Spin polarization of surface states on (100) $Pb_{0.73}Sn_{0.27}Se$

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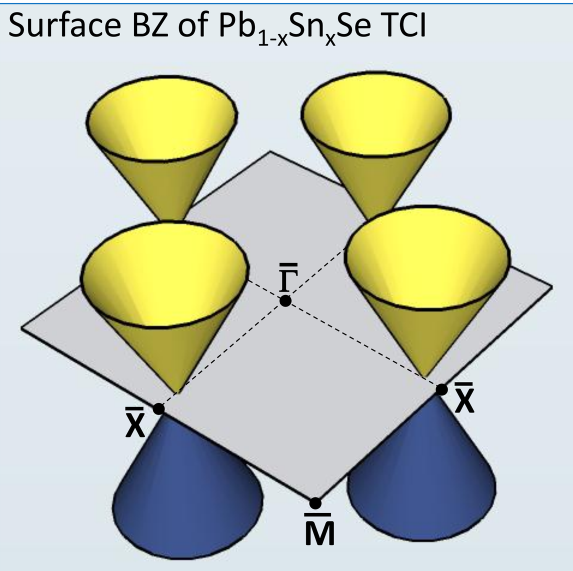
Introduction

The recent discovery of topological crystalline insulators (TCI) [1-3] (stimulated by theoretical considerations [4,5]) widened the range of solids considered as hosting topologically protected surface states by systems belonging to the family of IV-VI narrow band gap semiconductors. Our experiments aimed at revealing the topologically protected surface states on TCI, were successfully concluded by observation of such states on the (100) surface of $Pb_{1-x}Sn_xSe$ [1].

In TCIs, the crystalline symmetry replaces the role of time-reversal symmetry ensuring the topological protection in regular topological insulators (TI). The metallic surface states on $Pb_{1-x}Sn_xSe$ TCI are topologically protected by reflection symmetry of the crystal with respect to {110} (or equivalent) mirror planes (marked by dashed lines in the figure). Therefore, in this system four Dirac-like cones of the protected surface states appear close to the $\bar{X}$ points of the Brillouin zone (in contrast with TI systems). The ARPES and SRPES data (shown below) were collected for the set of two Dirac-like cones occurring on both sides of the $\bar{X}$ point (in the first and second surface Brillouin zones).

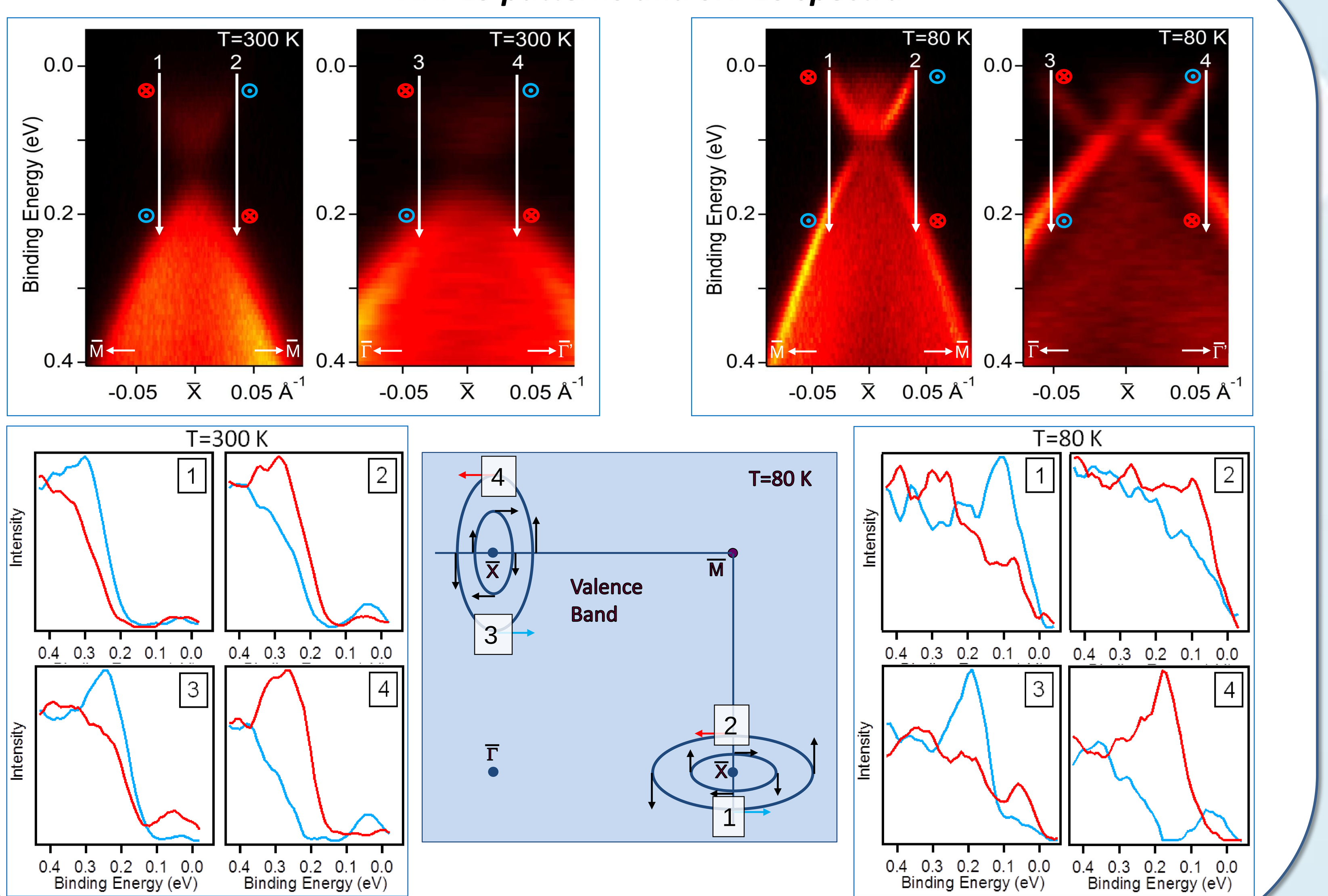
Surface BZ of $Pb_{1-x}Sn_xSe$ TCI



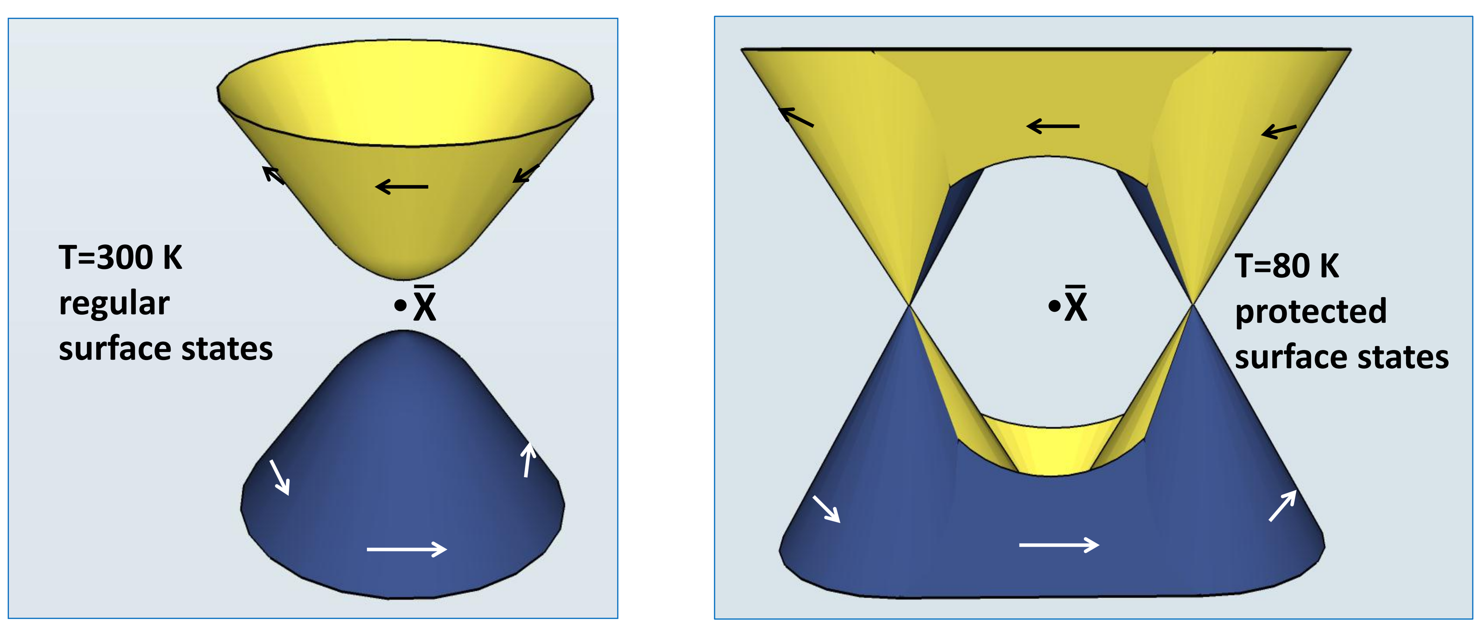
In $Pb_{1-x}Sn_xSe$ crystals the strong relativistic effects result in a remarkable compositional evolution of their band structure leading to zero gap state for a specific composition $x=x_c$. For lower and higher Sn compositions the energy gap is open, but the parity of electronic states at band edges is reversed. The crystal with inverted parity of the states at the band edges (for $x>x_c$) hosts the topologically protected surface states. Thus, the properties of both TCI and trivial phases can be investigated in a single experiment, while the transition from one phase to another is induced by the change in temperature. The reported experiments gave the evidence for the spin polarization of the surface states on the (100) surface of $Pb_{0.73}Sn_{0.27}Se$ in the TCI phase as well as in the trivial one.

[1] P. Dziawa, et al., Nat. Mater. **11**, 1023 (2012), [2] Y. Tanaka, et al., Nat. Phys. **8**, 800 (2012), [3] Su-Yang Xu, et al., Nat. Commun. **3**, 1192 (2012), [4] Liang Fu, Phys. Rev. Lett. **106**, 106802 (2011), [5] T.H. Hsieh, et al., Nat. Commun. **3**, 982 (2012).

ARPES patterns and SRPES spectra

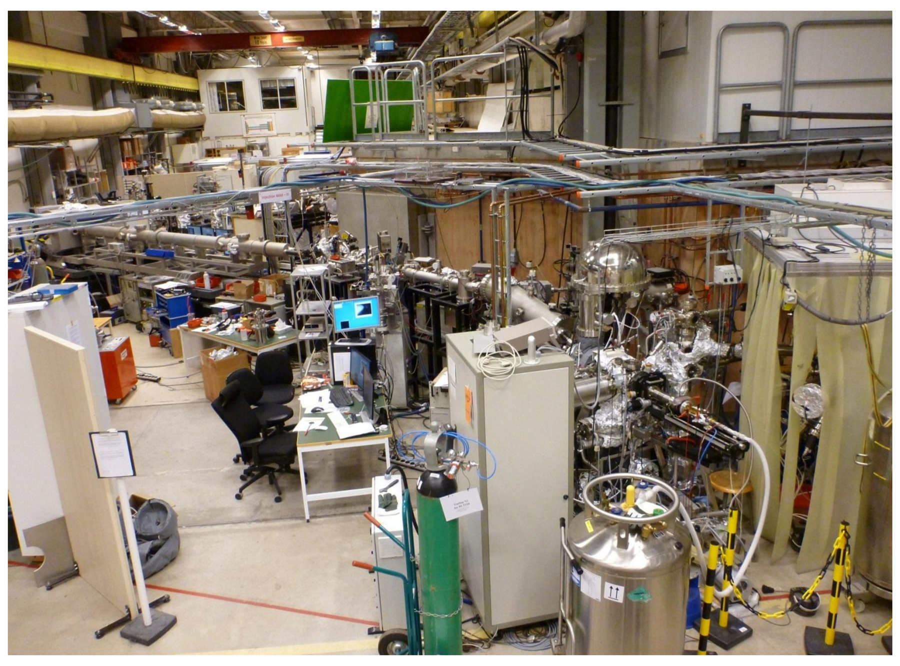


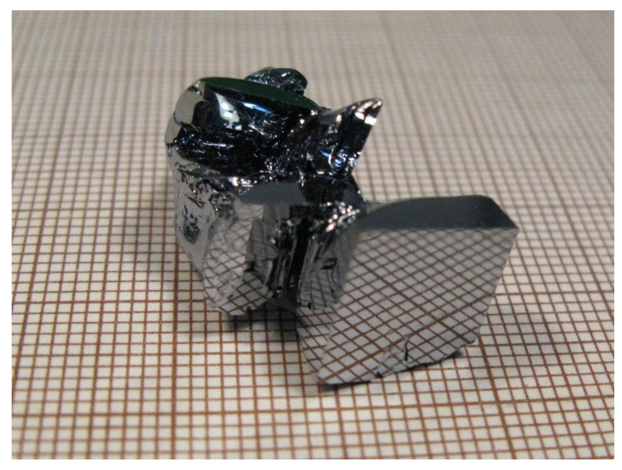
Summary of the experimental results
(the features of the spin texture revealed by SRPES)



Experimental methods

Since the band-structure inversion in $Pb_{0.73}Sn_{0.27}Se$ occurs at $T \approx 250$ K, the angle-resolved photoelectron spectroscopy (ARPES) and spin-resolved photoelectron spectroscopy (SRPES) measurements on cleaved (001) surfaces at temperatures $T \approx 80$ K (for the TCI phase) and $T \approx 300$ K (for the normal insulator phase) have been carried out at the I3 and I4 beamlines at the MAX-III synchrotron at MAX-lab, Lund University, Sweden. All experiments have been done under ultrahighvacuum conditions ($p \approx 3 \times 10^{-10}$ mbar) using linearly polarized light with a photon energy $h\nu = 18.5$ eV. The total energy resolution of the ARPES and SRPES experiments was 10 to 20 meV and 100 meV, respectively. The in-plane crystal-momentum resolution was 0.01 Å^{-1} for the ARPES measurements. The SRPES data acquisition integrated over a reciprocal-space area with a diameter of about 0.025 Å^{-1}.





The studied *n*-type single crystals have been grown by the self-selecting vapor growth method.

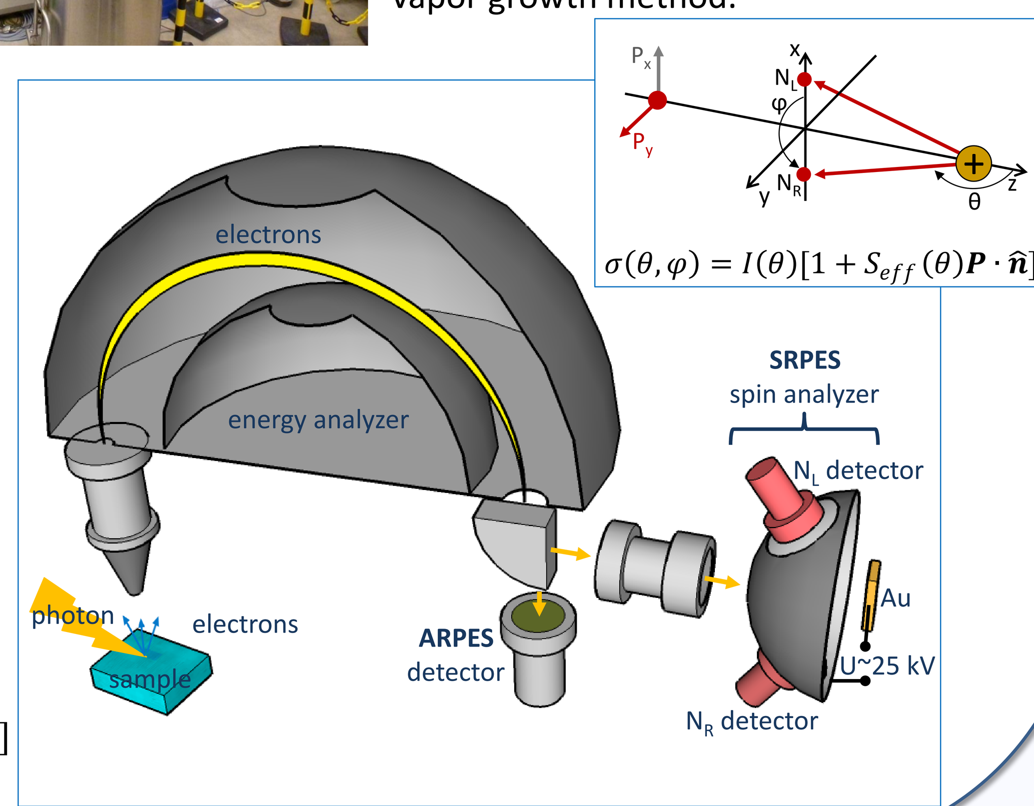
The scheme of the spin-resolved photoelectron spectroscopy experiment based on the use of a Mott spin detector.

The spin polarization $P(E)$ is given by:

$$S_{eff}\,P(E) = \frac{\hat{I}_R(E) - \hat{I}_L(E)}{\hat{I}_R(E) + \hat{I}_L(E)}$$

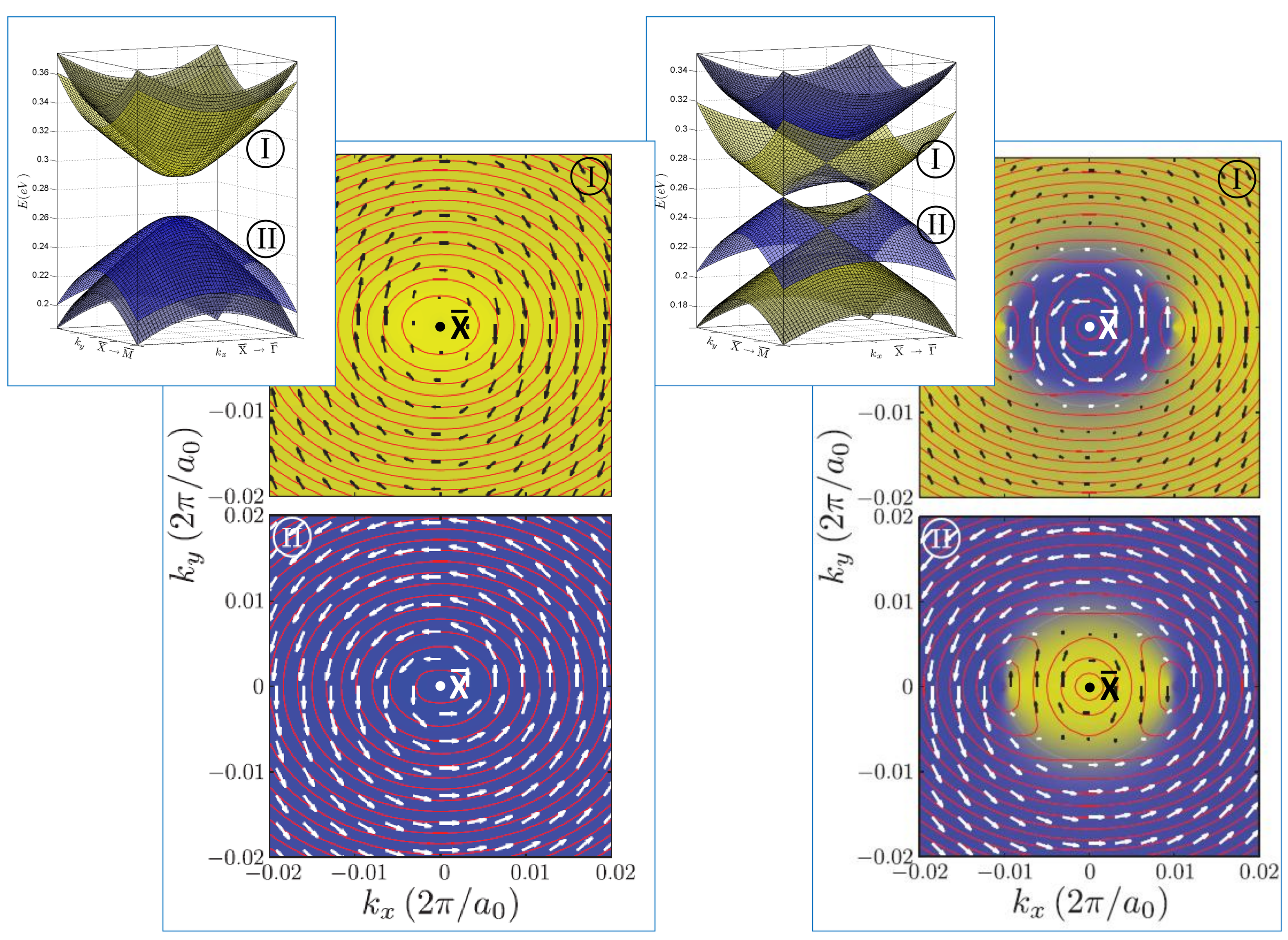
The absolute photoemission intensities (corrected for $S_{eff}<1$) are described by the formula:

$$I_{L/R}(E) = \frac{\hat{I}_R(E) + \hat{I}_L(E)}{2}[1 \pm P(E)]$$



Band structure calculations

The band structure and spin texture of the electronic surface states in $Pb_{0.73}Sn_{0.27}Se$ have been obtained by tight-binding calculations for a slab oriented in the [001] direction. The parameters for hypothetical bulk rock-salt SnSe were obtained from the parametrization of the DFT-LDA band structure by use of the simulated annealing method with the additional condition of a linear change of $E_g(x)$ in the mixed crystal.



CONCLUSIONS

- The spin-resolved photoemission experiments provided evidence for the spin polarization of surface states on (100) $Pb_{0.73}Sn_{0.27}Se$ in both cases: TCI phase and normal insulator.
- The experimental results are coherent with the results of corresponding tight-binding band structure calculations.

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