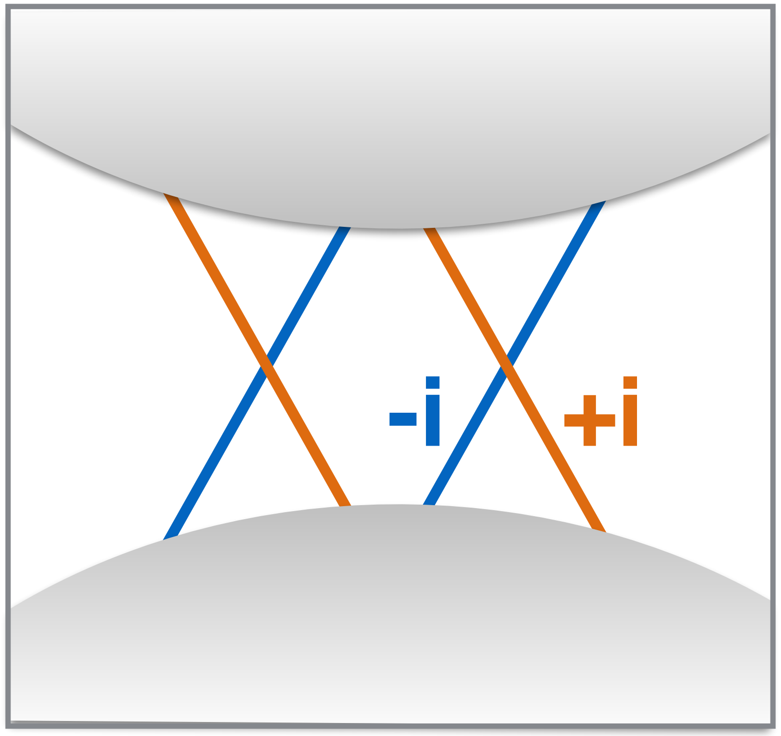
Edge modes at TCI surface steps

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







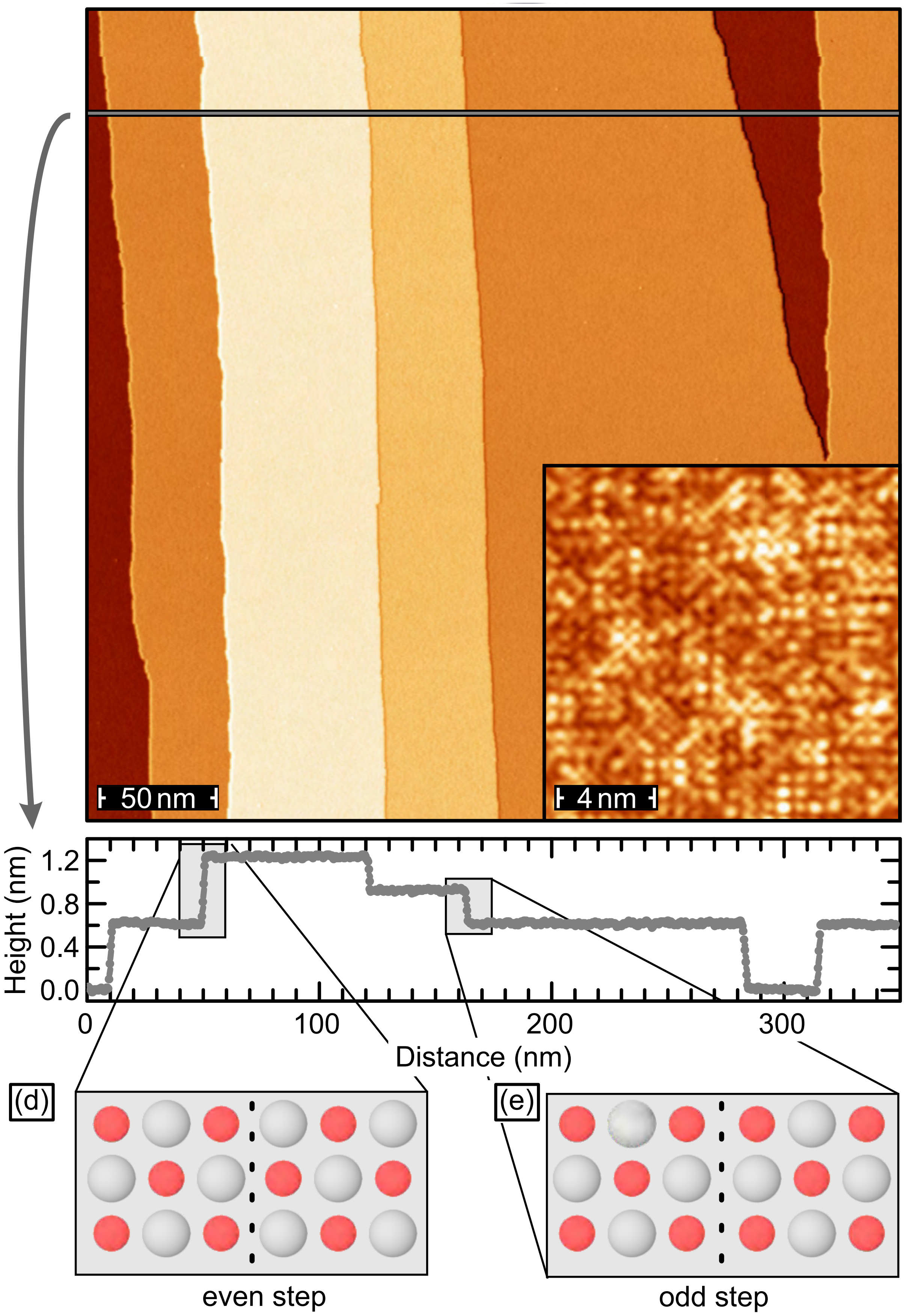
(Pb,Sn)Se: TCI with two pairs of Dirac cones,
protected by mirror Chern numbers

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

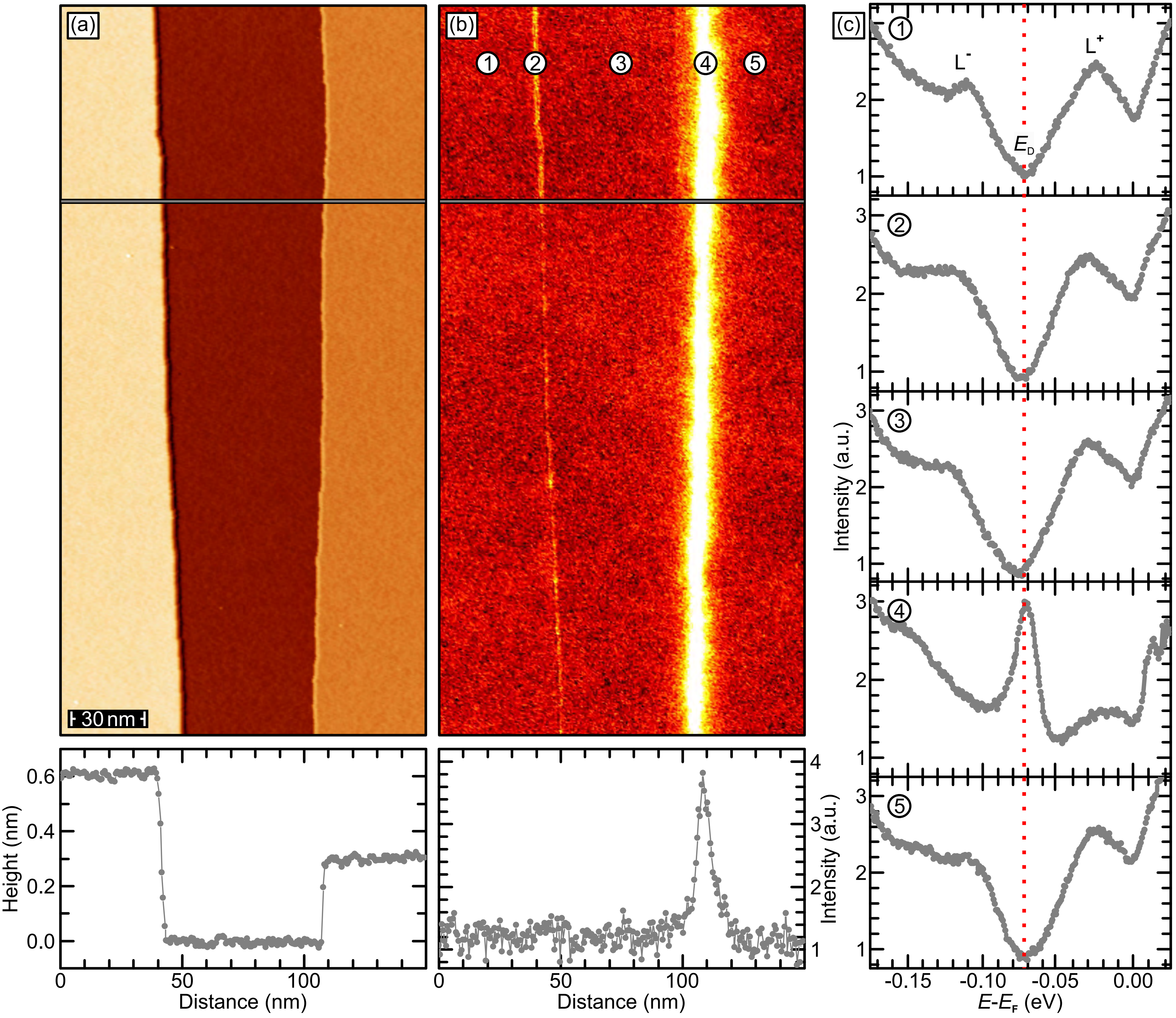
Step edges on topological crystalline insulators

Study step edges on the surface with STM

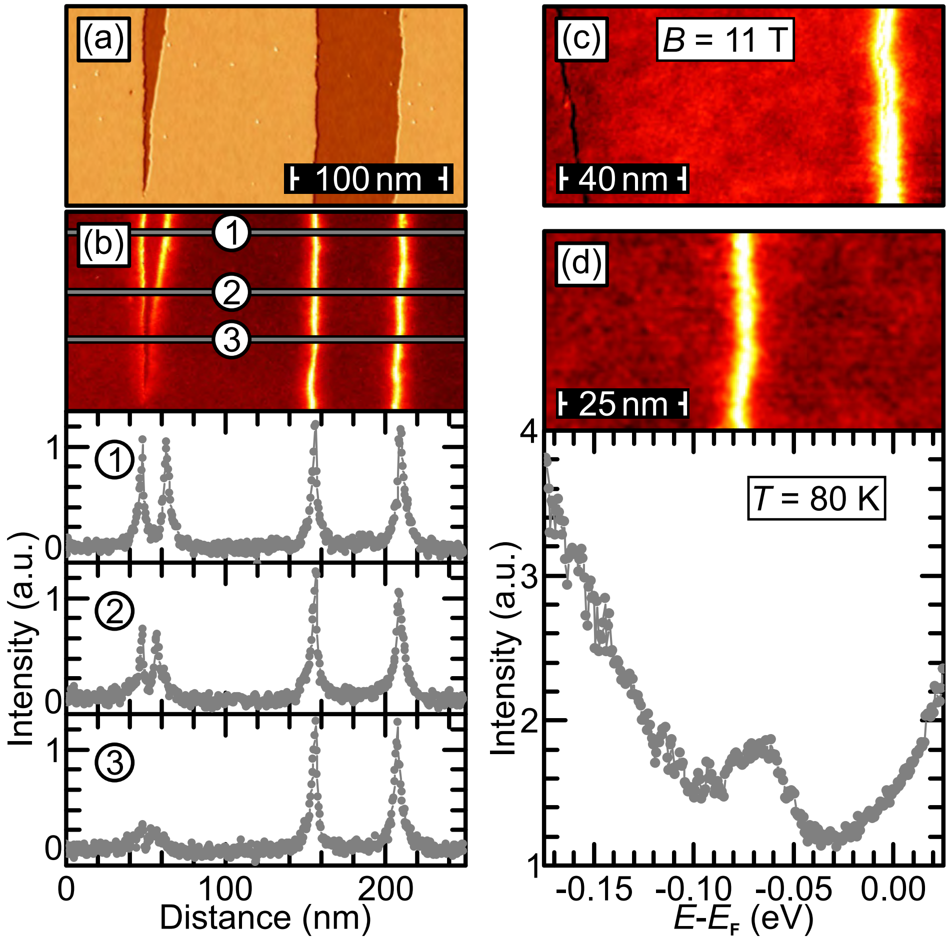
Pick (0,1) step edge orientation and distinguish **even and odd** steps



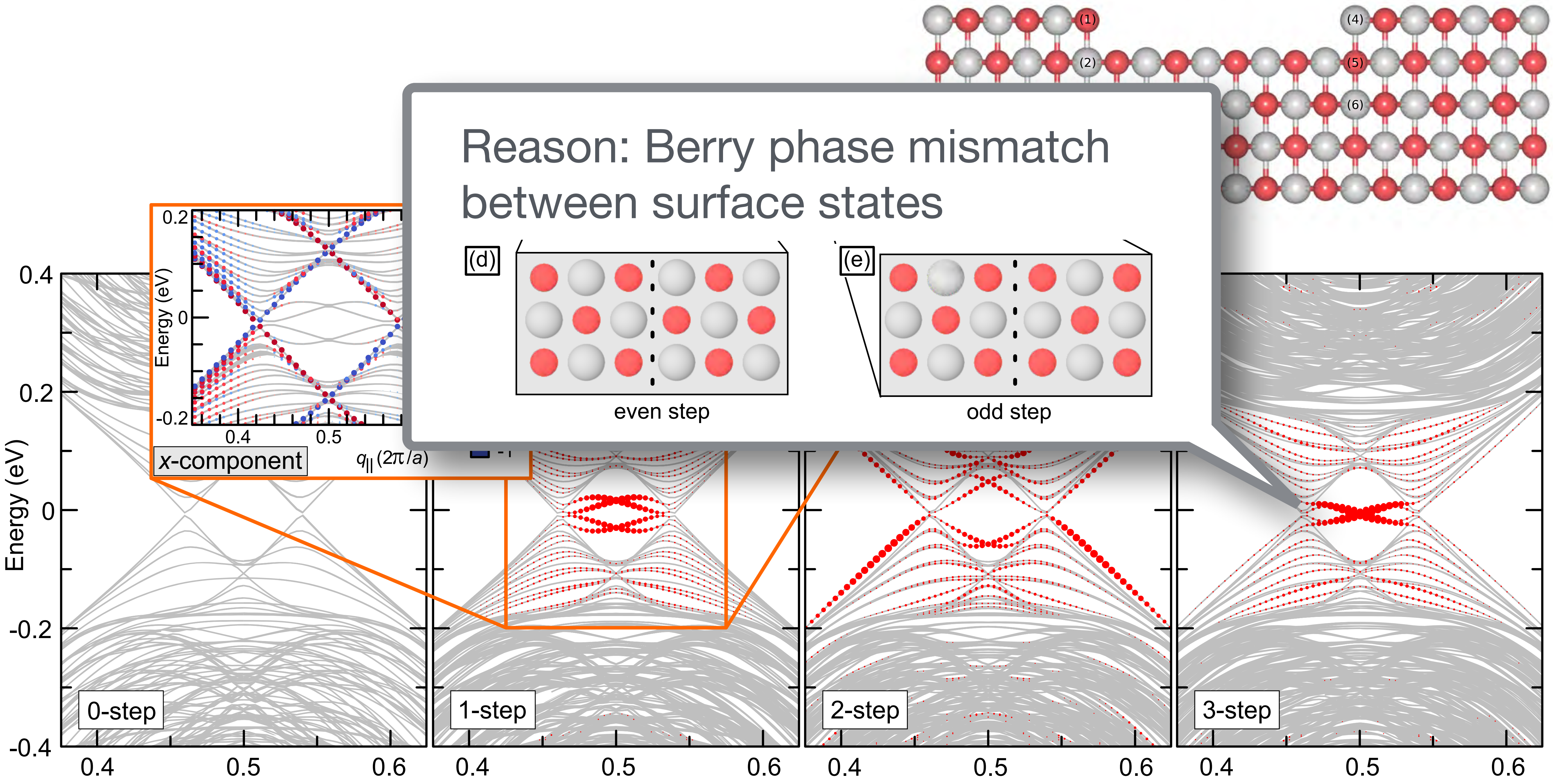
Large 1D DOS at odd steps only



Merging of step edges



Atomistic approach: DFT



Reason: Berry phase mismatch between surface states

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

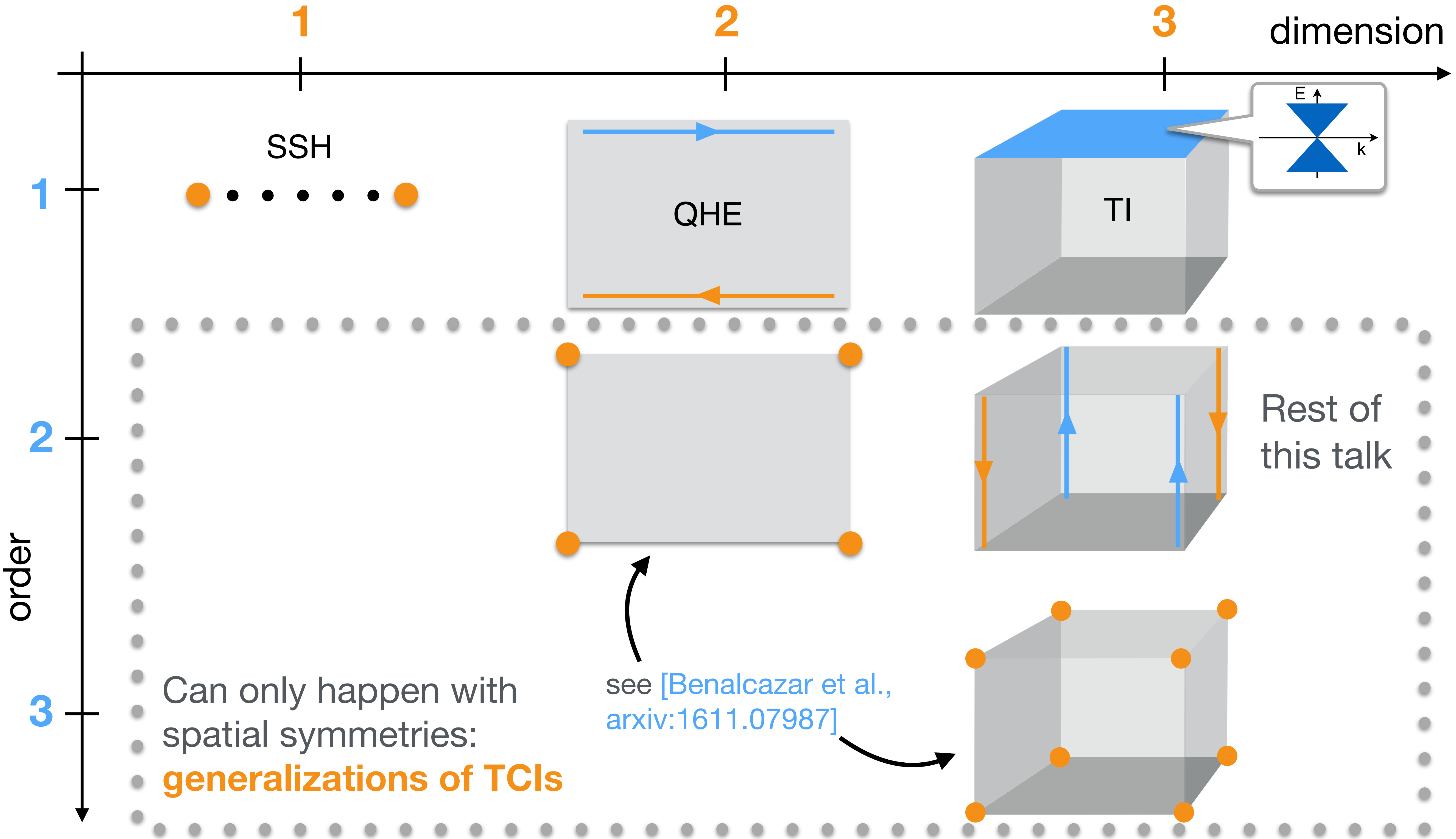
other dispersive features stem from finite size

2.

Higher-order topological insulators

Higher-order topological insulators

(d-m)-dimensional boundary components of a d-dimensional system are **gapless for m = N**, and are generically **gapped for m < N**



Rest of this talk

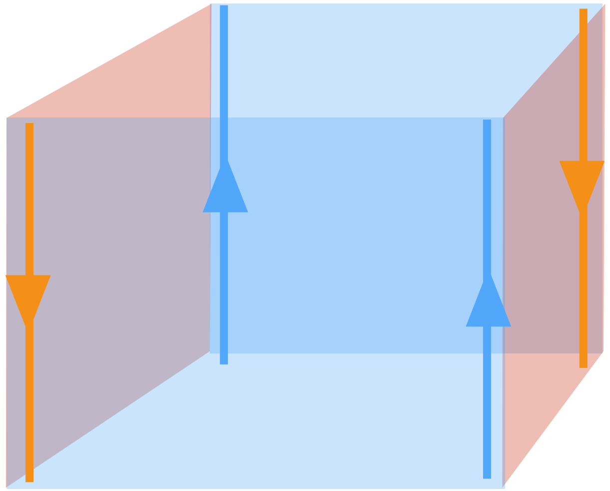
Can only happen with spatial symmetries: **generalizations of TCIs**

see [Benalcazar et al., arxiv:1611.07987]

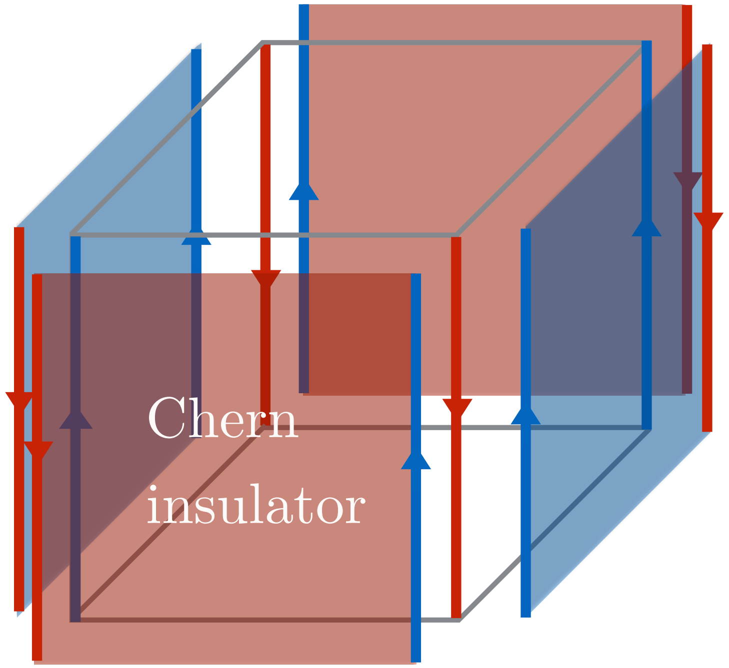
Construction of a 2nd order 3D TI

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**

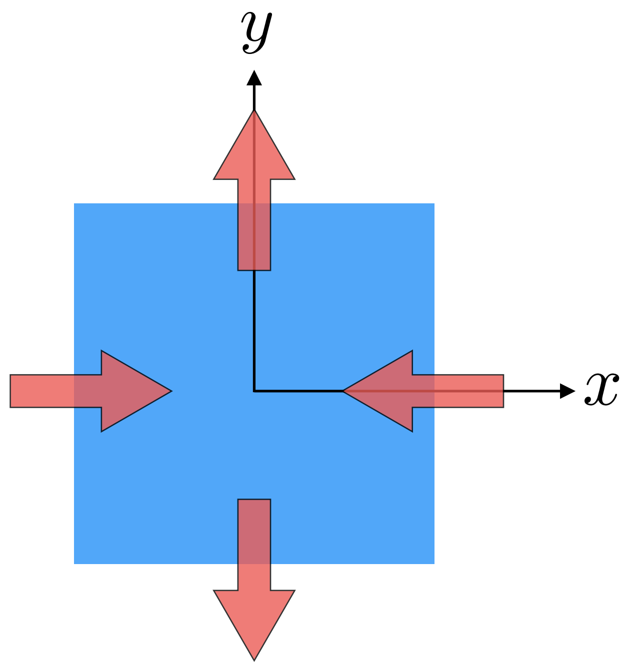


Odd number of hinge modes **stable** against any C_4T respecting surface manipulation

Bulk $\mathbb{Z}_2$ topological property

Construction of a 2nd order 3D TI

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

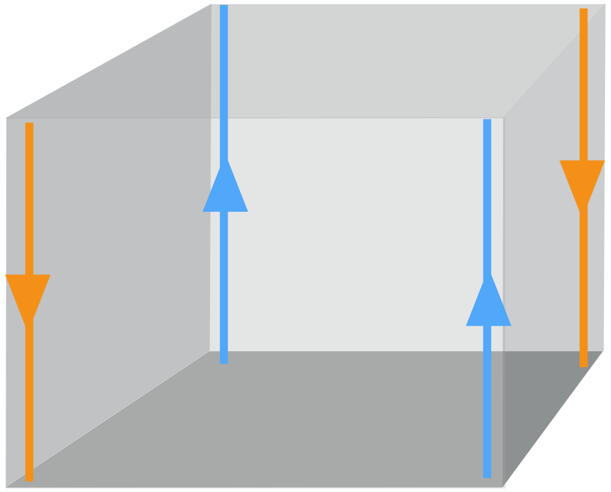


Bulk construction

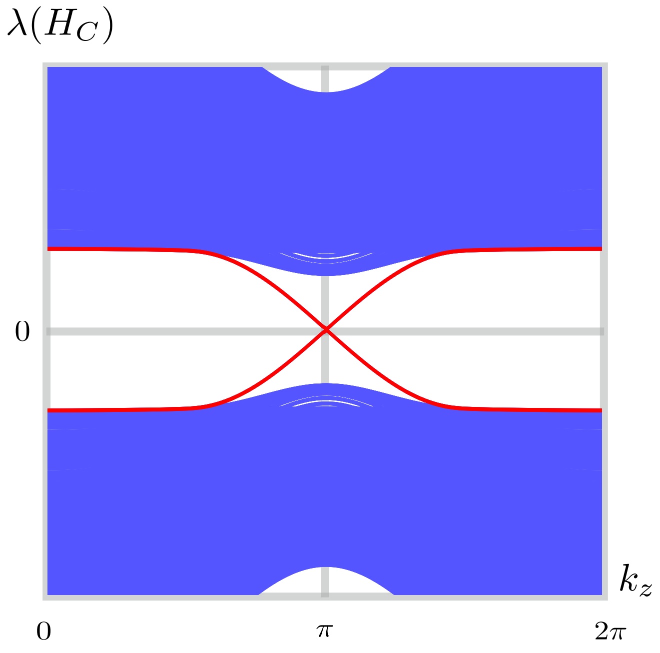
TI band structure plus (sufficiently weak) doble-q (π,π,0) magnetic order

Toy model

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



Spectrum of column geometry



Topological invariant of a 2nd order 3D TI

Topological invariant of 3D TI

Topological invariant:

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

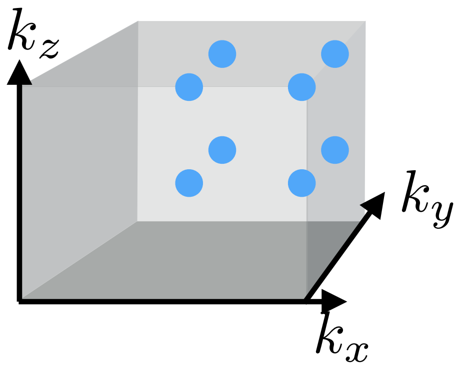
$$\mathcal{A}_{a;n,n'} = -\mathrm{i}\langle u_n | \partial_a | u_{n'} \rangle$$

$\theta = 0, \pi$ 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



Topological invariant of a 2nd order 3D TI

Same quantization with C₄T as with T alone:

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

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

Different from existing indices, because $\boxed{(C_4 T)^4 = -1}$

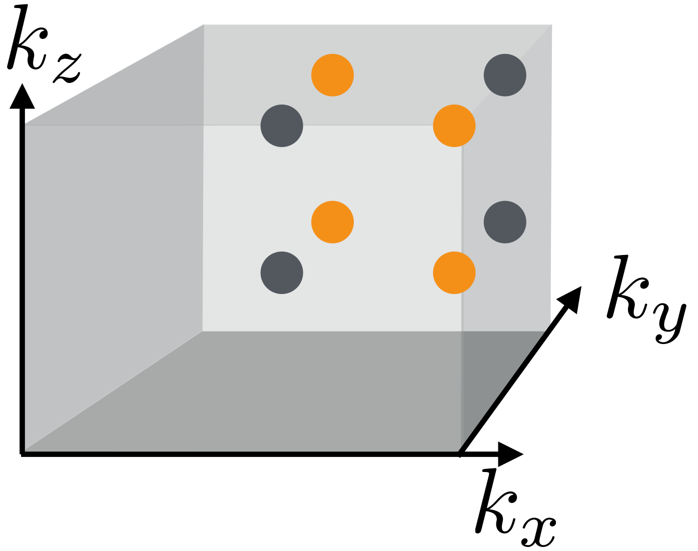
Case of additional **inversion times TRS**, IT, symmetry:
use $(IC_4)^4 = -1$ with eigenvalues $\xi_{\vec{k}}\{e^{i\pi/4}, e^{-i\pi/4}\}$ $\xi_{\vec{k}} = \pm 1$

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 C₄T invariant momenta

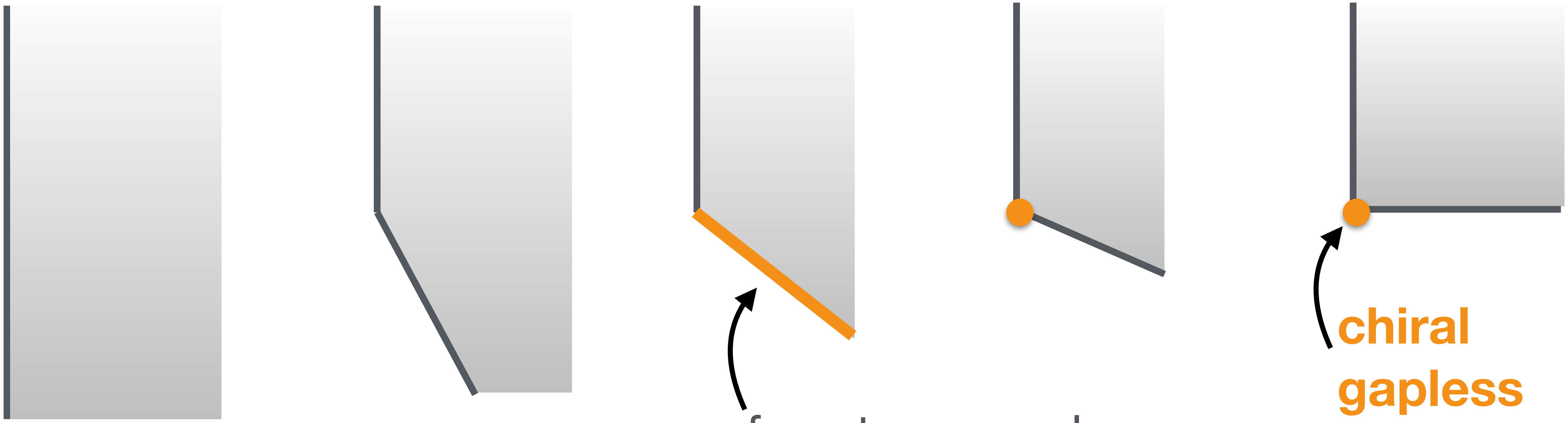
$$\boxed{(-1)^\nu = \prod_{\vec{k}\in\mathcal{I}_{\hat{C}_4^z\hat{T}}} \xi_{\vec{k}}}$$

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



Gapless surfaces?

consider adiabatically inserting a hinge



surface turns gapless
at some critical angle

**chiral
gapless
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.

2nd order 3D topological superconductor

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

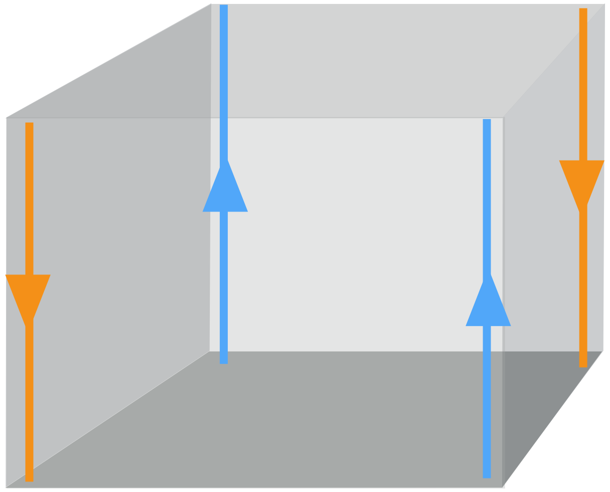
has a **particle hole symmetry** $P = \tau_y\sigma_y K$

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

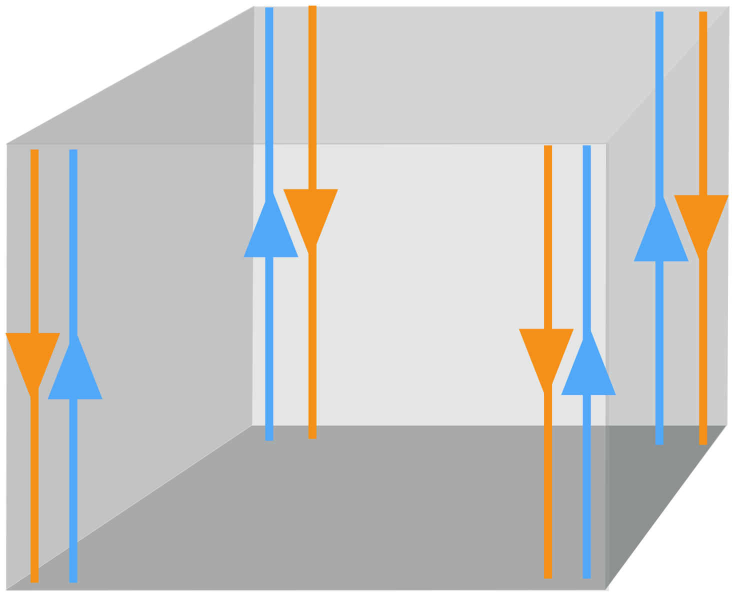
$p + \mathrm{i}d$ superconductor with chiral Majorana hinge modes



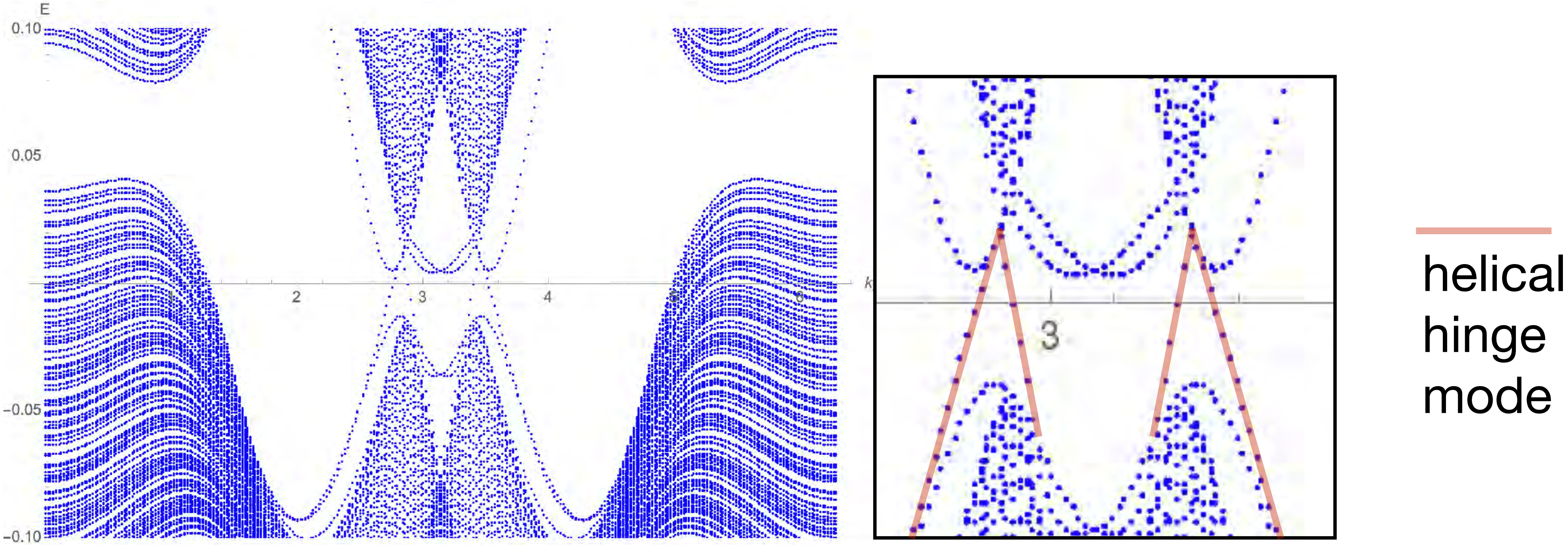
Time-reversal symmetric 2nd order 3D TI

Stabilized by mirror symmetries and TRS

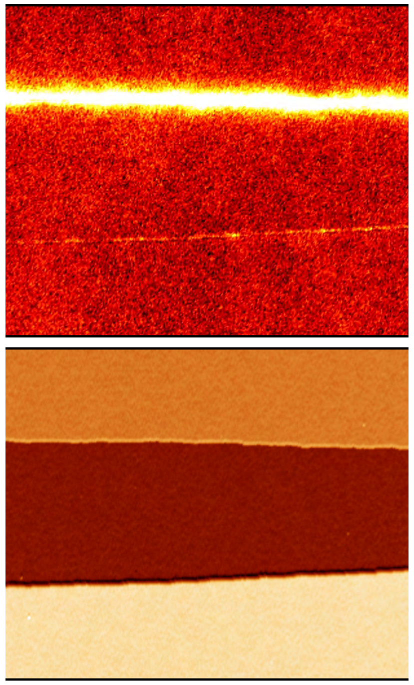
One Kramers pair of modes on each hinge



Example:

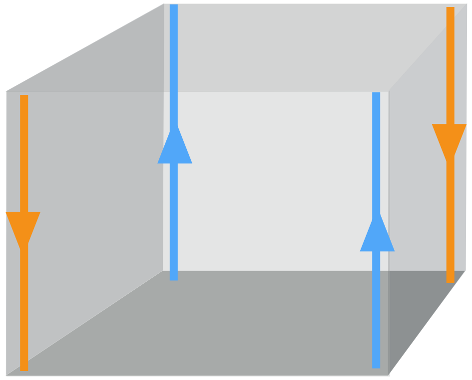


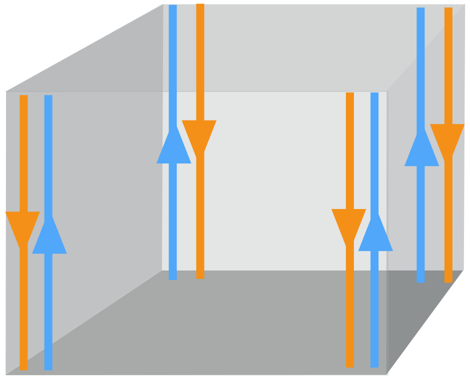
Summary



Edge modes at TCI surface steps

- 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





Higher-order topological insulators

new paradigm for topological phases protected by spatial symmetries

- hinge modes protected by 3D bulk invariant
- superconducting variant with Majorana hinges

TRB version

- single hinge like edge of QHE
- realizations in AFM spin-orbit coupled semiconductors?

TRS version

- single hinge like edge of QSHE