# One-dimensional Dirac modes of a pentagonal topological crystalline insulator nanowires

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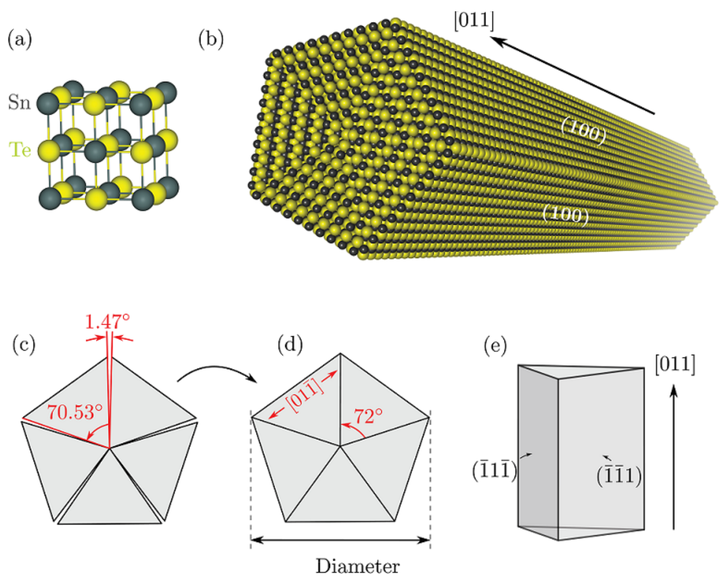
## IV-VI semiconductor pentagonal nanowires

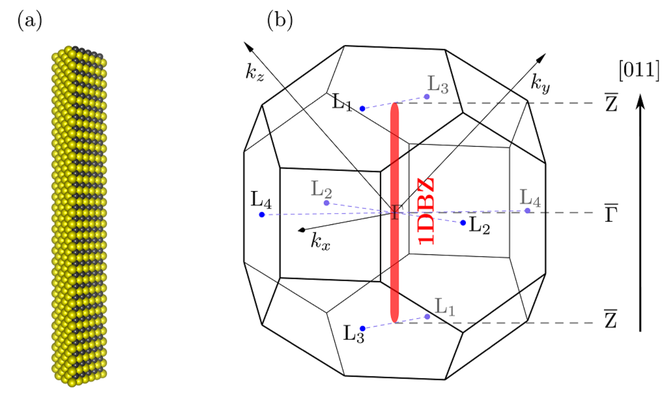
IV-VI compounds are categorized as a narrow bandgap semiconductors. In particular, SnTe has inverted band gap and is identified as a topological crystalline insulator (TCIs). The band gap occurs in four non-equivalent high symmetry $L$ points in the reciprocal space [1]. Five-fold NWs have been recently grown and demonstrated by transmission electron microscopic measurement [2].

- The NWs are grown along [011] direction
- They have five {111} twin plane (TP) boundaries; either exclusively cationic or anionic
- Five {100} free surfaces
- NWs have inherent circumferential strain ( by the angle $1.47°$)
- topological phase remains unchanged due to this strain
- The gap changes are less than 10% respect to unstrained bulk crystal for SnTe and less than 20% for $Pb_{0.6}Sn_{0.4}Se$

### Pentagonal modeled structure



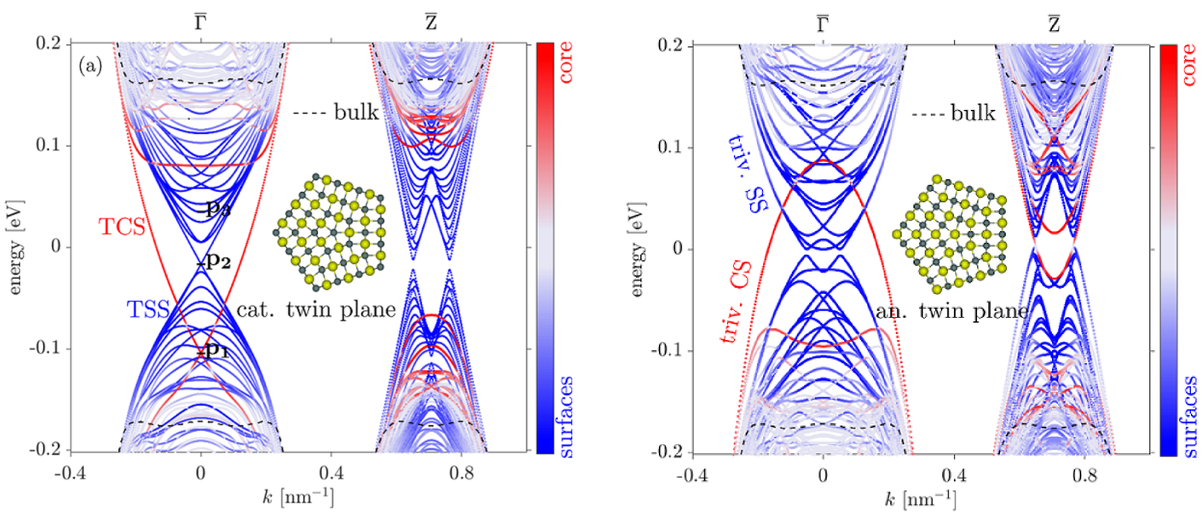

### 3D & 1D Brillouin zone




- Perspective of one triangle of pentagonal NW (Fig. a)
- The band gaps are placed in two distinct $\overline{\Gamma}$ and $\overline{Z}$ points in 1DBZ
- 1DBZ is the same for each triangle of NW

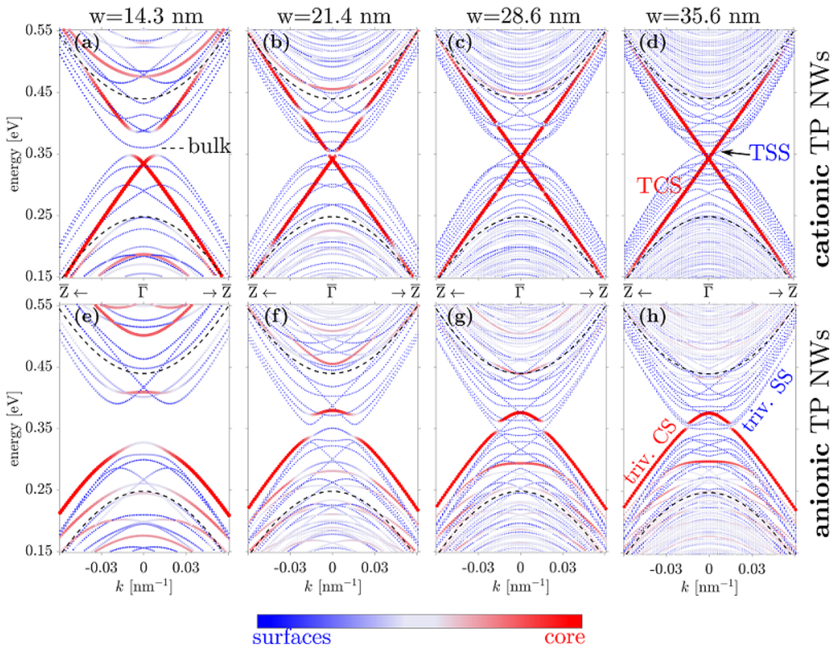
## Tight-binding band structure of pentagonal nanowires

Band structure calculations have been performed using simplified tight-binding (TB) parameterization with $p$ orbitals for SnTe and realistic $sp^3d^5$ parameterization for (Pb,Sn)Se [3]. The bulk band gaps are $-0.33$ eV for SnTe and $-0.19$ eV for $Pb_{0.6}Sn_{0.4}Se$.



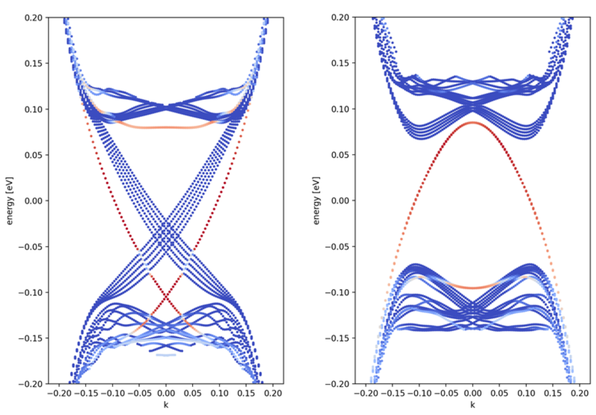

Right: Electronic structure for SnTe pentagonal NW with anionic TPs. Observation of topologically trivial (triv.) core states (CS) and surface states (SSs) obtained for 14 nm (20 rings) thickness.

Left: (a) Electronic structure for SnTe pentagonal NW with cationic TPs. Observation of topological CS and topological SSs obtained for 14 nm (20 rings). (b–d) Spatial distribution of localized CS (at $p_1$), hybridized hinge states (at $p_2$) and conventional TCI SSs (at $p_3$) presented by sum of the squared moduli of the wave functions, respectively.




Electronic structure for $Pb_{0.6}Sn_{0.4}Se$ pentagonal NW. Upper row: Topological CS is presented in cationic TPs. Due to confinement effect the CS hybridizes with SSs and open the gap (a,b). Lower row: Panels (e)-(f) represent the anti-crossing triv. CS for anionic TP NWs.

## Hinge states in a pentagonal NWs




- imposing perturbation to the atoms where located at the faces of pentagonal wire
- breaking all relevant mirror symmetries
- introducing on-site potential at each hinge (breaking $C_5$)

Left: Cationic TPs, one topological CS (red) and five topological hinge states. Right: Anionic TPs, no Dirac crossings become visible.

## Low-energy theory of the core and hinge states

**The k.p Hamiltonian** can be written as

$$H_\lambda(k_z) = \epsilon_{0,\lambda} + \begin{pmatrix} \Delta_\lambda & e^{\frac{i\pi}{10}} v_\lambda k_z \\ e^{-\frac{i\pi}{10}} v_\lambda k_z & -\Delta_\lambda \end{pmatrix} \quad (1)$$

where $C_5$ eigenvalue is

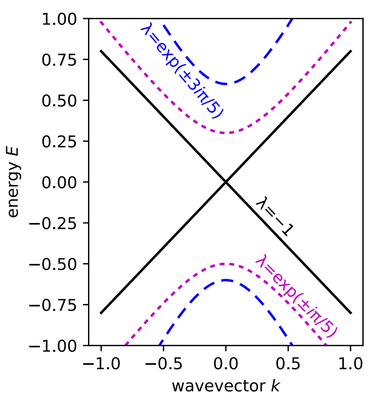
$$\lambda \in \left\{-1, e^{\frac{i\pi}{5}}, e^{-\frac{i\pi}{5}}, e^{\frac{3i\pi}{5}}, e^{-\frac{3i\pi}{5}}\right\} \quad (2)$$

The real valued parameters $\epsilon_{0,\lambda}$, $\Delta_\lambda$, and $v_\lambda$ satisfy constraints

$$\Delta_{\lambda^*} = -\Delta_\lambda, \quad v_{\lambda^*} = v_\lambda, \quad \epsilon_{0,\lambda^*} = \epsilon_{0,\lambda}. \quad (3)$$

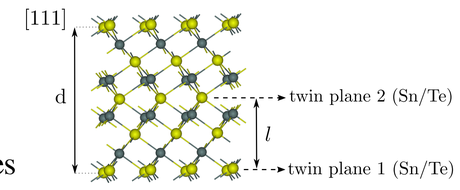
**Consequences:**

- symmetry dictates $\Delta_{-1} = 0$
- spectrum in the subspace $\lambda = -1$ is gapless (Dirac crossing)




## Topological phases of twin planes

[111] heterostructure constructed with twin planes $\Longrightarrow$

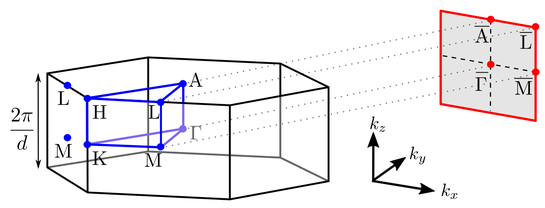



**Purpose:**

- influence of twin plane types on topological phases
- comparison with pentagonal NWs

**Method:**

- topological invariant calculations - mirror Chern number $C_m$ and $\mathbb{Z}_2$
- surface spectral Green's functions




Bulk BZ and surface BZ of a [111] heterostructure.

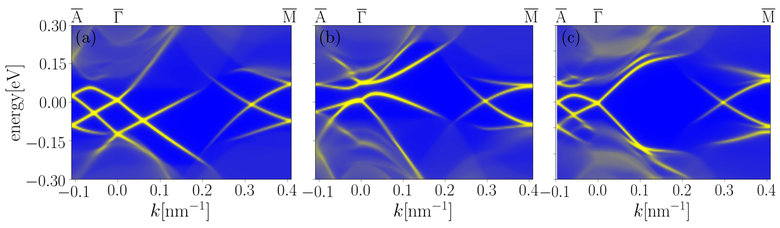



Figure: The $(10\bar{1})$ surface spectrum calculated for $d = 16$ monolayer height for both cationic (a) and anionic (b) TPs. (c) The spectral solutions for $d = 18$ monolayer height, hosting alternate TP kind. Table: The mirror Chern number $C_m$ and $\mathbb{Z}_2$ invariants calculated for 3D heterostructures grown along [111] direction.

| layers | cat-cat | | an-an | | cat-an | |
|---|---|---|---|---|---|---|
| | $C_m$ | $\mathbb{Z}_2$ | $C_m$ | $\mathbb{Z}_2$ | $C_m$ | $\mathbb{Z}_2$ |
| 4 | 0 | 0 | 0 | 0 | – | – |
| 6 | – | – | – | – | 0 | 0 |
| 8 | 4 | 0 | 2 | 0 | – | – |
| 10 | – | – | – | – | 3 | 1 |
| 12 | 4 | 0 | 2 | 0 | – | – |
| 14 | – | – | – | – | 3 | 1 |
| 16 | 4 | 0 | 2 | 0 | – | – |
| 18 | – | – | – | – | 3 | 1 |

## Conclusions

In $C_5$-symmetric NW, the Dirac point exists only in $C_5 = -1$ subspace when the five TPs dividing the NW segments are cationic. However, exact crystalline symmetry is not necessary for the crossing to emerge. The Dirac point still persists even after $C_5$ is weakly broken, because topological CS or topological hinge states are protected by time-reversal symmetry.

The core and hinge topological states can be interpreted as hybridized edge states of five twin boundaries which effectively act as quantum spin Hall insulators.

## References and Acknowledgment

[1] T. H. Hsieh et al., Nat. Commun. **3**, 982 (2012)
[2] D. Janaszko et al, the XVII$^{th}$ International Conference on Electron Microscopy (2020)
[3] P. Dziawa et al., Nat. mater. **11**, 1023 (2012)

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