Mirror and Spin Chern Number Analysis of Band Structure Topology of PbTe and SnTe

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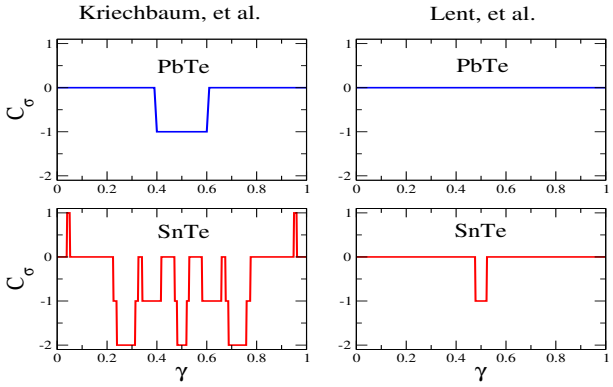
PbTe and SnTe belong to narrow gap IV–VI semiconductors family. From the band structure topology point of view they are trivial, and nontrivial insulators, respectively. This difference is related to the so called inverted band structure for SnTe (negative energy gap) where in the vicinity of the L points in the Brillouin zone the valence band wavefunctions, contrary to the PbTe case, are built from cation orbitals. However, due to peculiarity of the band structure (4 nonequivalent L points) the widely used criterion based on Z_2 topological index for both semiconductors suggests their triviality. In order to distiguish these two compounds, another criterion, the mirror Chern number (MCN), must be invoked [1].

Let us notice that in the paper [1] the conclusions concerning the values of MCN (0 for PbTe and -2 for SnTe) were drawn from the analysis of the Berry's curvature at two L points of the Brillouin zone only. In the present work we calculate numerically MCN for these two compounds using two different tight binding model parametrizations (TBMP) described in [2] and [3]. We show that the results depend on the used parametrization. For TBMP proposed in [2] we obtain -1 and -3 for PbTe and SnTe, respectively, while for TBMP assumed in [3] the corresponding numbers are 0 and -2.

For these two compounds we show that another topological index, the spin Chern number (SCN) [4] may also be applied to distinquish between normal and inverted band structures. The method of analysis of band structure topology is borrowed from Yang at al. [5]. Let $\mathbf{b_1}$, $\mathbf{b_2}$ and $\mathbf{b_3}$ be the translation vectors in the reciprocal lattice. For a given $0 \leq \gamma \leq 1$, treated as a parameter, the set of vectors $\alpha\mathbf{b_1} + \beta\mathbf{b_2} + \gamma\mathbf{b_3}$ with $0 \leq \alpha, \beta \leq 1$ constitute a two dimensional cell in the reciprocal lattice for which the SCN, $C_\sigma(\gamma)$, may be calculated numerically.



The results shown in the nearby figure clearly indicate that like in the case of MCN the SCN also depends on the parametrization.

In the paper the possible sources of these differences are discussed.

We present also the analogous results obtained from density functional theory calculations.

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[2] M. Kriechbaum, *et al.*, *IEEE J. Quant. El.* **24**, 1727 (1988)
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