Topological electronic structure of twin boundaries and twinning superlattices in SnTe

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Twinning superlattices

Topological crystalline insulators (TCIs) are materials in which crystal symmetry protects the non-trivial topology of the electronic band structure [1]. In SnTe the negative bulk band gap leads to Dirac-like metallic surface states which are protected by {110} mirror symmetries [2,3]. In the present work, we perform theoretical study in SnTe twinning superlattices (TSLs) with rock-salt structures grown along [111] direction.

✓ there exist two {111} twin planes (TPs) in the supercell (Fig. a); either cationic or anionic

✓ the atomic stacking sequence is changed due to a twin plane

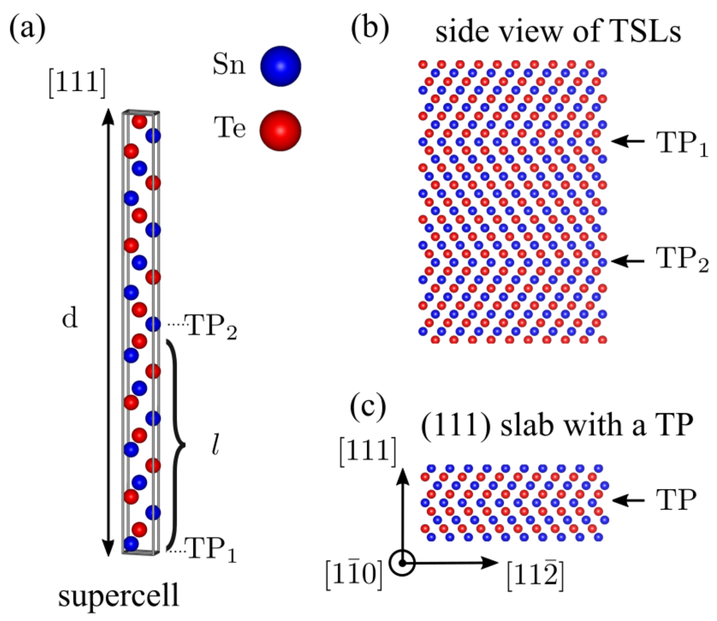
Calculations:

➢ mirror Chern number C_m and Fu-Kane $\mathbb{Z}_2$ invariant

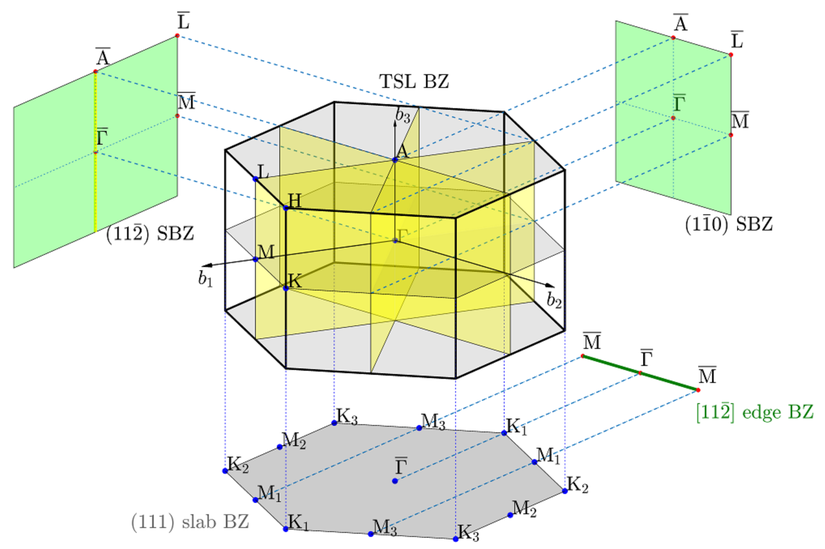
➢ (mirror) Berry curvature

➢ surface/edge spectral Green's function & band structures

Twinning superlattice structure

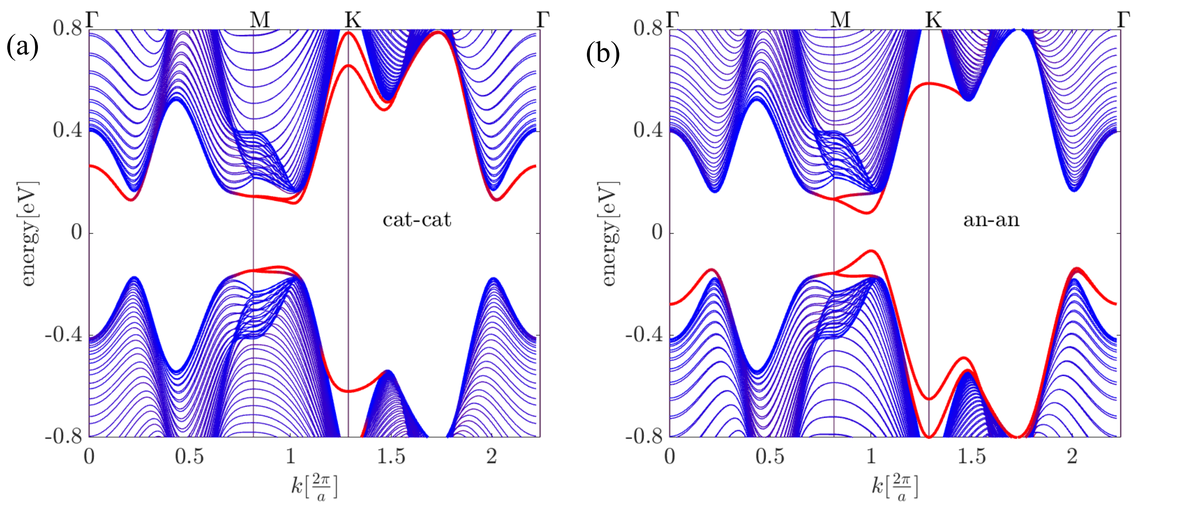


3D bulk, 2D surface & 1D edge Brillouin zone



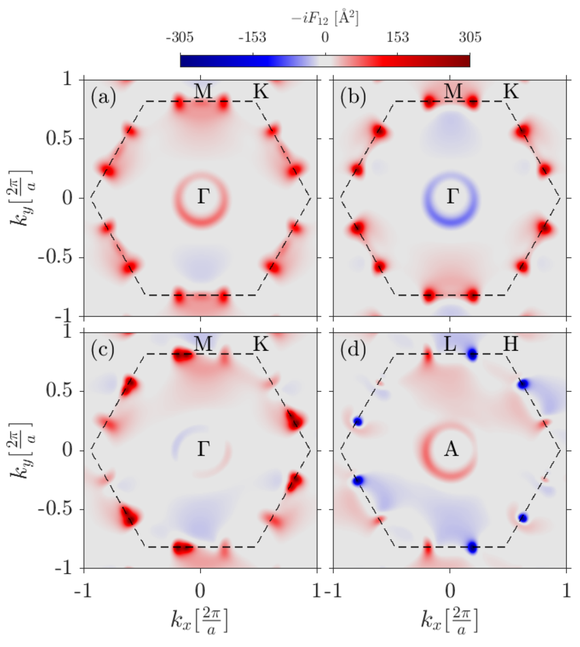
Tight-binding calculations: 3D bulk superlattices

- SnTe bulk crystal band gap → −0.33 eV
- only p orbitals parameters
- atoms near TPs → red
- intermediate atoms → blue



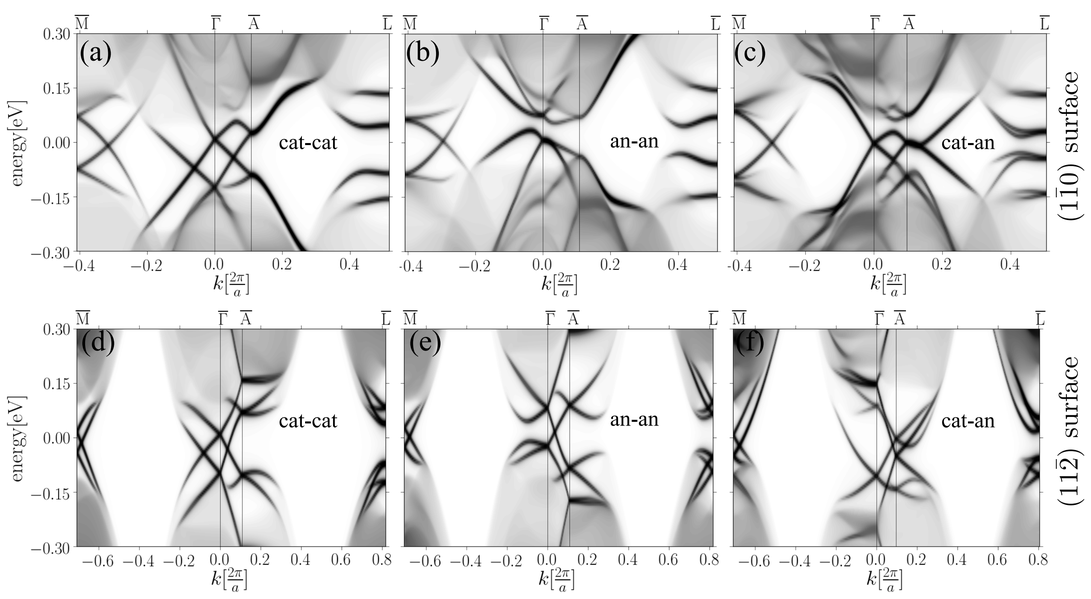
The calculated band structures of a 200 monolayer-height (ca. 36.1 nm) [111]-oriented SnTe TSLs. Colors indicates the weight of atoms to the wave functions.

TSLs	$\mathbb{Z}_2$	$C_m^{(\Gamma MK)}$	$C_m^{(ALH)}$	$C_m^{(AL\Gamma M)}$
cat-cat ($d \geq 8$, $l \in$ even)	(0;0,0,0)	4	0	2
an-an ($d \geq 8$, $l \in$ even)	(0;0,0,0)	2	0	2
cat-an ($d \geq 10$, $l \in$ odd)	(0;0,0,1)	3	1	2



- all kinds of TSLs are identified as a TCIs
- cat-an TSL is also a weak topological insulator
- curvature extrema are correlated with localization of wave functions on TPs in the vicinity of Γ and M_i and contribute $\pm 1/2$ to the Chern number C_m
- a cationic TP has $C_m^{(TP:cat)} = 2$ while anionic has $C_m^{(TP:an)} = 1$

Left: Berry curvatures associated with $+i$ (111) mirror subspace. (a) and (b) calculated for cat-cat and an-an TSLs with 16 atomic layer supercell, respectively. (c) and (d) show curvatures for cat-an TSLs with 18 monolayers.

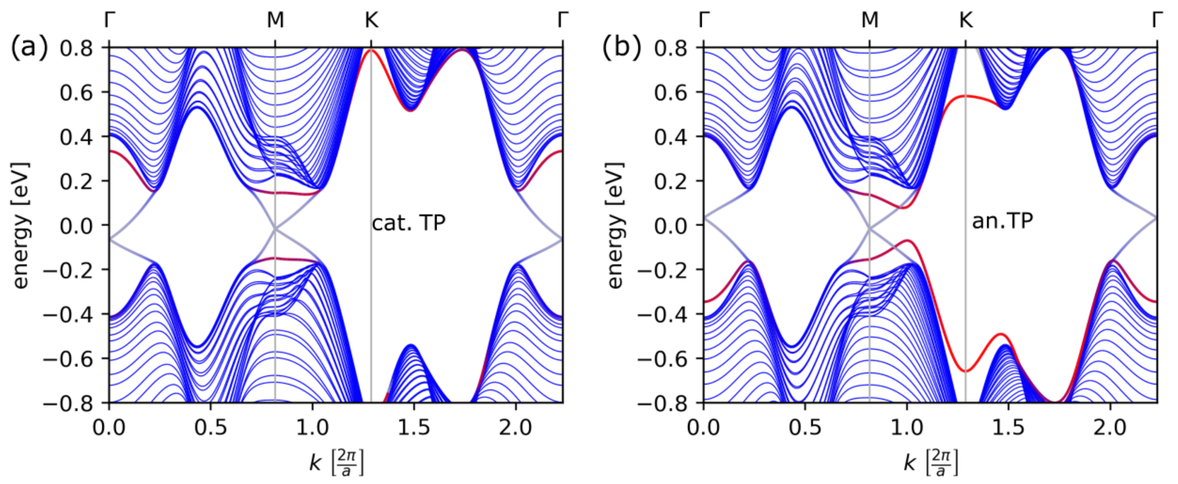


Surface spectral functions of TSLs along $(1\bar{1}0)$ (top row) and $(11\bar{2})$ (bottom row). The spectra calculated for $d = 16$ monolayer height for same kind TPs. The thickness for cat-an TSLs is $d = 18$ atomic layers.

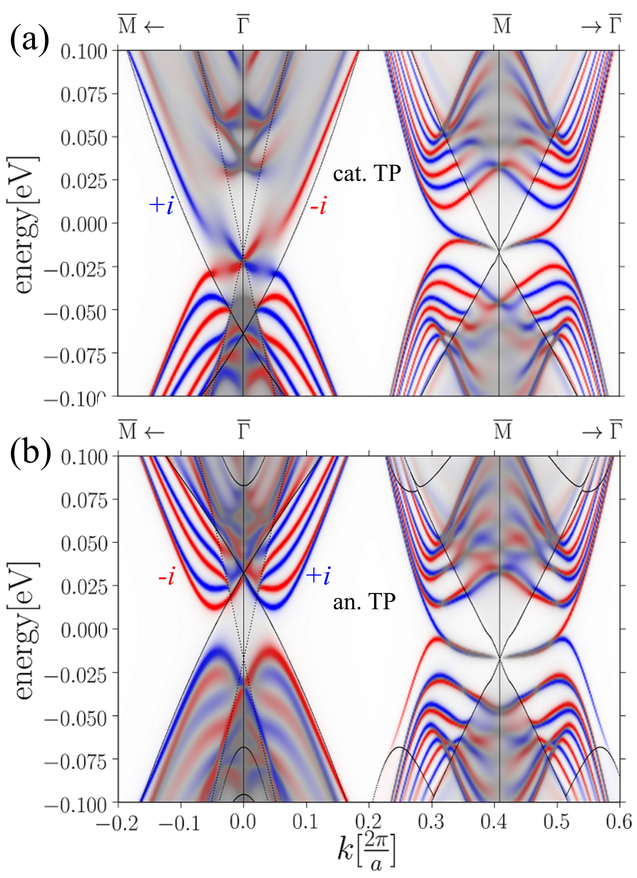
Tight-binding calculations: (111) slab with single TP

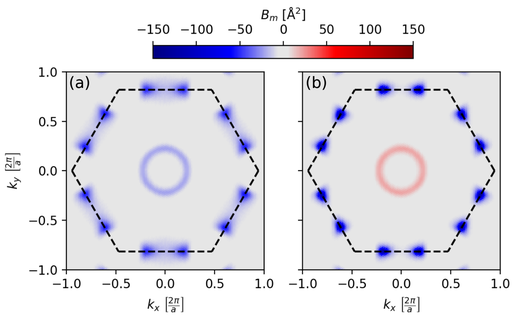
➢ **Purpose**: to find the influence of a single TP on topological phases

- atoms near TPs → red
- atoms near surfaces → gray
- intermediate atoms → blue



The calculated band structures of [111]-oriented twinned SnTe slabs with 121 atomic layers (ca. 21.8 nm) thickness.





Right: Mirror Berry curvatures of (111)-oriented twinned crystal slabs with (a) a cationic and (b) an anionic TP in the middle.

Consistently with 3D TSLs:

- cationic twin boundary has $C_m = 2$
- anionic twin boundary has $C_m = 1$

For tuning the surface energy:

- onsite potential added to the outermost layers

Left: Edge spectra of a cationic TP (a) and an anionic TP (b) along $[11\bar{2}]$ 1DBZ. Local extrema of the 2D bands projected to the edge shown by black dotted lines. $+i$ and $-i$ denote (111) mirror subspaces.

Conclusions

We found that the cationic TP is topologically distinct from the anionic case due to the opposite sign of Berry curvatures around Γ point.

We show that for a large enough distance between $TP_{(1)}$ and $TP_{(2)}$/surface:

1. The results at $\bar{\Gamma}$ are pertained to the properties of the electronic states localized at TPs.
2. The edge states at $\bar{M}$ are not confined to the TP

References and Acknowledgment

[1] L. Fu, Phys. Rev. Lett. **106**, 106802 (2011)

[2] T. H. Hsieh et al., Nat. Commun. **3**, 982 (2012)

[3] Y. Ando et al., Annu. Rev. Condens. Matter Phys. **3**, 361 (2015)

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