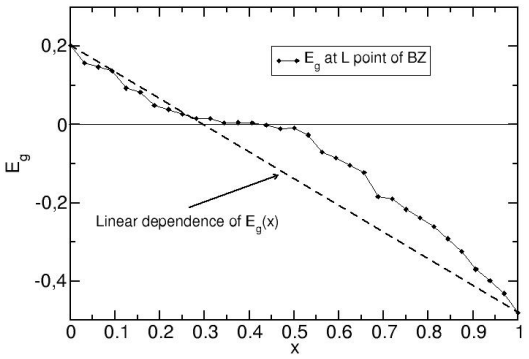
Pecularities of band structure and topological properties of $Pb_{1-x}Sn_xTe$ alloys

A. Łusakowski[1], P. Bogusławski[1,2], and T. Story[1]

[1] *Institute of Physics PAS, Al. Lotników 32/46, PL-02-668 Warszawa, Poland*
[2] *Institute of Physics, University of Bydgoszcz, ul. Chodkiewicza 30, 85-072 Bydgoszcz, Poland*

The main difference between the band structures of PbTe and SnTe is the order of levels at the L point of the Brillouin Zone: in PbTe, the symmetry of the valence band maximum (conduction band minimum) is L_{6+} (L_{6-}), while in the topologically non-trivial SnTe the order is inverted, which is referred to as the inverted band structure with a negative energy gap E_g. Current interest is focused on the $Pb_{1-x}Sn_xTe$ alloy because the varying Sn content, temperature, or the applied external pressure enables to study the transition between topologically trivial and nontrivial phases. Previous theoretical studies of such alloys were conducted within the Virtual Crystal Approximation (VCA), which essentially leads to linear dependencies of the alloy properties on composition. Importantly, within the VCA, the alloy has the full point and translational symmetry of the rock salt structure. In contrast, in real alloys there always is a chemical disorder, and those symmetries are missing.

Our goal is to study the influence of the chemical disorder on both the band structure and topological properties of $Pb_{1-x}Sn_xTe$. To this end, we consider alloys with supercells containing 8, 16 and 64 atoms with varying compositions and spatial distributions of cations obtained with the special quasi-random structures method. Ab initio LDA calculations with the spin-orbit coupling included are done with the OpenMX code.



The dependence of the band gap E_g on x for 64-atom supercell, shown in the Figure, is strongly non-linear. Instead of the sharp transition from the direct to the inverted structure, there is a wide composition range $0.3 < x < 0.5$ with the zero gap. Second, the band gap bowing (i.e. non-linearity of $E_g(x)$) is convex and concave below and above the transition, respectively.

For smaller supercells we perform calculations varying the lattice constants a, which mimics the changes of the temperature or application of hydrostatic pressure. The analogous anomalies, i. e. the absence of sharp transition between direct and inverted structures are also found. After the initial reduction of E_g for decrease of a, there is a considerable interval of the lattice constants when the energy gap is zero. In this interval the topological indices, the Mirror and Spin Chern Numbers assume almost random highly non-monotonic values. Finally, a further decrease of a leads to the opening of the (negative) gap.

We explain that all these unexpected behaviours are caused by the presence of chemically different species (Pb and Sn) in the alloy, which leads to additional splittings of the energy bands. In addition, the chemical disorder leads also to a decrease of the crystal symmetry and has an additional influence on the band structure energy levels.

Acknowledgements:
Work supported partially by NCN Grant Nr. UMO-2016/23/B/ST3/03725