Surface states of the topological crystalline insulator $Pb_{0.4}Sn_{0.6}Te$

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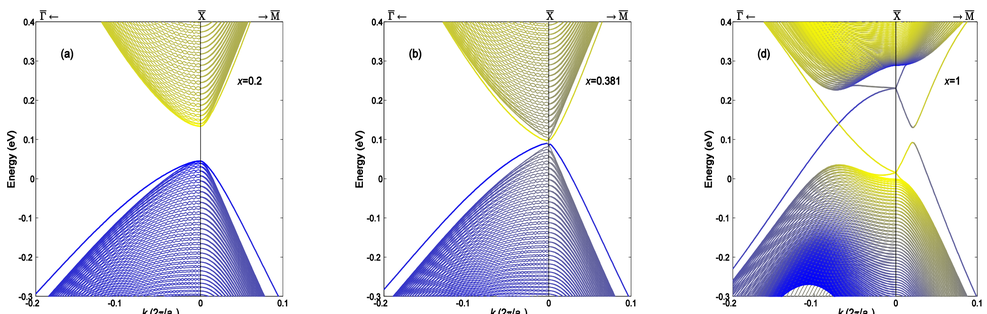
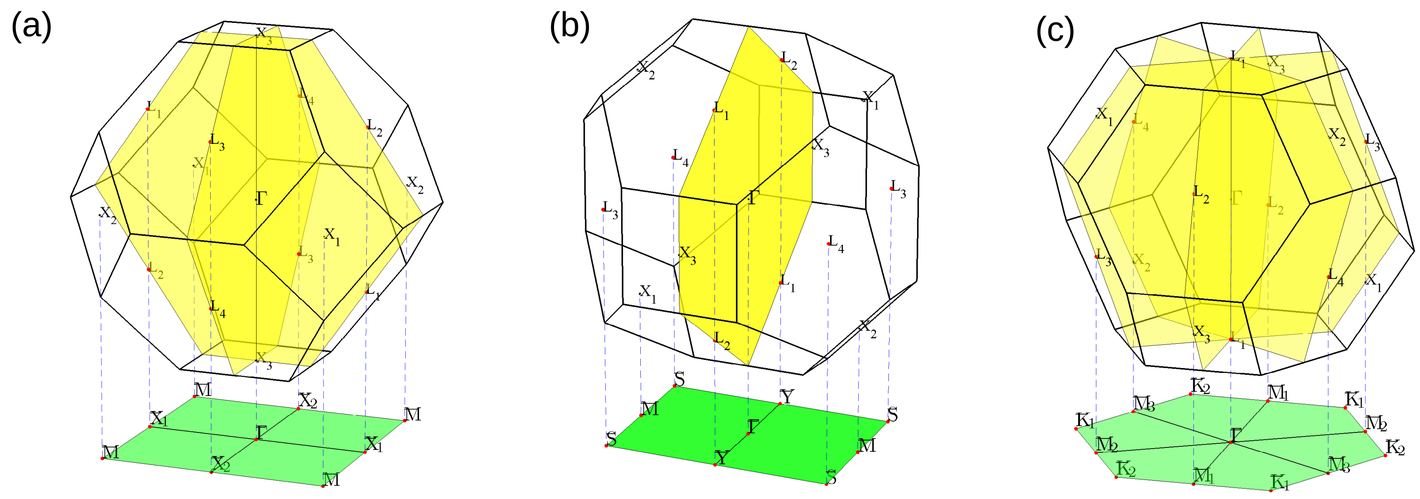
Topological insulators are new quantum materials that behave as insulators in their interior while permitting the movement of charges on their surfaces which are protected by time-reversal symmetry. Recently, it has been theoretically predicted[1] and experimentally proved[2] that SnTe belongs to a new class of topological materials, namely, topological crystalline insulators (TCI), in which crystalline mirror symmetry replaces the role of time-reversal symmetry in topological protection. Using a tight-binding approach, we study theoretically the nature of surface states in $Pb_{0.4}Sn_{0.6}Te$. In this rock-salt TCI, the surface states with nontrivial Dirac-like energy spectrum can form at many crystal surfaces symmetric about {011} mirror plane. The number of Dirac points in the surface Brillouin zone (BZ) corresponds to four *L*-points. Apart from the {001} oriented cleavage surface, also the surface states for {011} and {111} families has been studied.

(001) Surface electronic band structure - phase transition by changing the composition



Band structure of $Pb_{1-x}Sn_xTe$ 90 nm [001] oriented slab for different compositions. It shows the phase transition from ordinary to topological insulator by changing x. For $x > x_0$ we have obtained surface states with expected properties[2].
They have closed gaps in $\overline{\Gamma}$-$\overline{X}$ directions protected by {011} mirror symmetry.
The blue to yellow color coding indicates again the contributions of the cation (yellow) and anion (blue) p-orbitals to the wavefunctions.

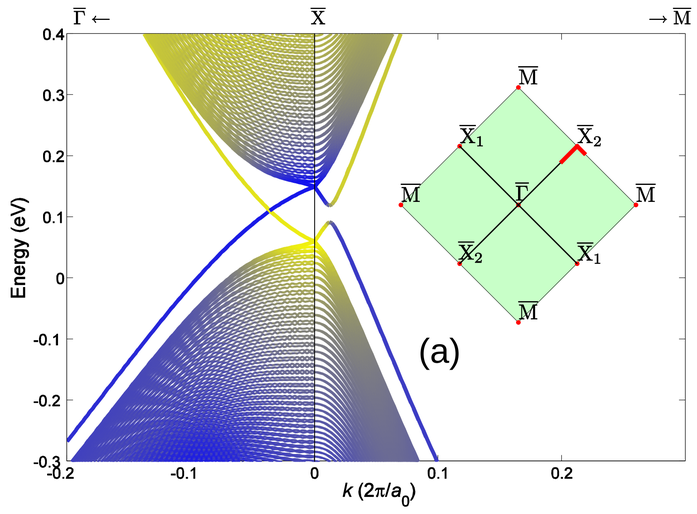
Brillouin zone and its projections into different 2D BZ



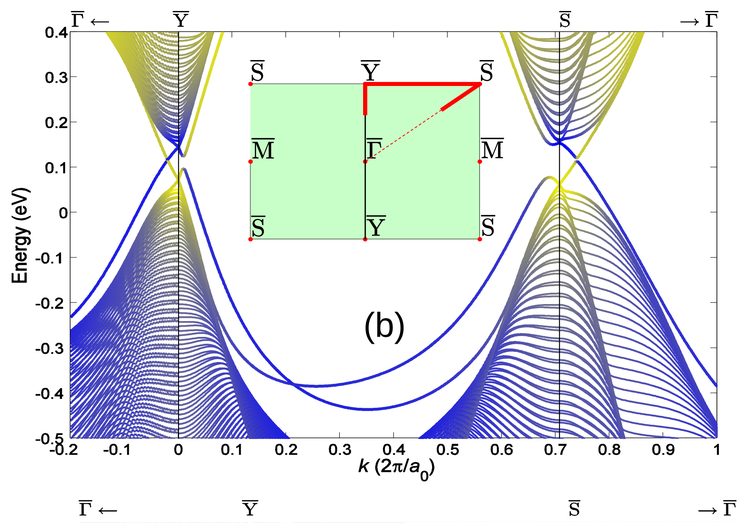
The Brillouin zone for the (a) [001], (b) [011] and (c) [111] oriented rock-salt crystal with the corresponding 2DBZs (in green). The {011} mirror planes of all surfaces are marked in yellow. In the 2DBZs the {011} mirror plane symmetry lines are also depicted.

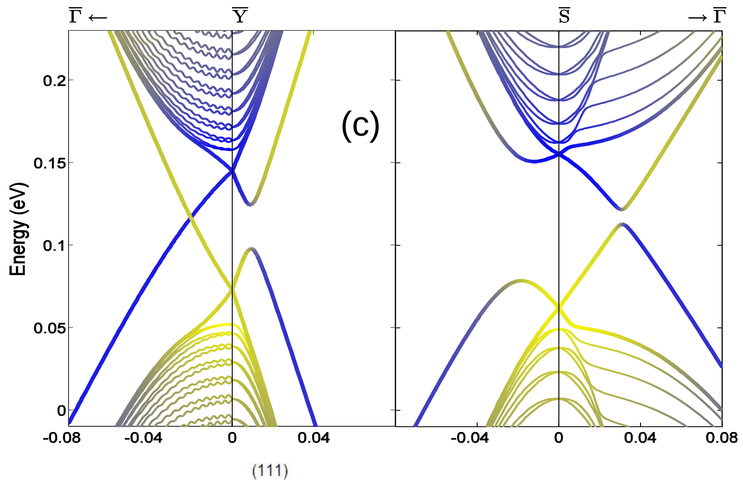
Calculation of band structures have been done by tight binding method with nearest neighbor interactions and sp^3d^5 parameterization taken from *Carig S. Lent et al.*[3]. The mixed crystal is described by virtual crystal approximation. To explore the properties of PbSnTe surface states we have used a slab geometry with two surfaces separated enough far (~80-90 nm) to be assured there is no interaction between them.

(001) Surface

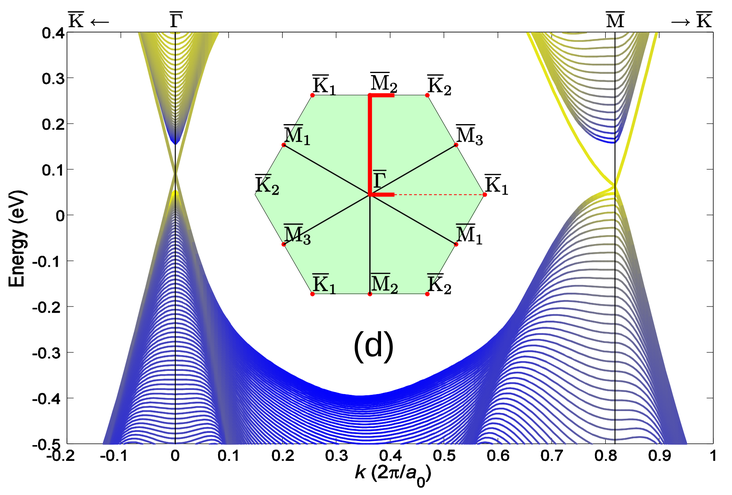


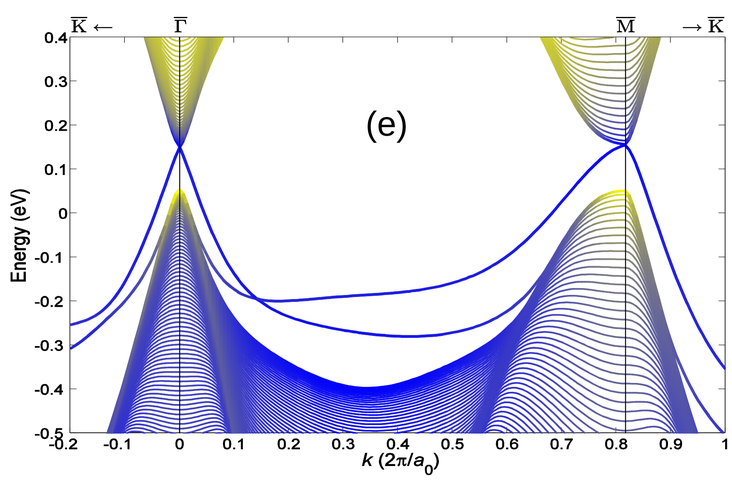
(011) Surface



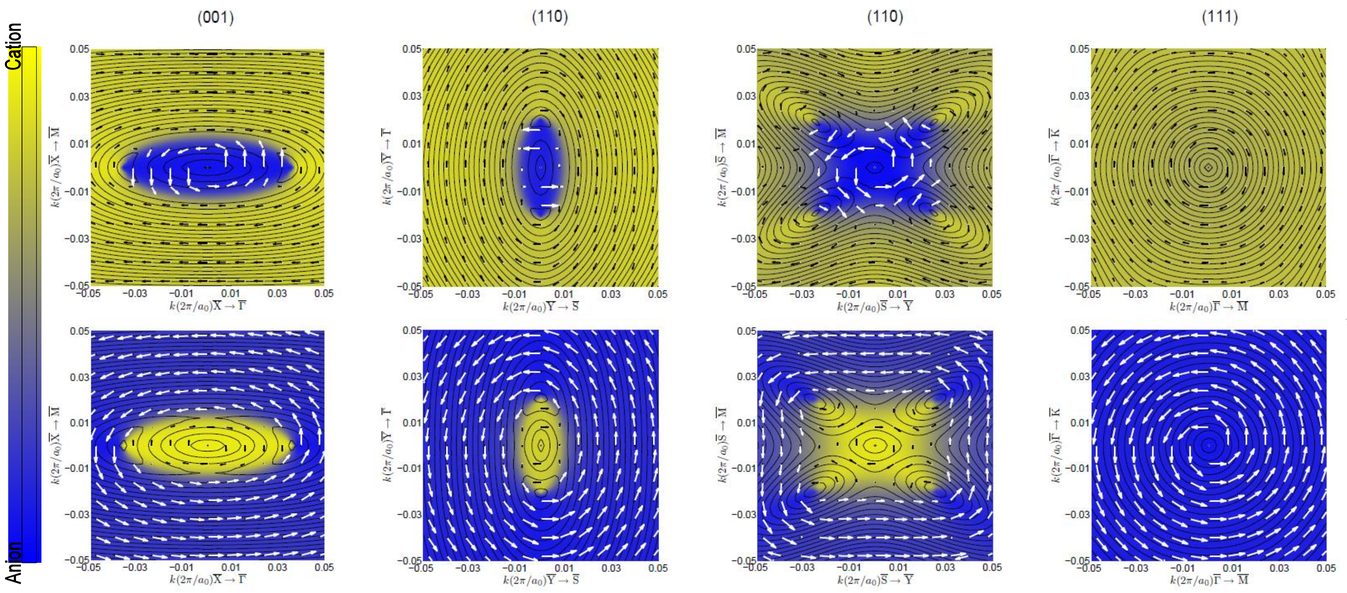


(111) Surface





(a) The calculated band structure of a [001] oriented $Pb_{0.4}Sn_{0.6}Te$ slab along $\overline{\Gamma}\,\overline{X}\,\overline{M}$ direction.
(b)The band structure of a [011] oriented slab, for the *k* wave vectors shown in the inset by the red line. The zoomed view (c) of the band structure in the vicinity of the $\overline{Y}$ and $\overline{S}$ points of the 2DBZ has been obtained for a thicker slab. (d) The band structure of a [111] oriented slab for the *k* wave vectors of the 2DBZ along the $\overline{K}\,\overline{\Gamma}\,\overline{M}\,\overline{K}$ pass, as shown in the inset by the red line. The band structure of a slab with cations at the surfaces is presented in (d), with anion surfaces in (e).



Contour plots of the constant-energy lines of the [001], [011] and [111] surface states of $Pb_{0.4}Sn_{0.6}Te$ above (upper row) and below (lower row) the Dirac point. For the [001] surface the plots are around the $\overline{X}$ point of the 2DBZ, for [110] around two, $\overline{Y}$ (left) and $\overline{S}$ (right), points and for [111] in the vicinity of the $\overline{\Gamma}$.
For the [111] oriented surface, in the upper panel the result obtained for the cation-ended slab is shown, while the lower panel shows the result for the anion-ended slab. The arrows indicate the in-plane spin texture, the arrows' size the degree of spin polarization. The blue to yellow color coding indicates again the contributions of the cation (yellow) and anion (blue) p-orbitals to the wavefunctions, as shown in the bar.

These results have been comprehensively shown in upcoming paper[5] with more details.

Conclusions:

- For compositions higher than x_0 the gapless, spin non degenerate, helical surface states are formed.
- Chiral spin texture at (001), (011) and (111) surfaces has been predicted for (Pb,Sn)Se and (Pb,Sn)Te. Our calculations show a “multi-vortical” spin structure for the (001) and (011) surface states due to double *L* points projections. For the (111) anion and cation surfaces a “single-vortical”spin texture is anticipated. In the case of (001) surface of (Pb,Sn)Se spin structure has been confirmed by SARPES measurements[4].

Refrences:
1- T. H. Hsieh et al., Nature Communications, **3**, 982 (2012)
2- P. Dziawa et al., Nature Materials, **11**, 1027 (2012)
3- C. S. Lent et al., Superlattices and Microstructures, **2**, 491 (1986)
4- B. M. Wojek et al., Phys.Rev.B, **87**, 115106 (2013)
5- S. Safaei et al., Phys.Rev.B, **88**, 045305 (2013)