Topological crystalline insulators

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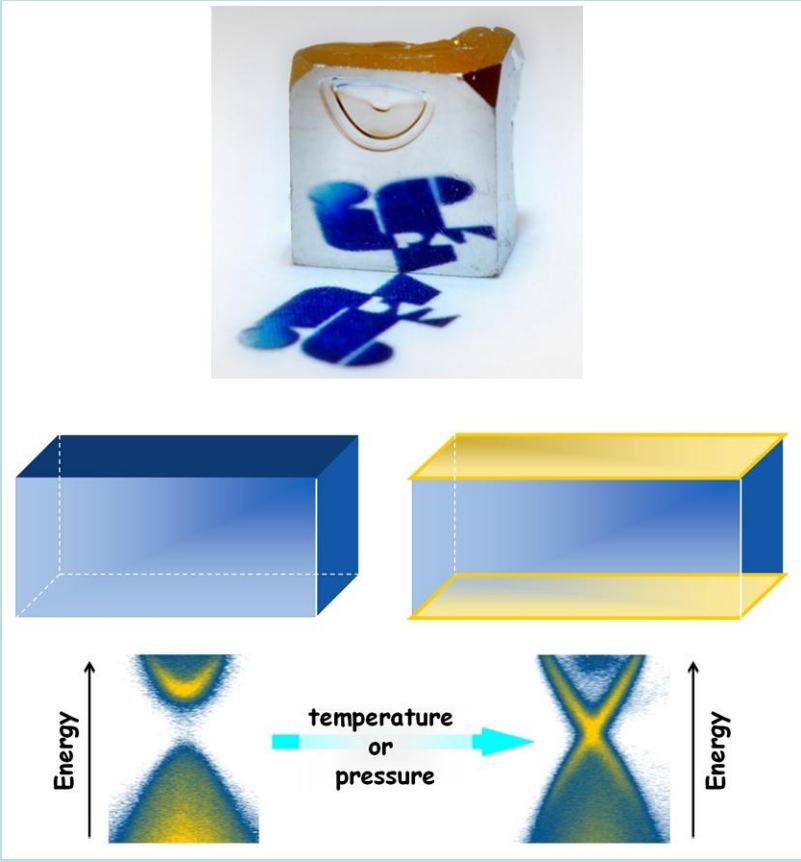


Topological crystalline insulators - outline

1. Introduction – topological crystalline insulators (TCI) vs topological insulators (TI)

2. IV-VI semiconductors as topological insulators

3. $Pb_{1-x}Sn_xSe$ monocrystals – growth , structural, chemical and electric characterization

4. Angle- and spin-resolved photoemission experiments

5. Electronic band structure calculations

6. Magneto-transport studies

7. Summary and future outlook

$Pb_{1-x}Sn_xSe$ as topological crystalline insulator

Crystal growth: A. Szczerbakow (IP PAS)

Structural and chemical characterization:
W. Domuchowski, E. Łusakowska, A. Reszka (IP PAS)

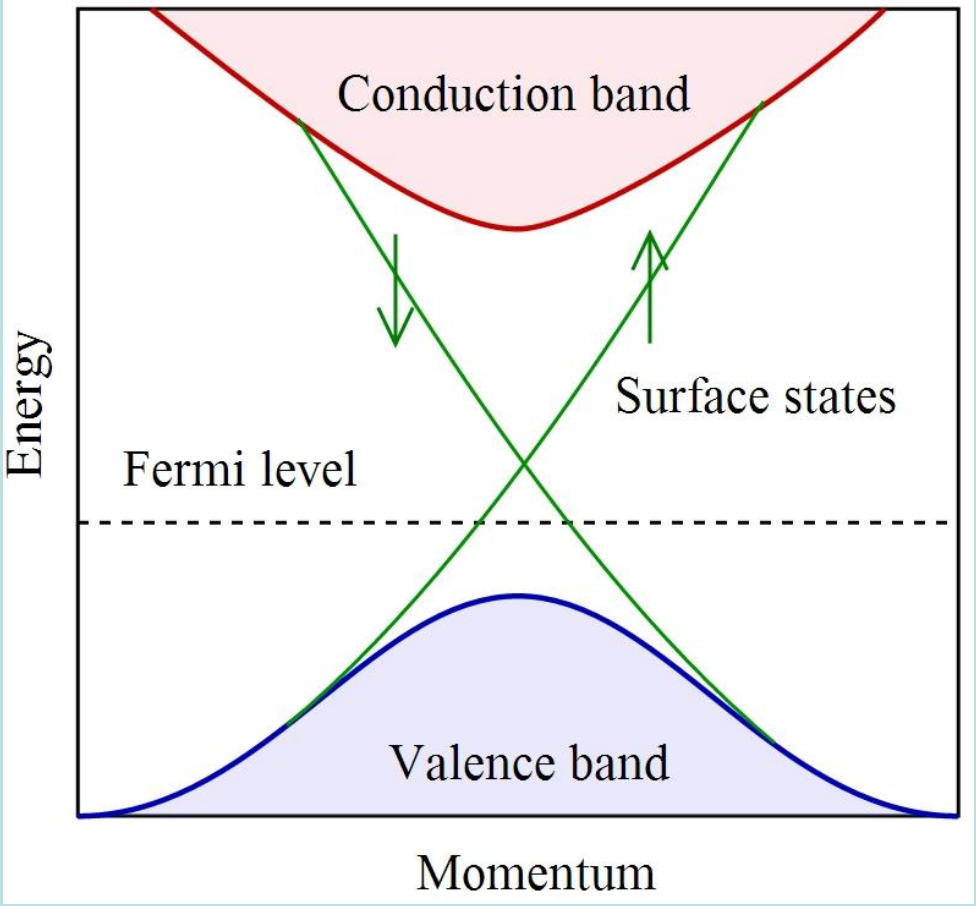
Magneto-transport studies – K. Dybko, M. Szot (IP PAS)

Band structure calculations – R. Buczko (IP PAS)

Photoemission measurements at Lund University (synchrotron facility) and KTH Stockholm (laser facility):
P. Dziawa, B.J. Kowalski (IP PAS), T. Balasubramanian (Lund), M.H. Berntsen, O. Tjernberg, B.M. Wojek (KTH)

TS

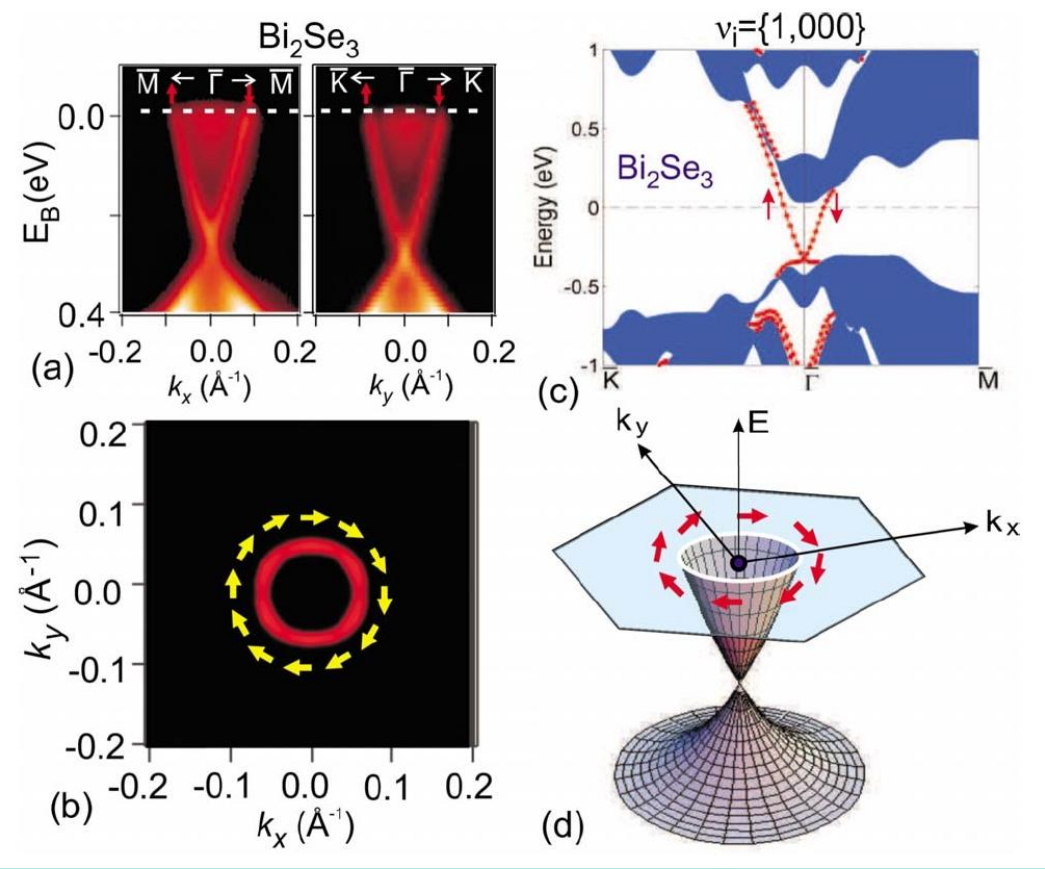
Topological insulators: key physical factors



- **Inverted c-band and v-band symmetry**
- **Odd number of Dirac cones**
- **Strong spin-orbit coupling $E_{so} \approx E_G$**

- **Metallic, helical Dirac electronic surface states**
- **Topological protection**

Topological insulators - materials

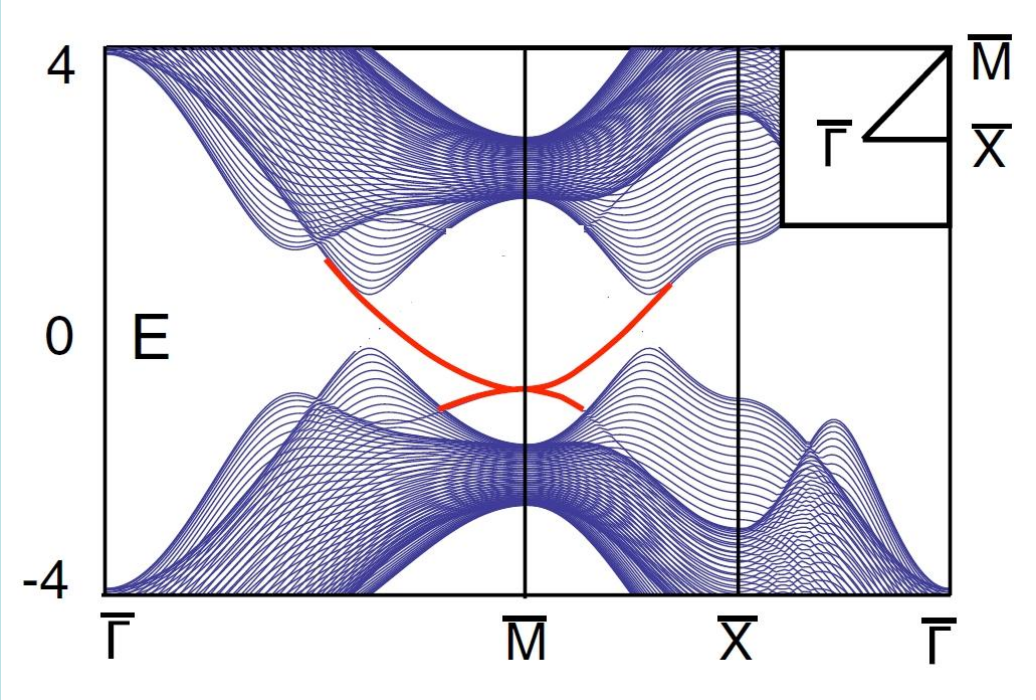


- **3D**
- **$Bi_{1-x}Sb_x$**
- **Bi_2Se_3**
- **Bi_2Te_3**

- **2D**
- **HgTe/CdTe QW**

M.Z. Hasan, C.L. Kane, Rev. Modern Phys. 82, 3045 (2010)

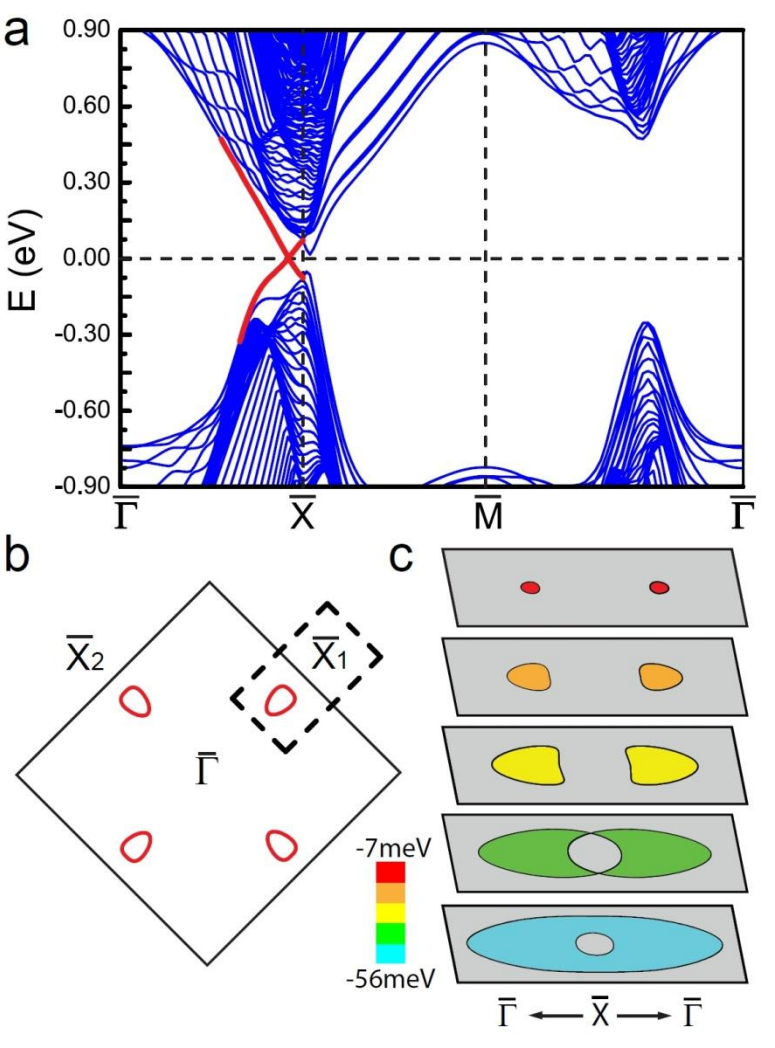
Topological crystalline insulators: theoretical idea



Theoretical analysis of electronic band structure of tetragonal crystal with 4-fold surface symmetry. Topologically protected surface TCI states (red) are expected even in materials with no spin-orbit coupling.

L. Fu, Phys. Rev. Lett. 106, 106802 (2011).

Topological crystalline insulators
SnTe - theoretical analysis

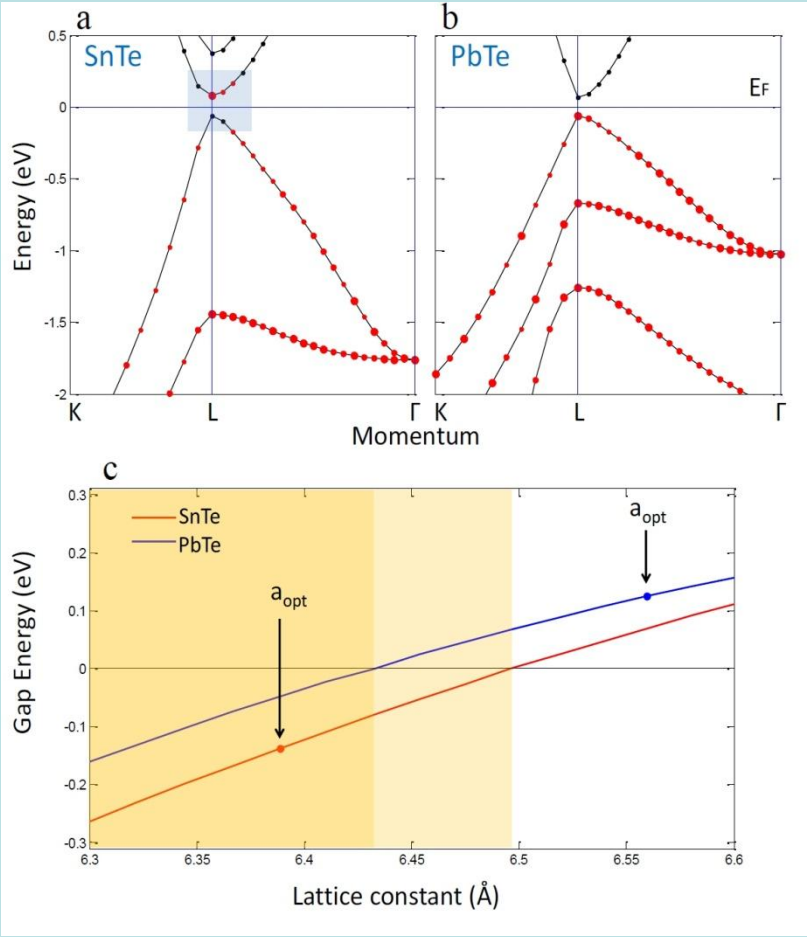


SnTe - TCI states with 4 Dirac cones nearby X-points of the surface Brillouin zone

Lifshitz transition - Topological changes of Fermi surface

T.H. Hsieh et al, Nature Commun. 3, 982 (2012).

Topological crystalline insulators: SnTe vs PbTe – theoretical analysis

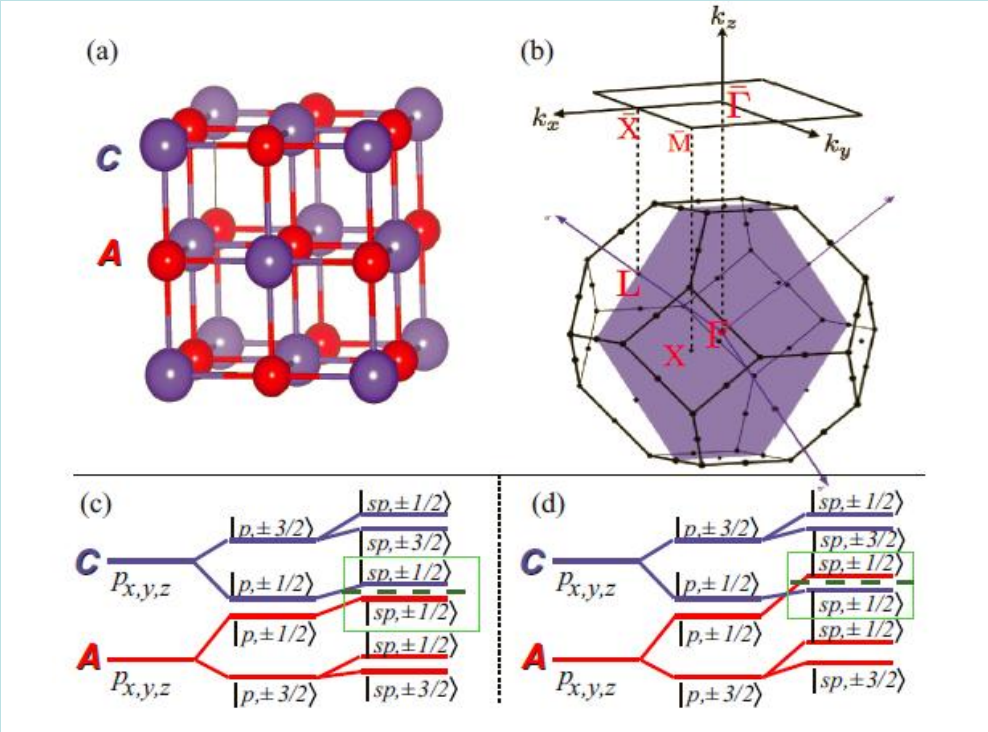


PbTe – trivial band insulator
$E_G>0$

SnTe – topological insulator (TCI)
$E_G<0$

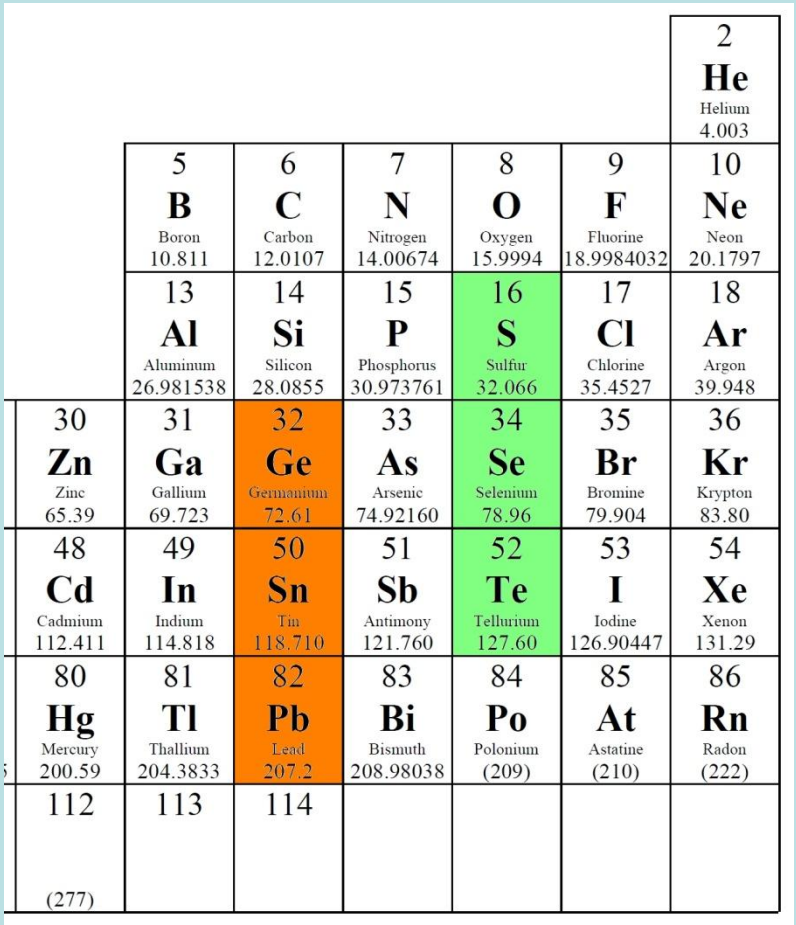
T.H. Hsieh et al,
Nature Commun. 3, 982 (2012).

Band inversion in IV-VI semiconductors



P. Barone et al., Phys. Rev. B 88, 045207 (2013)

IV-VI semiconductor family



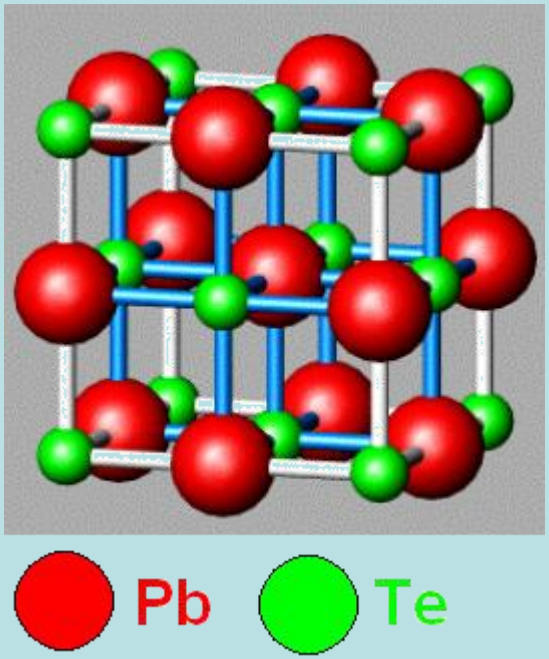
						2 **He** Helium 4.003
	5 **B** Boron 10.811	6 **C** Carbon 12.0107	7 **N** Nitrogen 14.00674	8 **O** Oxygen 15.9994	9 **F** Fluorine 18.9984032	10 **Ne** Neon 20.1797
	13 **Al** Aluminum 26.981538	14 **Si** Silicon 28.0855	15 **P** Phosphorus 30.973761	16 **S** Sulfur 32.066	17 **Cl** Chlorine 35.4527	18 **Ar** Argon 39.948
30 **Zn** Zinc 65.39	31 **Ga** Gallium 69.723	32 **Ge** Germanium 72.61	33 **As** Arsenic 74.92160	34 **Se** Selenium 78.96	35 **Br** Bromine 79.904	36 **Kr** Krypton 83.80
48 **Cd** Cadmium 112.411	49 **In** Indium 114.818	50 **Sn** Tin 118.710	51 **Sb** Antimony 121.760	52 **Te** Tellurium 127.60	53 **I** Iodine 126.90447	54 **Xe** Xenon 131.29
80 **Hg** Mercury 200.59	81 **Tl** Thallium 204.3833	82 **Pb** Lead 207.2	83 **Bi** Bismuth 208.98038	84 **Po** Polonium (209)	85 **At** Astatine (210)	86 **Rn** Radon (222)
112 (277)	113	114				

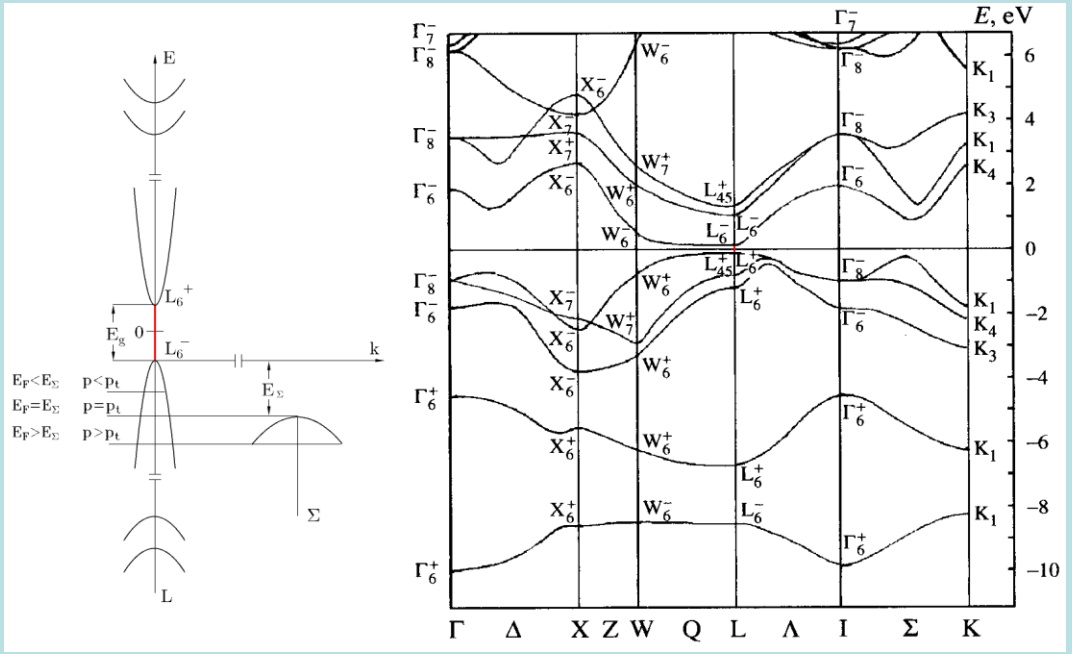
- **Binary compounds:**
- **PbTe, PbSe, PbS, SnTe, GeTe**

- **Substitutional solid solutions:**
- **$Pb_{1-x}Sn_xTe$, $Pb_{1-x}Sn_xSe$**

- **Diluted magnetic semiconductors:**
- **$Sn_{1-x}Mn_xTe$, $Ge_{1-x}Mn_xTe$**

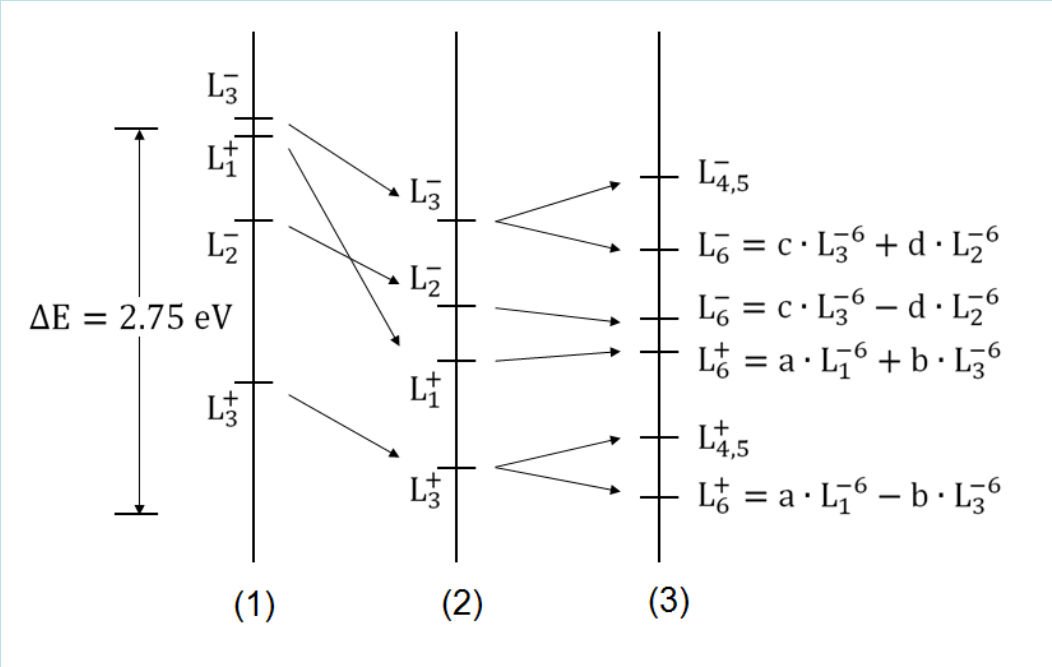
IV-VI semiconductors

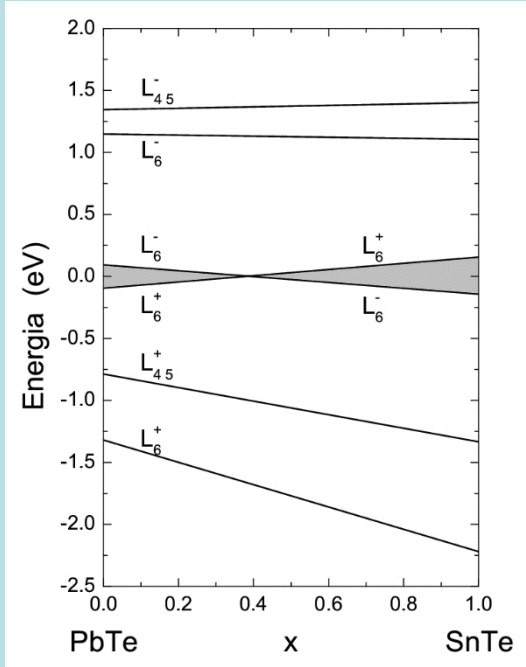




Rock-salt crystal structure.
Narrow-gap materials (0-0.3 eV) with a direct gap at 4 equivalent L-points .
Strong (1 eV) relativistic interactions (spin-orbit and Darwin terms).
Small effective masses and high mobilities of electrons and holes.
Materials for thermoelectric generators and mid-infrared lasers and detectors.

Electron band structure of IV-VI semiconductors



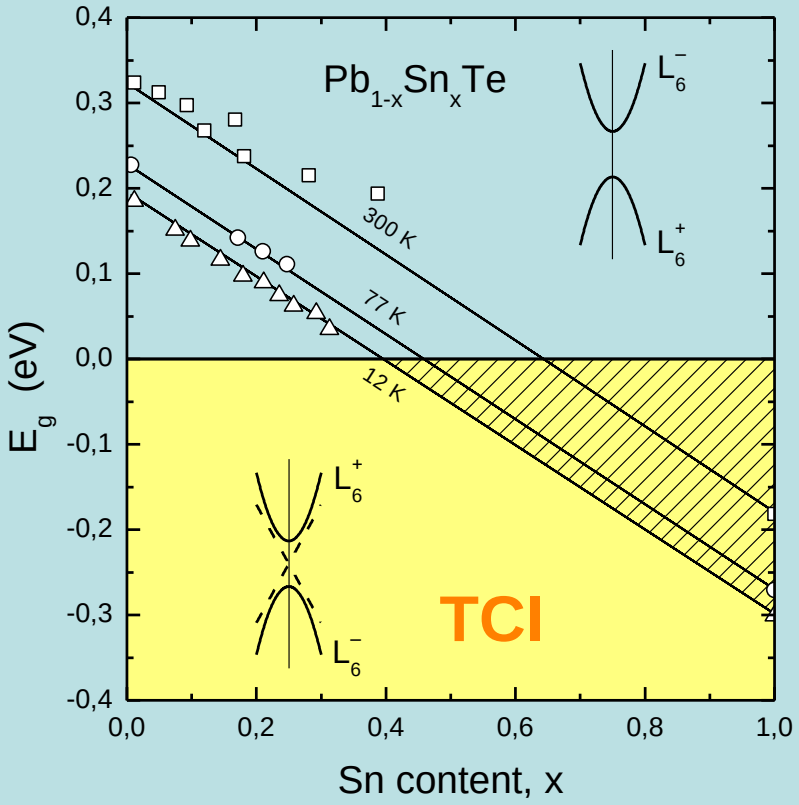


Relativistic interactions in PbTe and $Pb_{1-x}Sn_xTe$

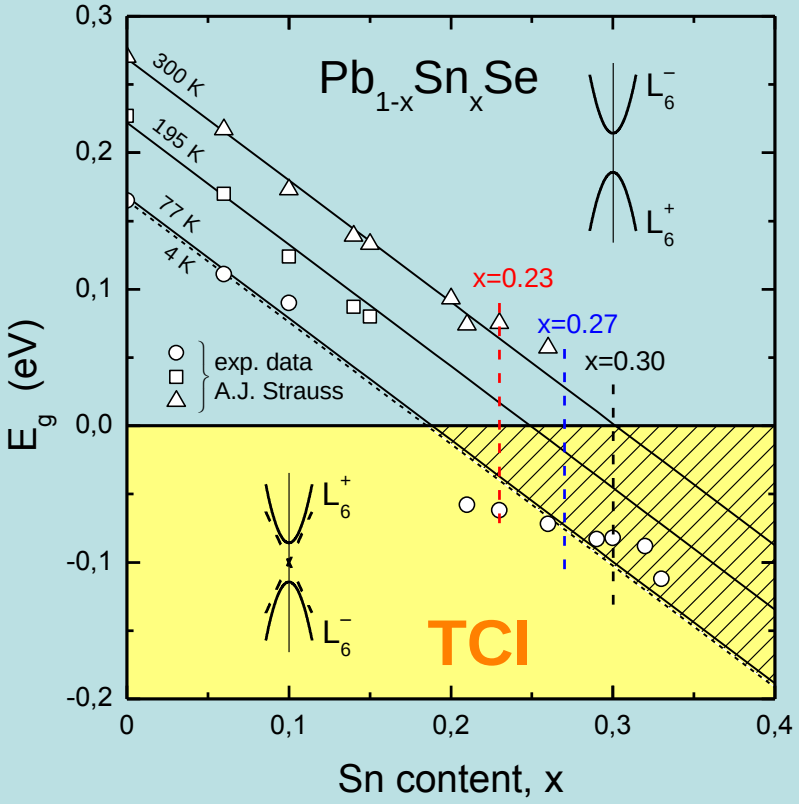
$$\hat{H} = \frac{\hat{p}^2}{2m_0} + U - \frac{\hat{p}^4}{8m_0^3c^2} + \frac{\hbar^2}{8m_0^3c^2}\nabla^2 U + \frac{\hbar}{4m_0^3c^2}\hat{\sigma}(\nabla U \times \hat{p})$$

$Pb_{1-x}Sn_xTe$ substitutional solid solutions

R. Dornhaus, G. Nimtz, and B. Schlicht,
Springer Tracts in Modern Physics vol. 98, Narrow-Gap Semiconductors
(Springer, Berlin, 1983)



$Pb_{1-x}Sn_xSe$ substitutional solid solutions

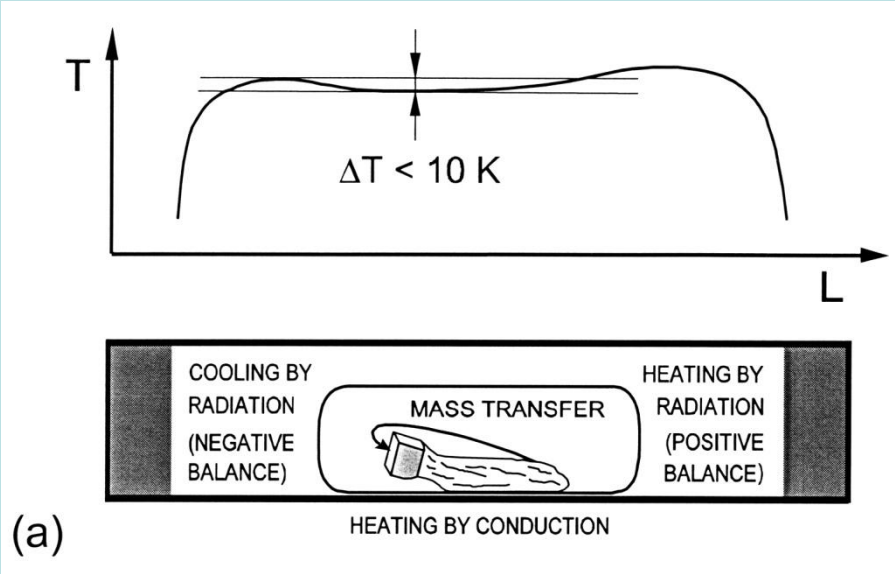


Idea of our TCI project

- $Pb_{1-x}Sn_xSe$ monocrystals ($0.18<x<0.3$) to observe temperature-driven topological phase transition from trivial insulator to the TCI state
- n-type crystals required for $x>x_c$ (TCI states occupied)
- cleaving at UHV conditions as a versatile method of preparing high crystal quality, atomically clean (001) surfaces
- no surface reconstruction expected
- only $Pb_{1-x}Sn_xSe$ crystals fulfil all these conditions
- $Pb_{1-x}Sn_xTe$ ($x>x_c$) and SnTe crystals are heavily p-type doped by electrically active native defects (metal vacancies).

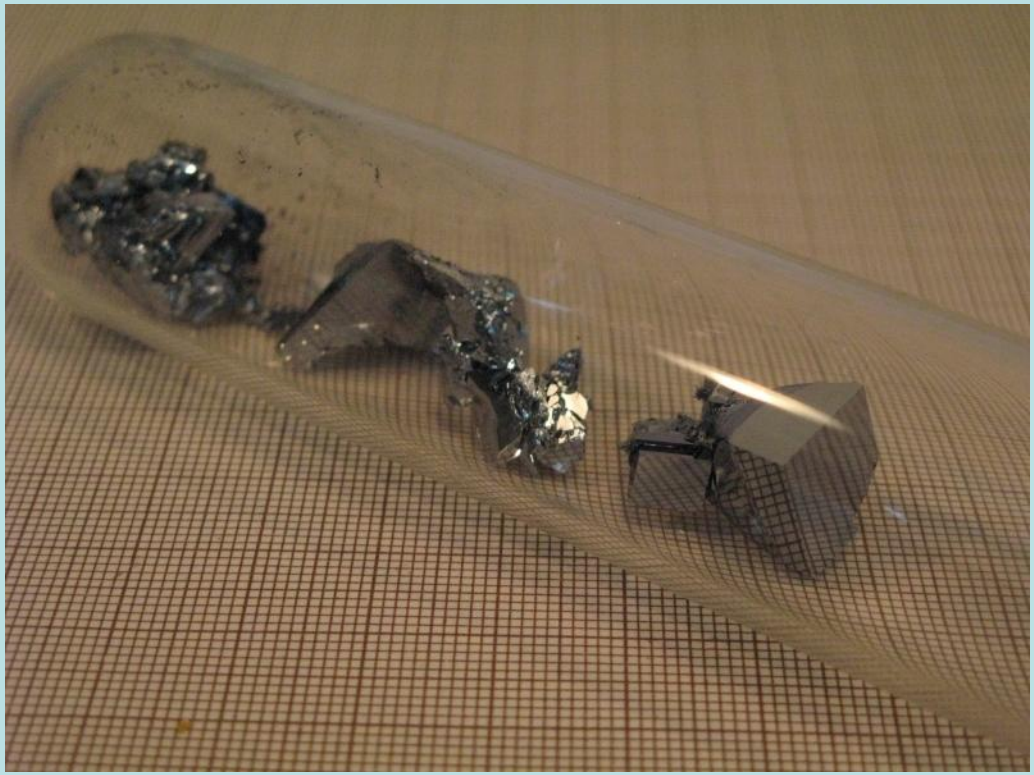
Growth of $Pb_{1-x}Sn_xSe$ and $Pb_{1-x}Sn_xTe$ bulk monocrystals

- Self-selecting vapor growth (SSVG) – A. Szczerbakow
- Natural (001) crystal facets – cleavage planes
- Stoichiometry control of n – and p-type conductivity
- Highly homogeneous chemical composition of solid solutions



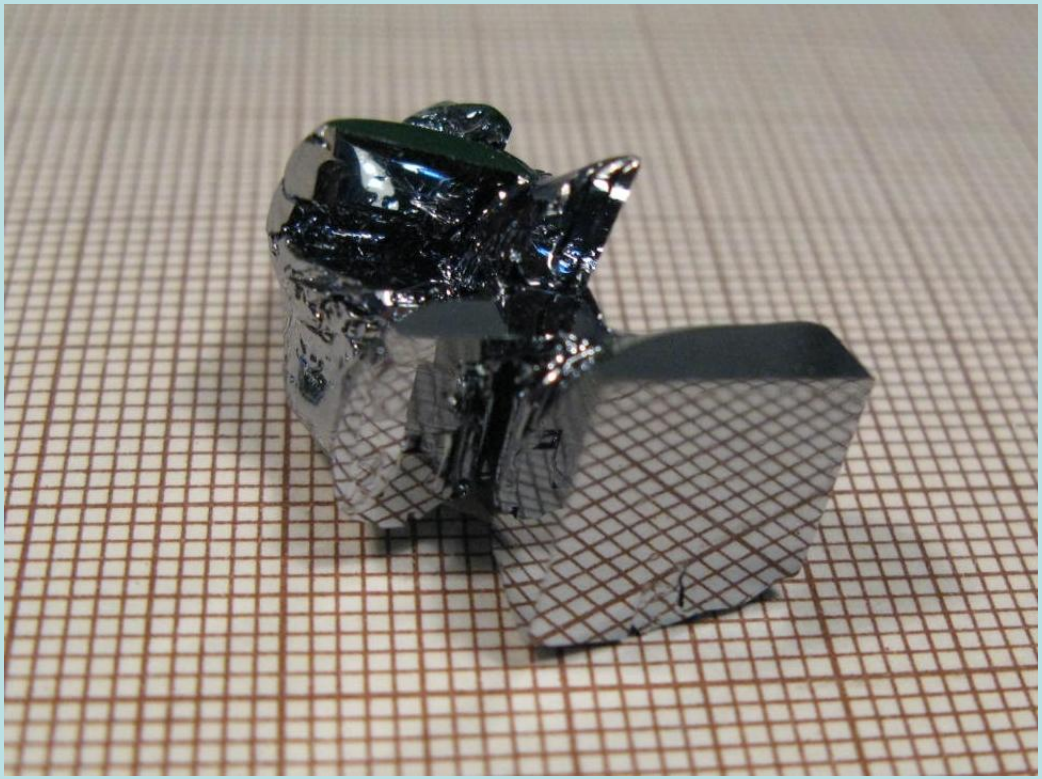
A. Szczerbakow et al.:
J. Cryst. Growth 139, 172 (1994);
Prog. Cryst. Growth Charact. Mater. 51, 81 (2005).

Growth of bulk PbSnSe crystals by SSVG method

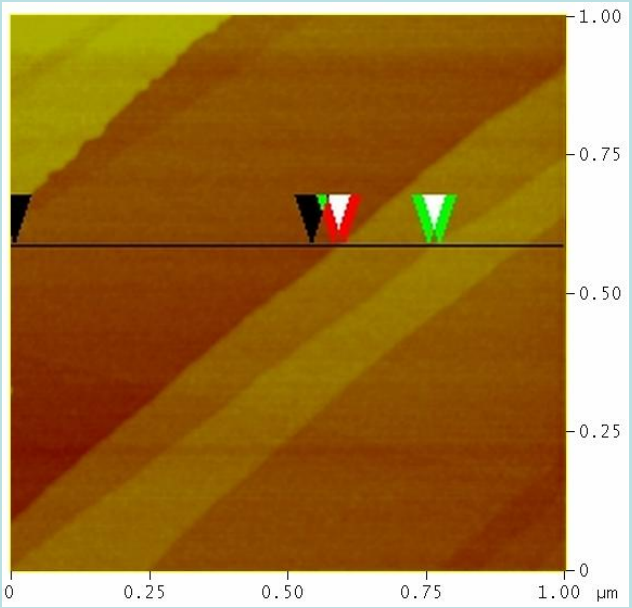


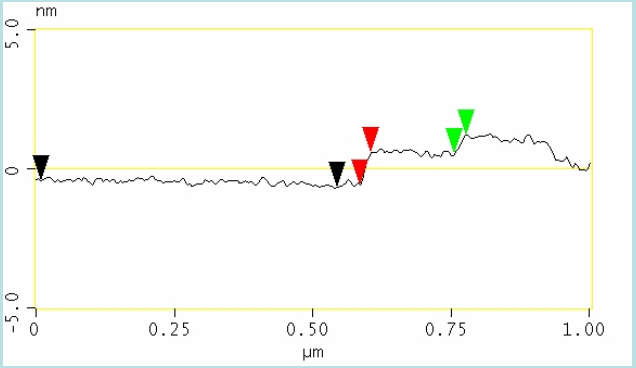
- A. Szczerbakow, $Pb_{0.76}Sn_{0.24}Se$ monocrystal

$Pb_{0.77}Sn_{0.23}Se$ monocrystal grown by self-selecting vapor growth



Structural and chemical characterization

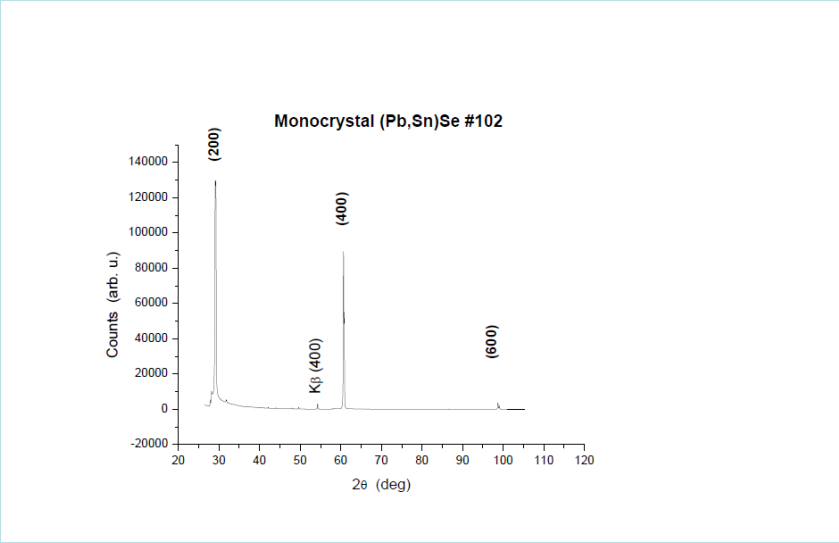




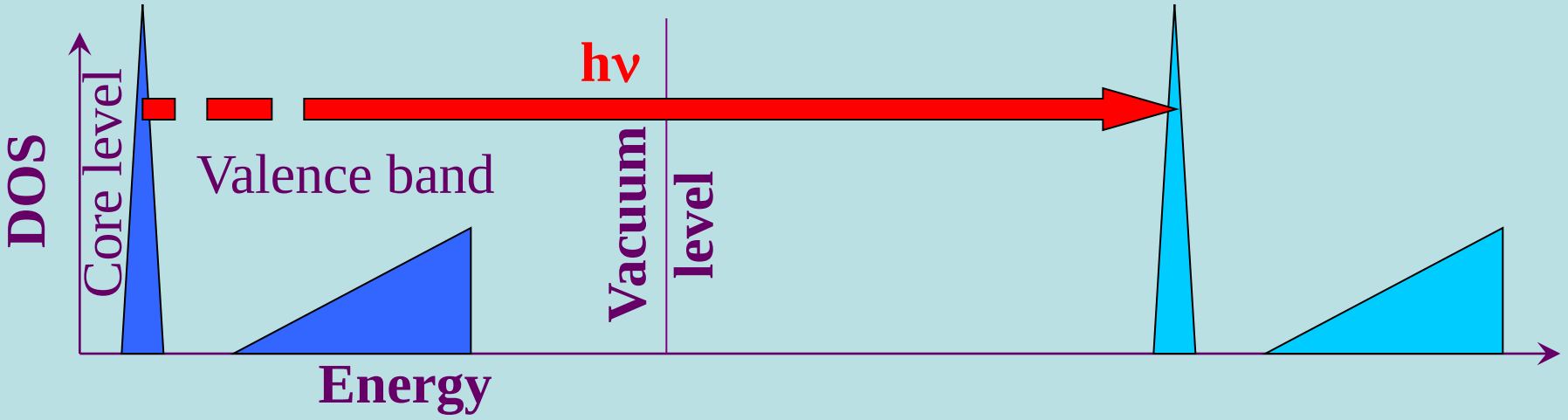
X-ray diffraction (XRD)

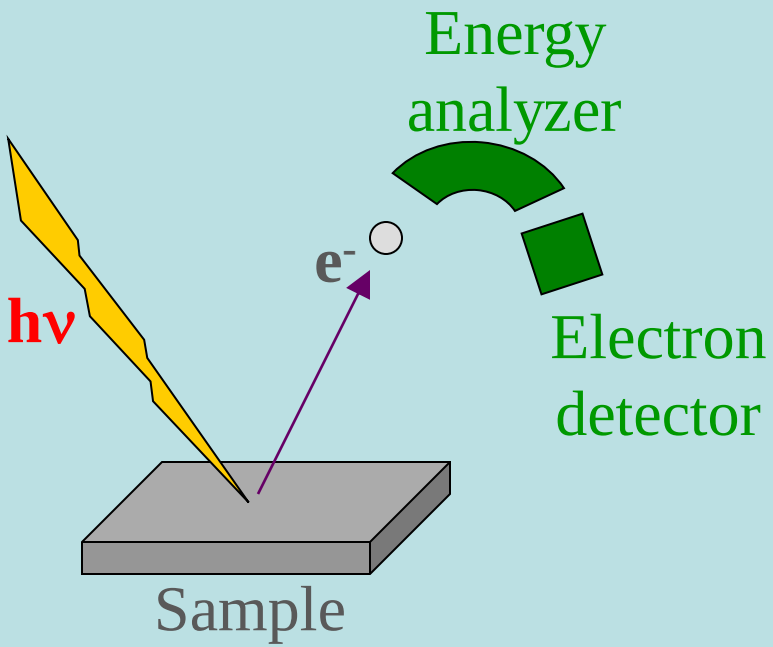
EDX chemical analysis

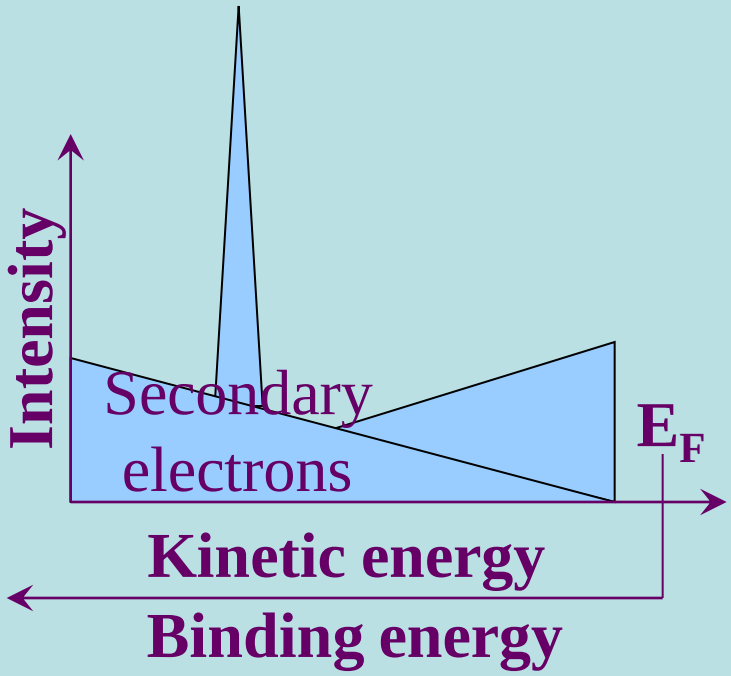
Surface morphology analysis by AFM microscopy



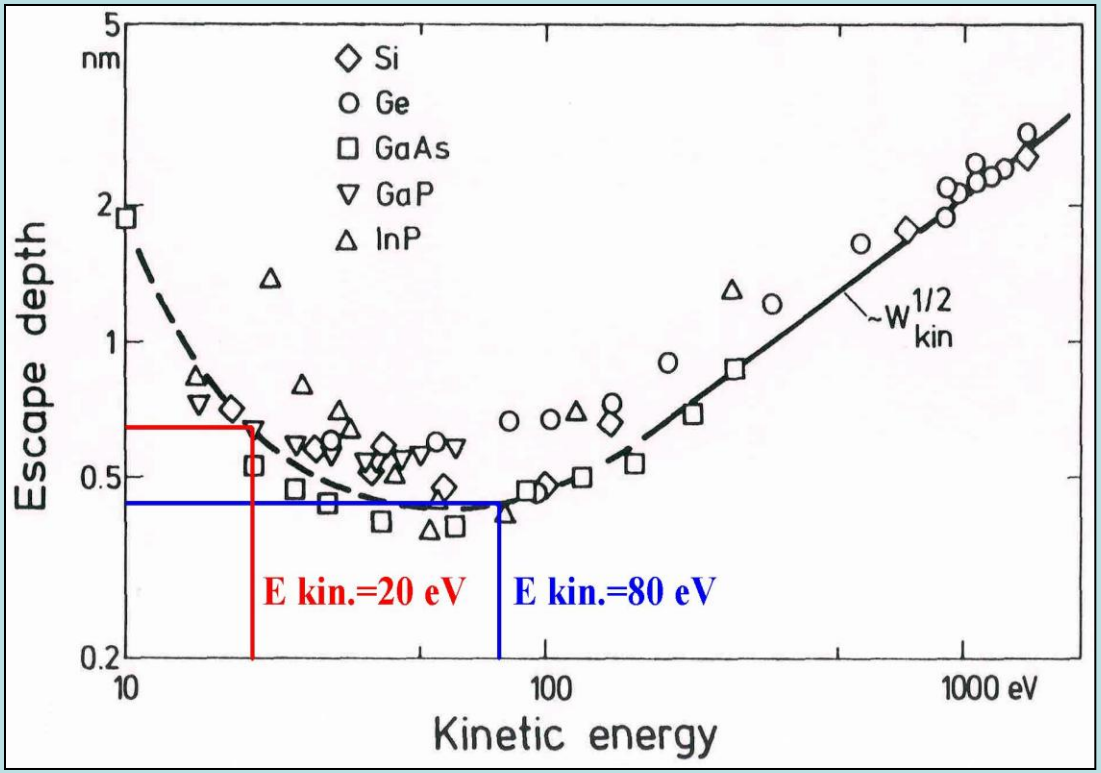
Photoemission electron spectroscopy

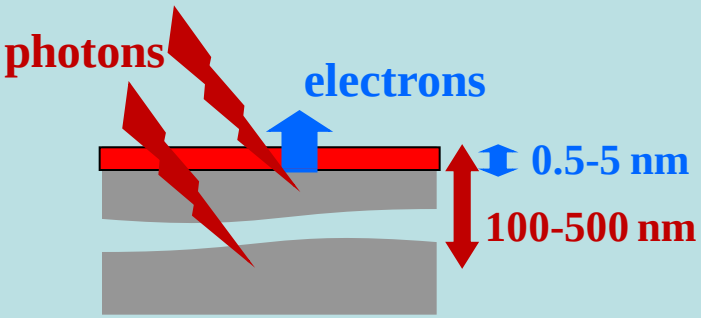






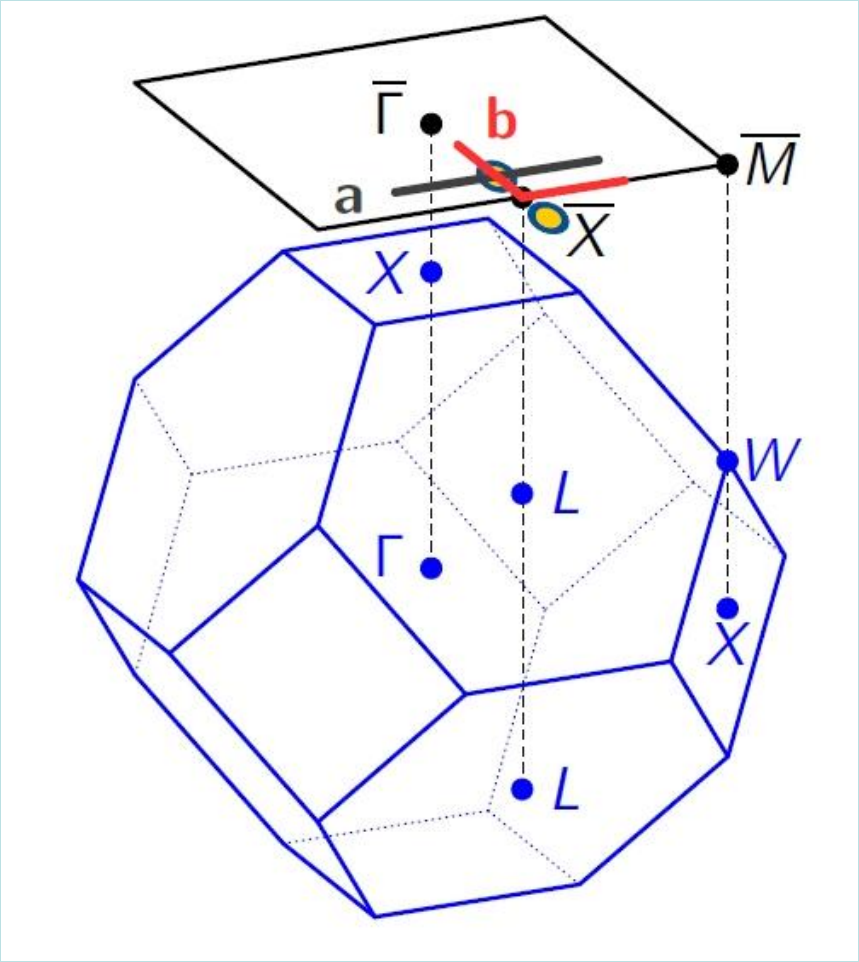
Photoemission – crystal surface sensitive technique





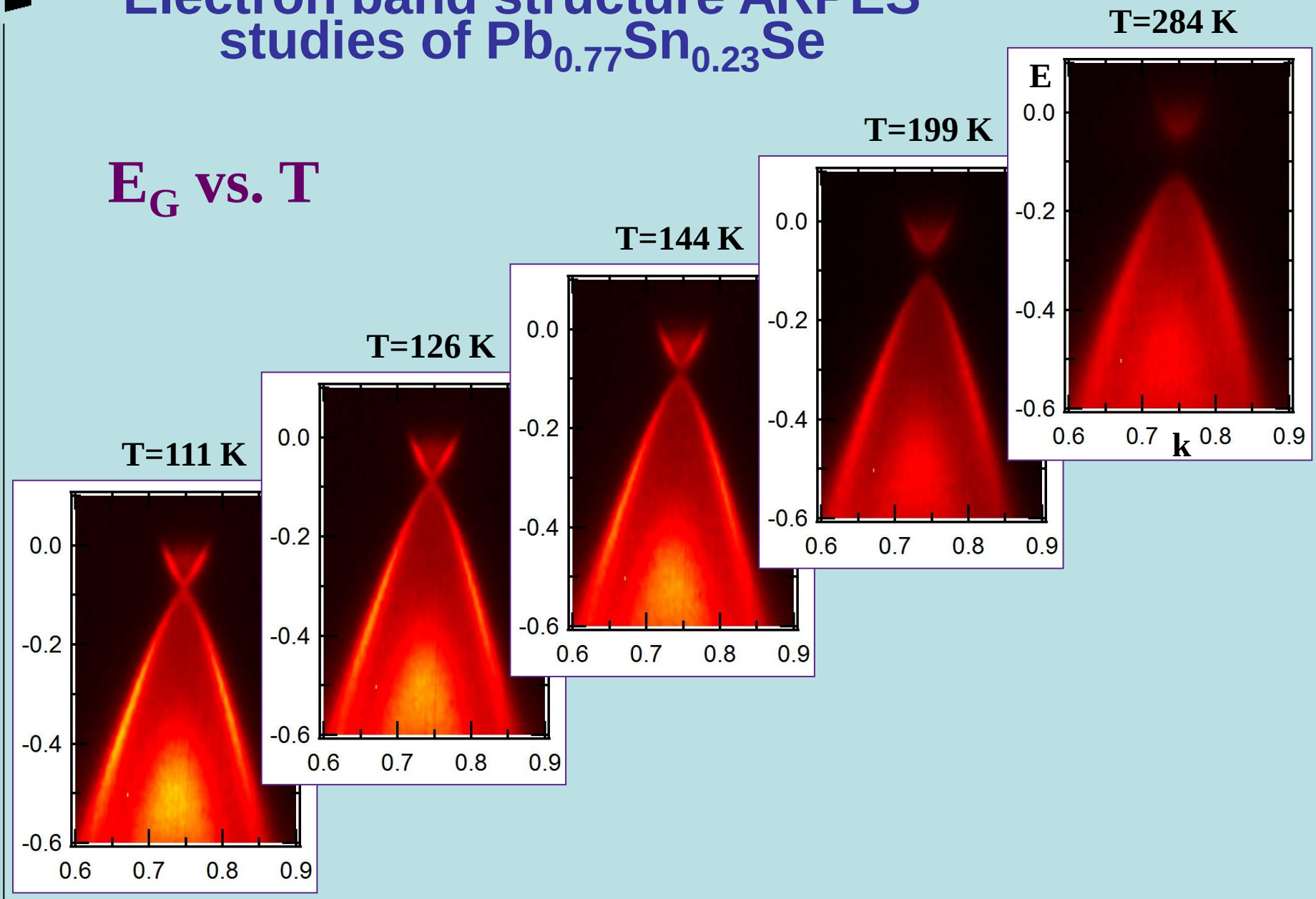
W. Mönch „Semiconductor surfaces and interfaces” 1993

Brillouin zone for (001) surface

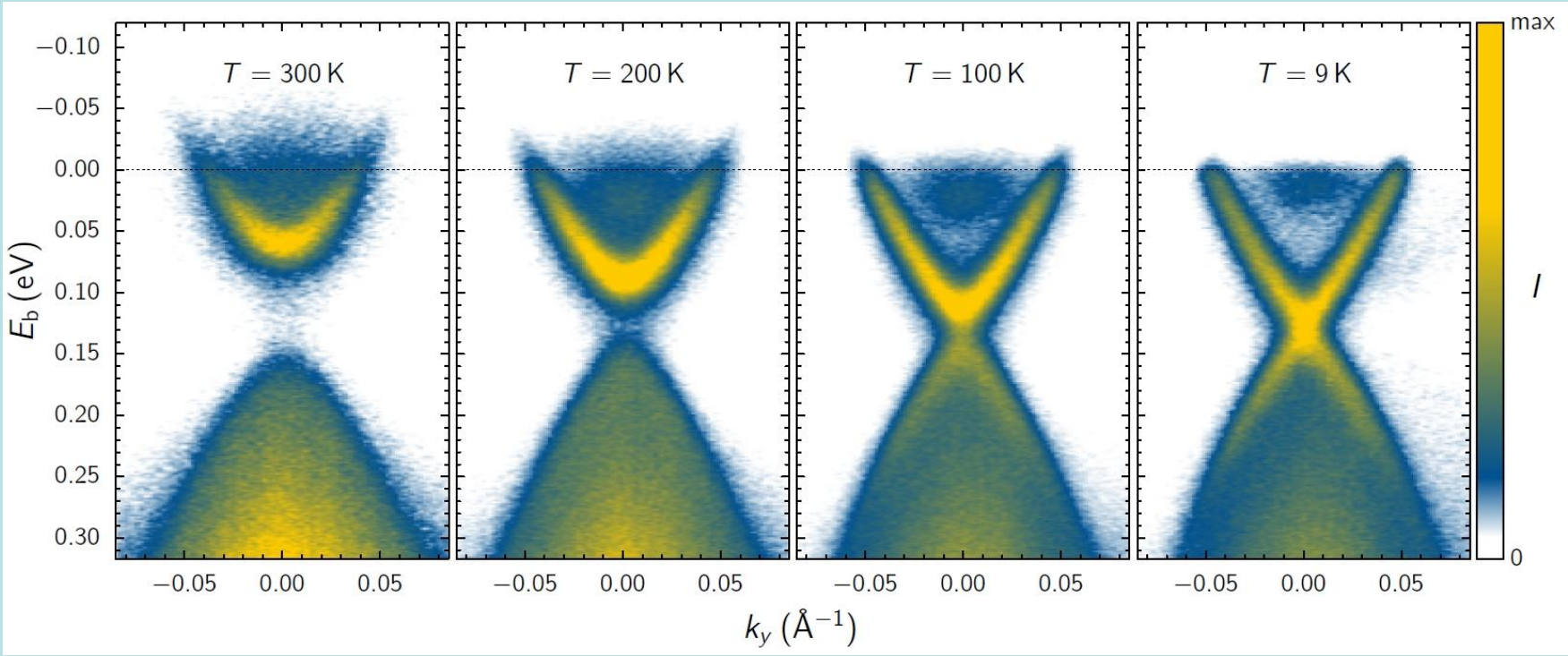


Electron band structure ARPES studies of $Pb_{0.77}Sn_{0.23}Se$

E_G vs. T

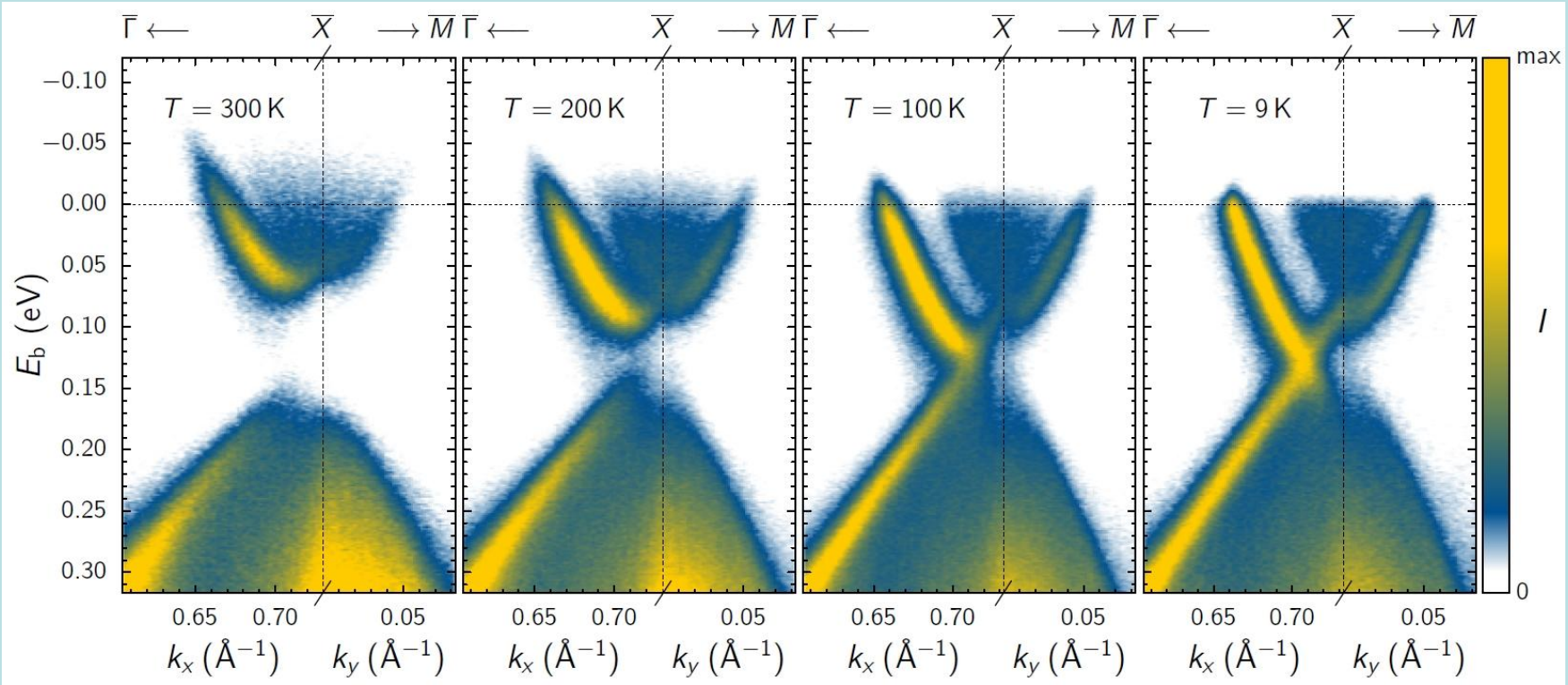


Electron band structure of $Pb_{0.77}Sn_{0.23}Se$ ARPES experimental studies



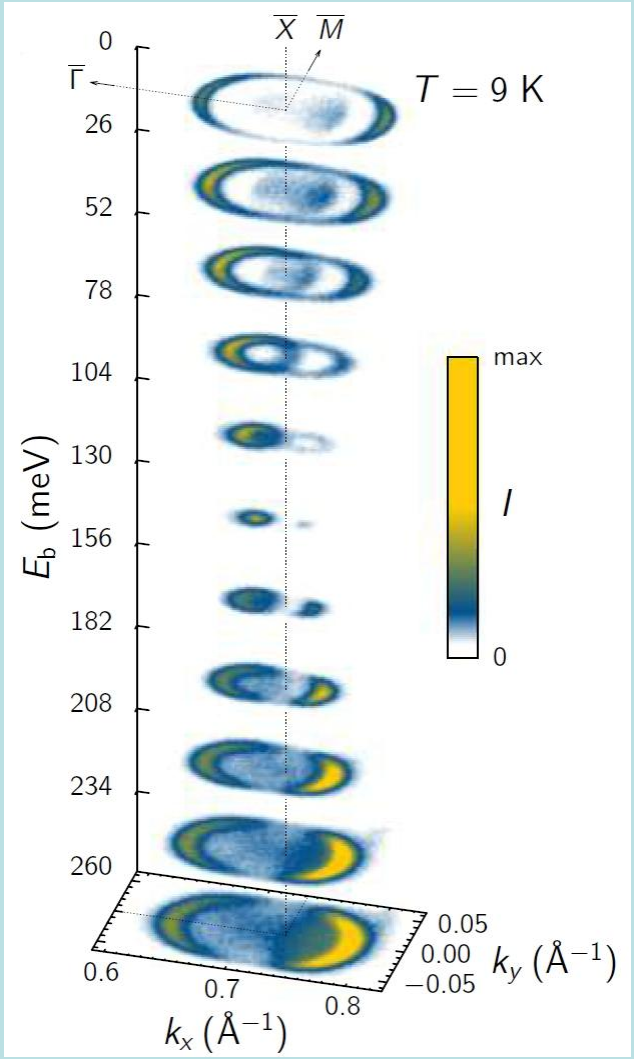
- **Energy dispersion relation for temperature varying across band inversion point**

Electron band structure of $Pb_{0.77}Sn_{0.23}Se$ ARPES experimental studies



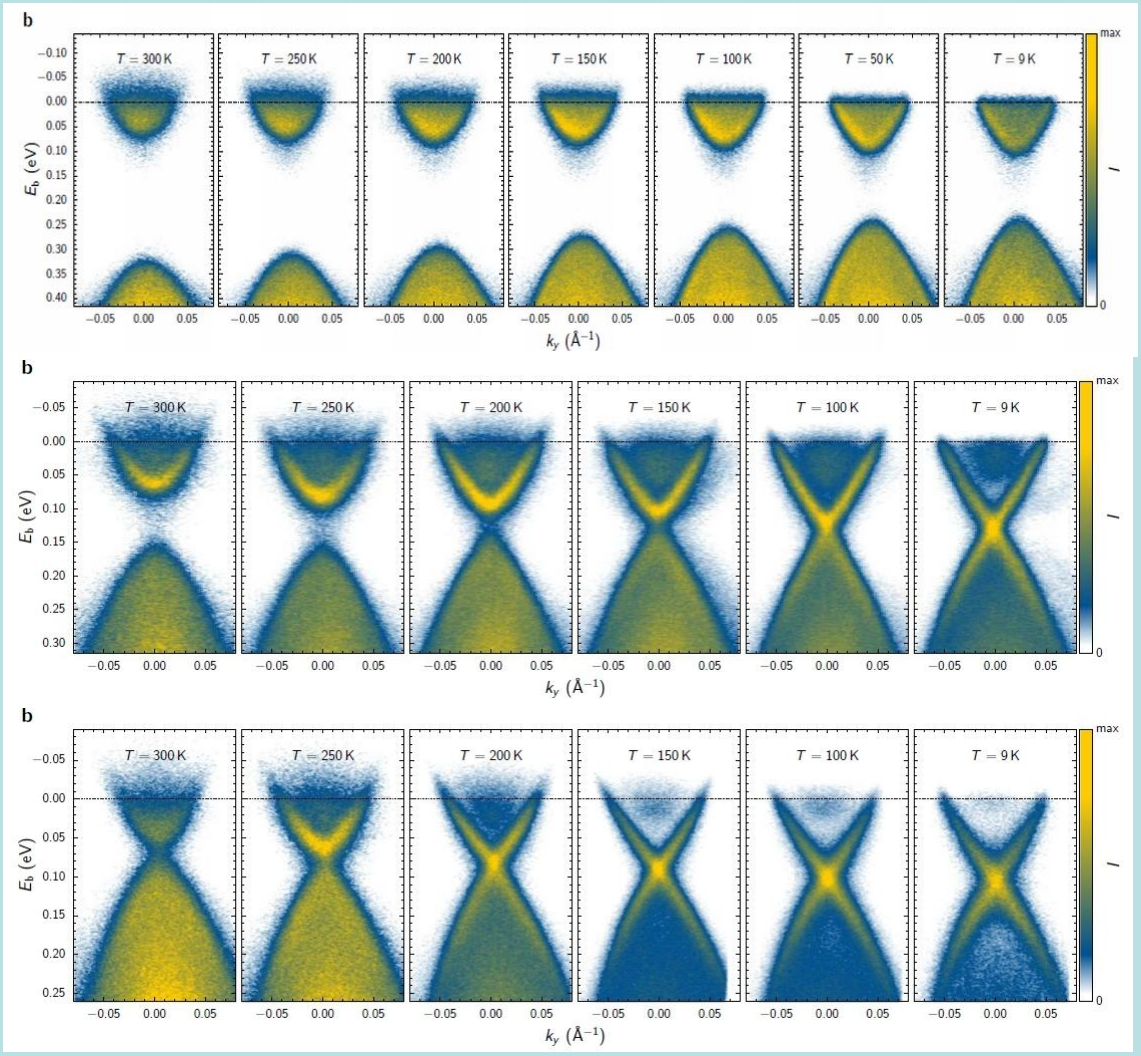
- **Energy dispersion E(k) for X-Γ and X-M directions in surface Brillouin zone**

Electron band structure of $Pb_{0.77}Sn_{0.23}Se$ ARPES experimental studies



- **Fermi surface cuts $E(k_x, k_y)$ for varying binding energy E_b**

Trivial insulator (PbSe) vs topological crystalline insulator ($Pb_{1-x}Sn_xSe$)



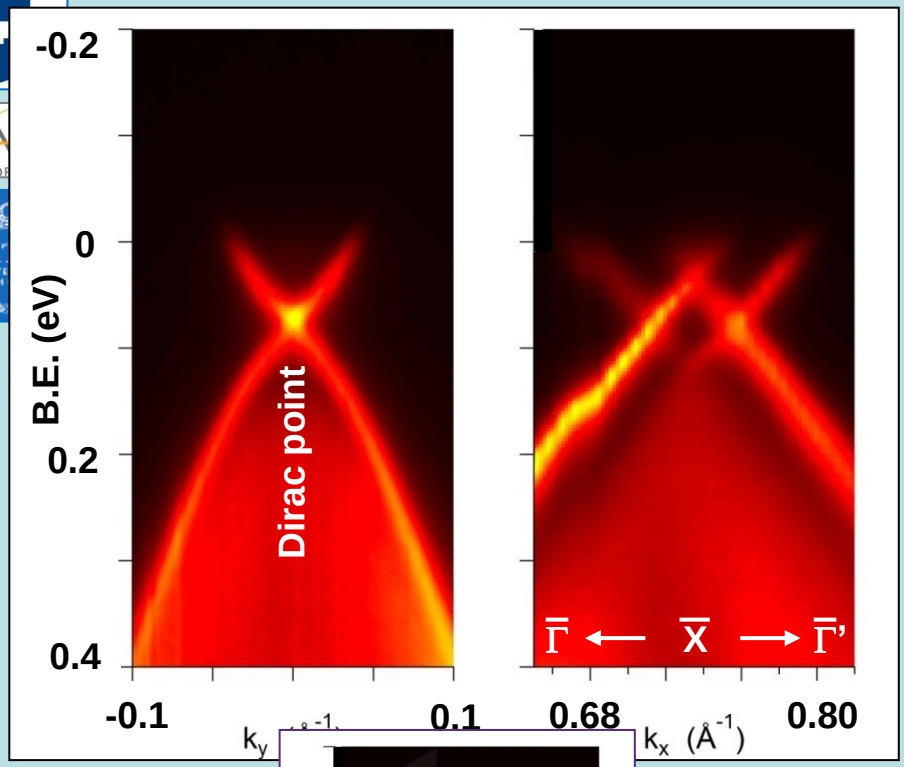
PbSe (x=0)

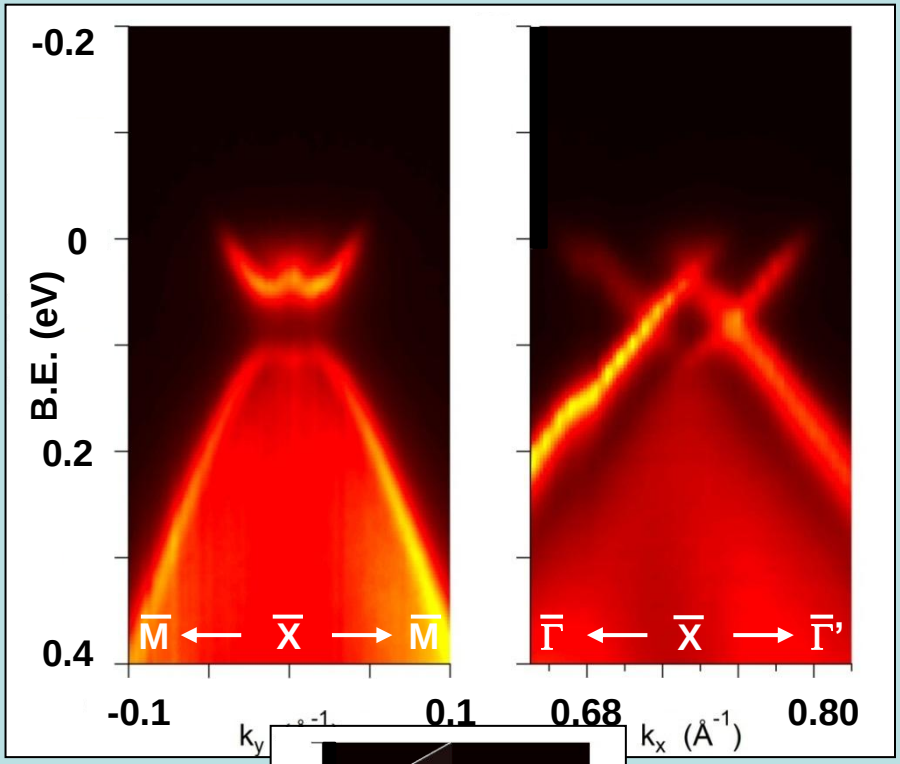
x=0.23

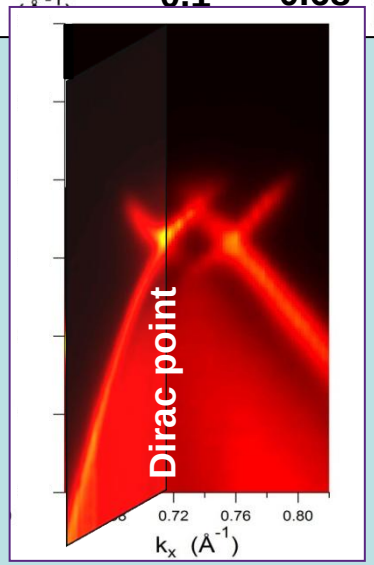
x=0.30

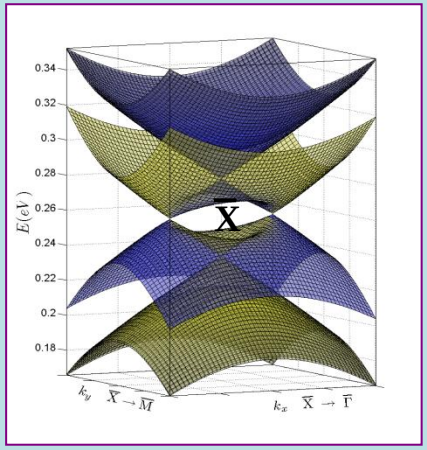
B.M. Wojek et al. 2012

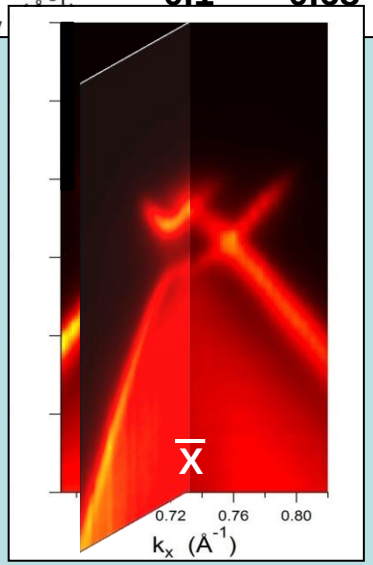
$Pb_{0.67}Sn_{0.33}Se$, T=87 K, hν=18.5 eV





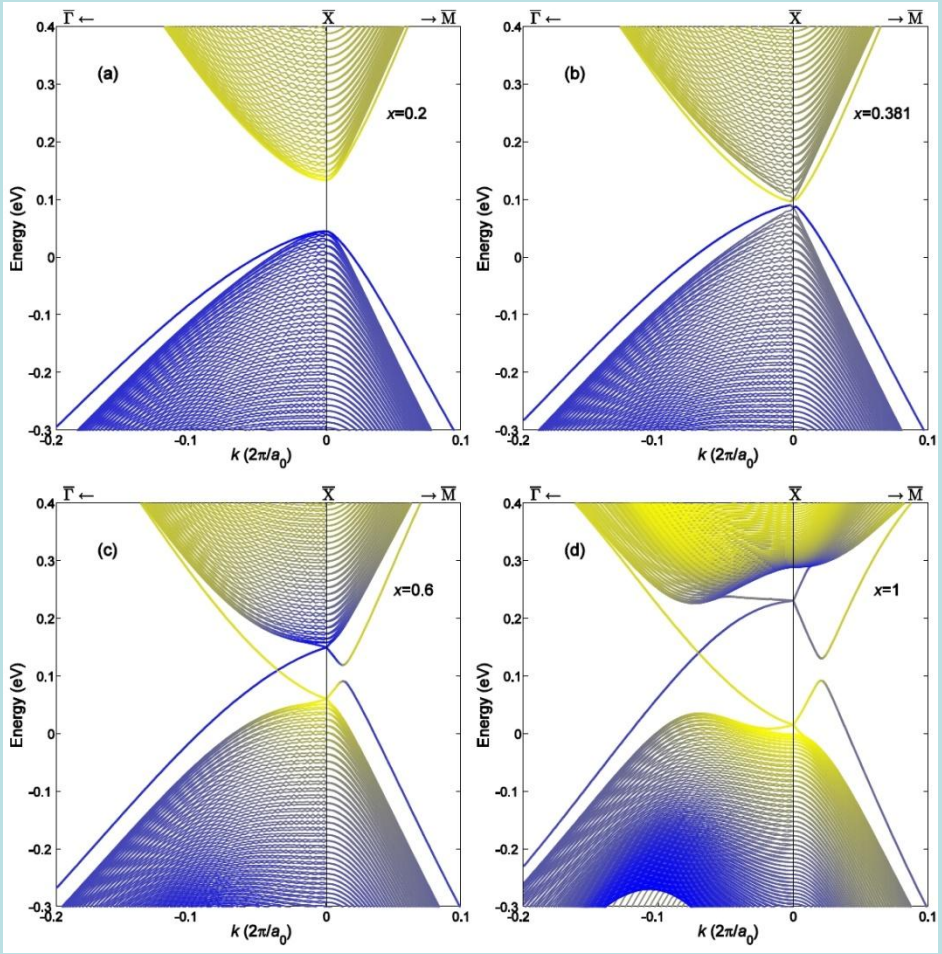






Theory-
R. Buczko, P. Kacman, S. Safaei

Band structure of $Pb_{1-x}Sn_xTe$: tight binding calculations

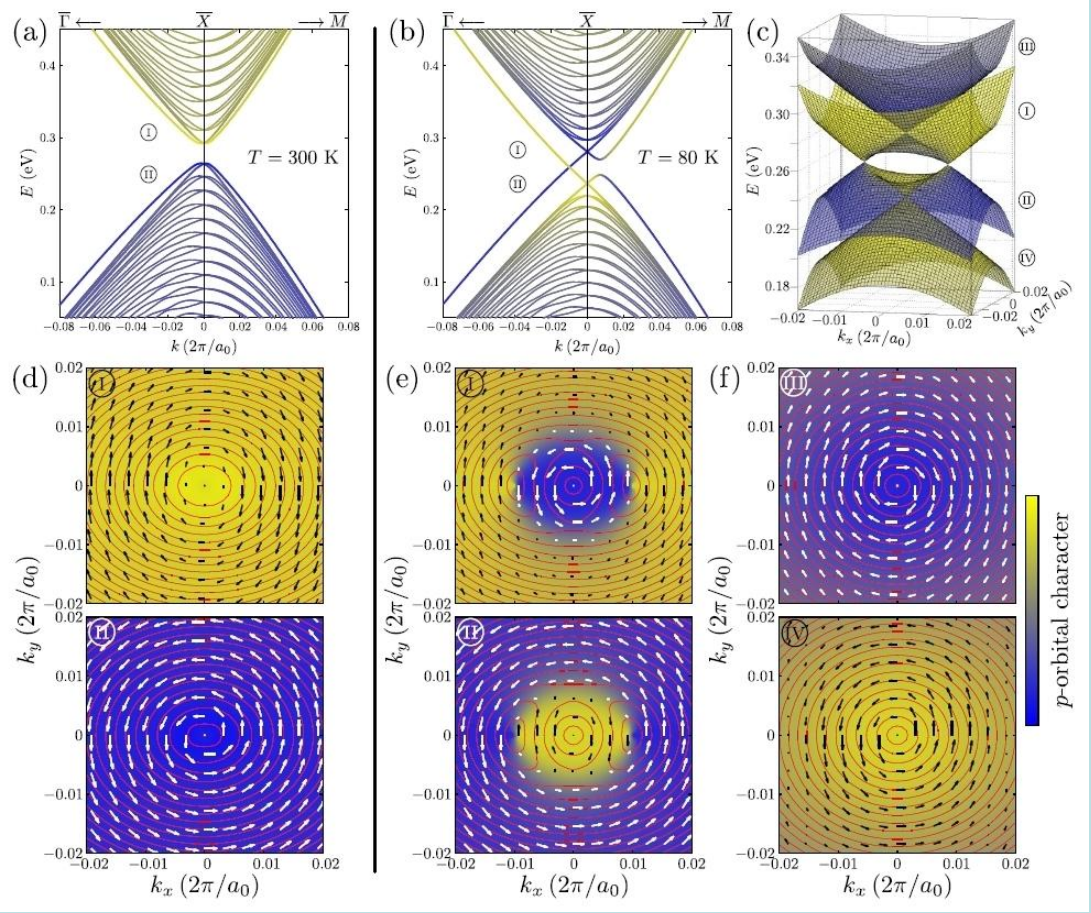


- PbSnTe in band inversion region:

- A) band insulator
- B) zero bulk band gap
- C) inverted gap - TCI
- D) SnTe – TCI

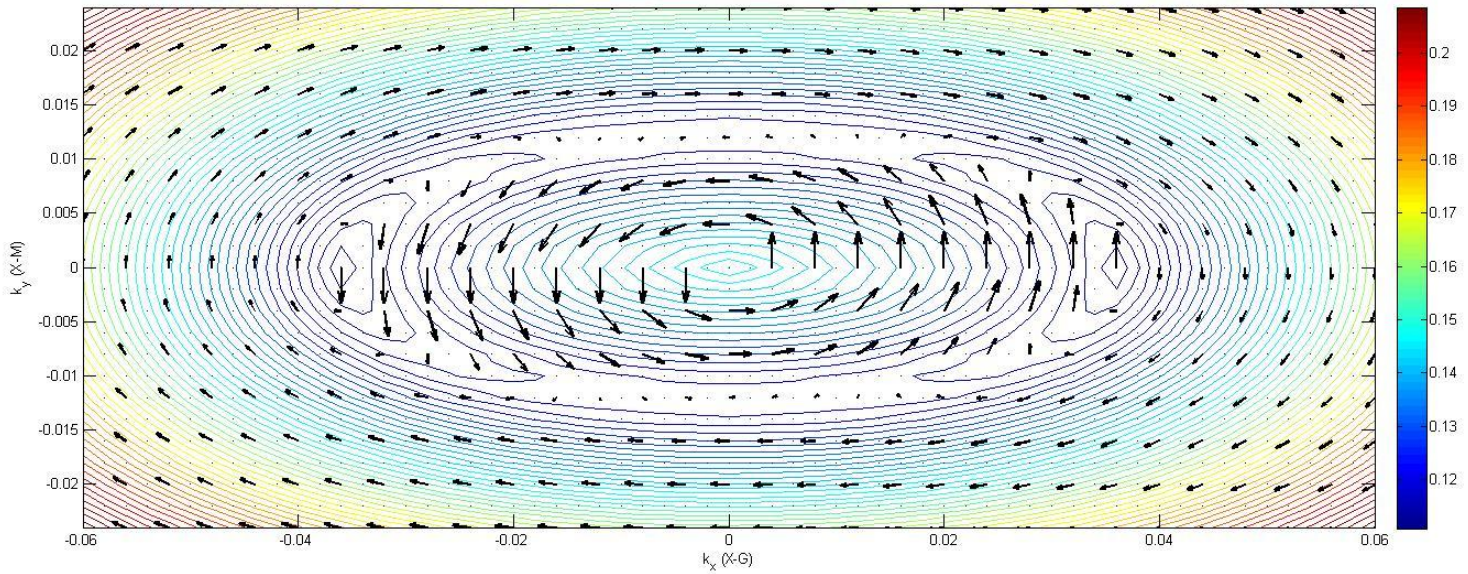
Yellow – p-type cation orbitals
Blue – p-type anion orbitals

Spin polarization of TCI states: tight binding model – $Pb_{0.76}Sn_{0.24}Se$



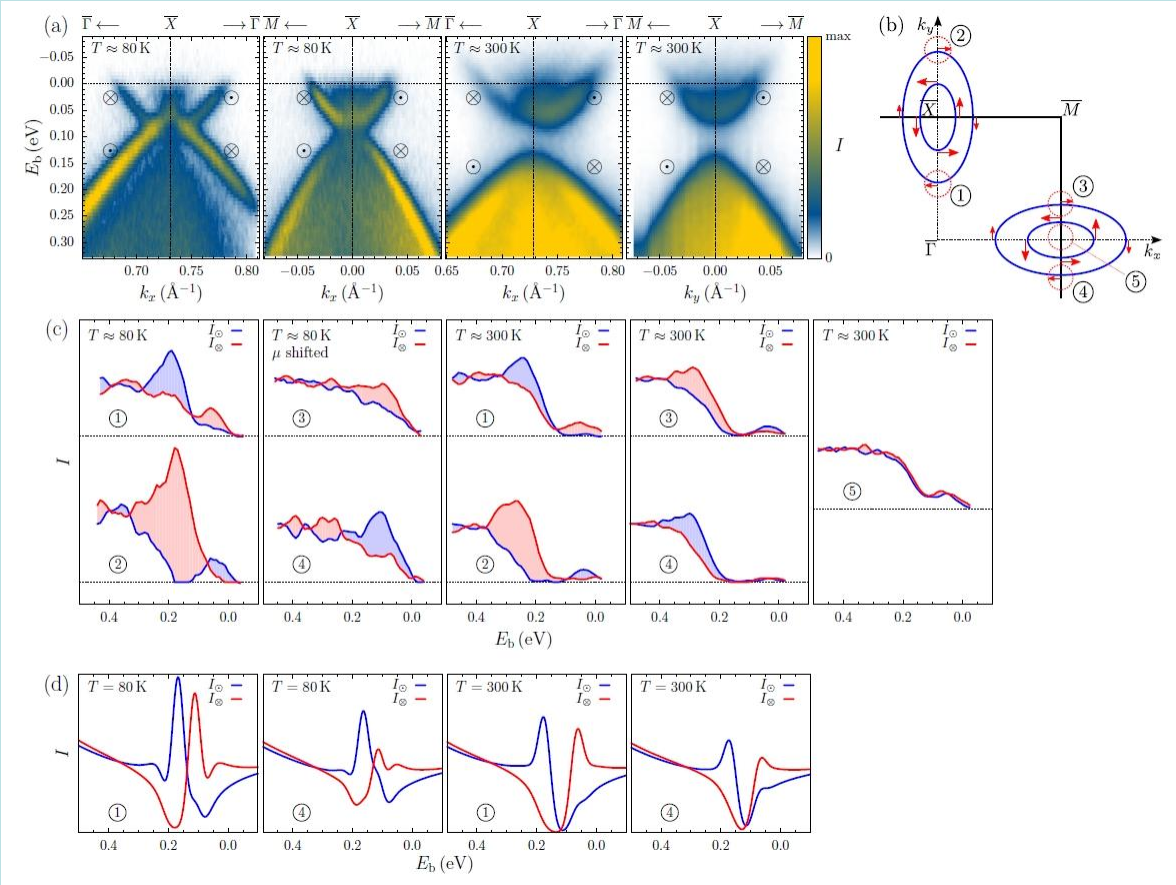
B.M. Wojek, R. Buczko et al. Phys. Rev. B 87, 115105 (2013)

Spin polarization of TCI states in SnTe



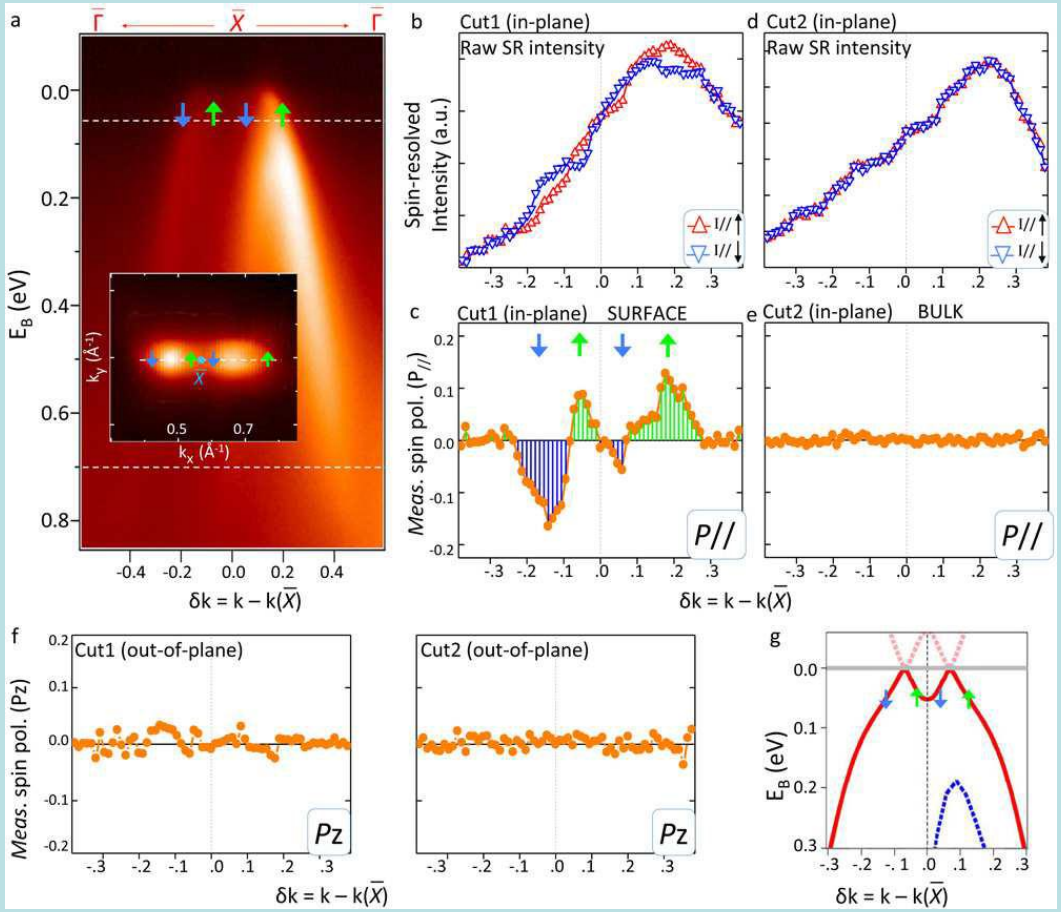
S. Safaei, P. Kacman, R. Buczko, Phys. Rev. B 88, 045305 (2013)
tight binding calculations

Spin polarization of TCI states: SRPES experiment – $Pb_{0.76}Sn_{0.24}Se$



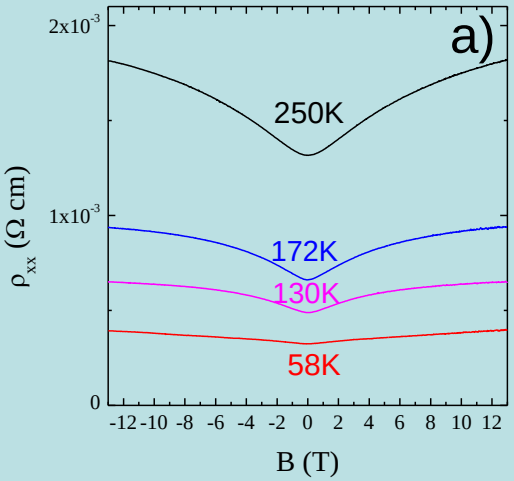
B.M. Wojek, R. Buczko et al. Phys. Rev. B 87, 115106 (2013)

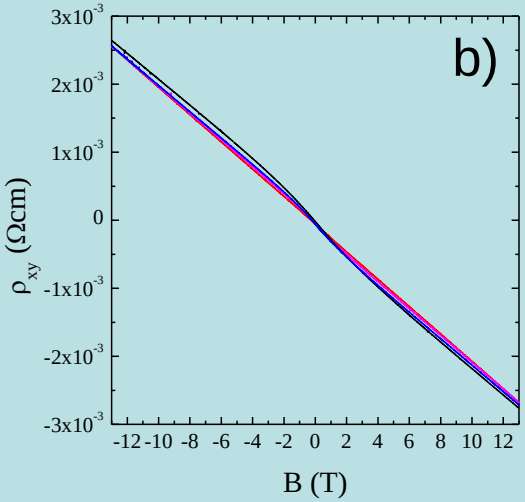
Spin polarization of TCI states: SRPES experiment – $Pb_{0.6}Sn_{0.4}Te$

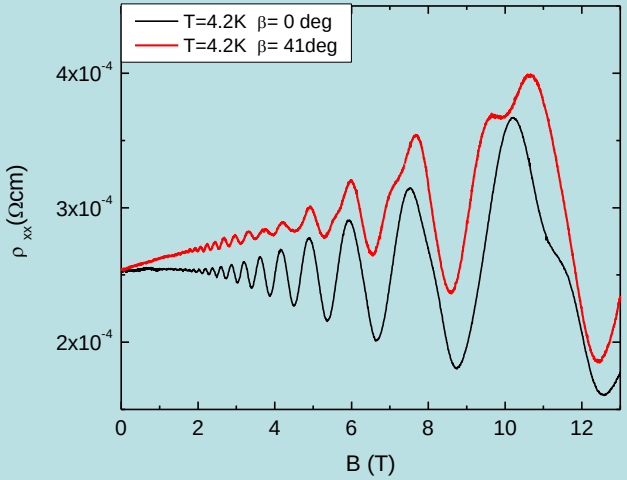


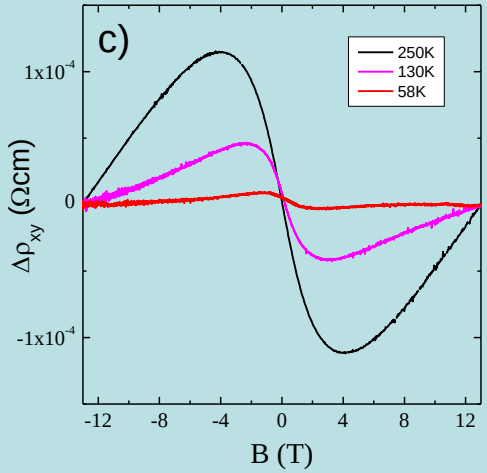
- S-Y Xu, … M.Z. Hasan, Nat. Commun. 3, 1192 (2012).

$Pb_{0.77}Sn_{0.23}Se$: magneto-transport

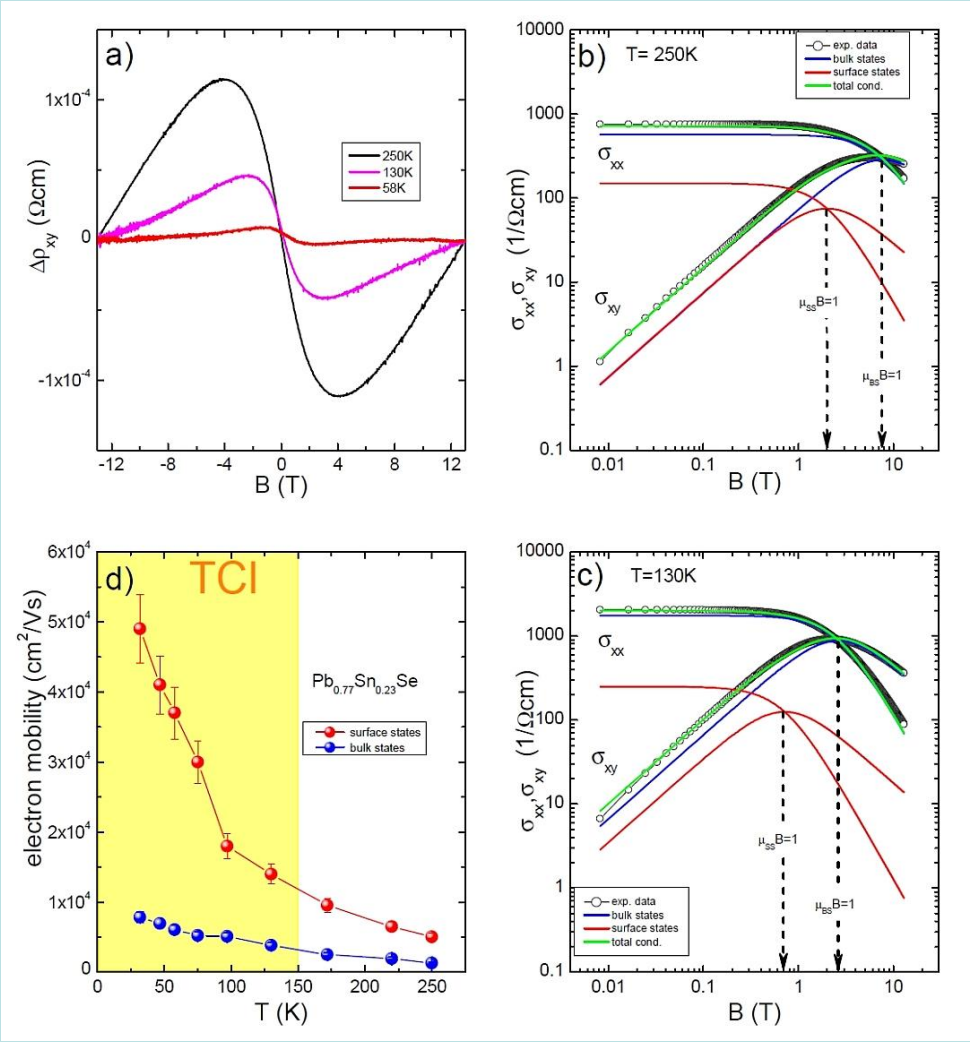








$Pb_{0.77}Sn_{0.23}Se$: magneto-transport



Drude model for magneto-conductivity

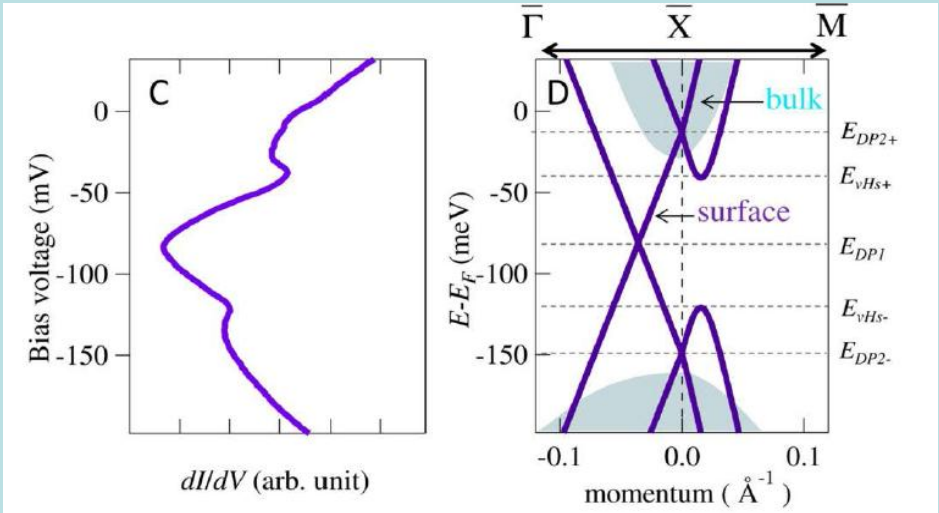
Two parrallel conduction channels

Fitting of electron transport parameters

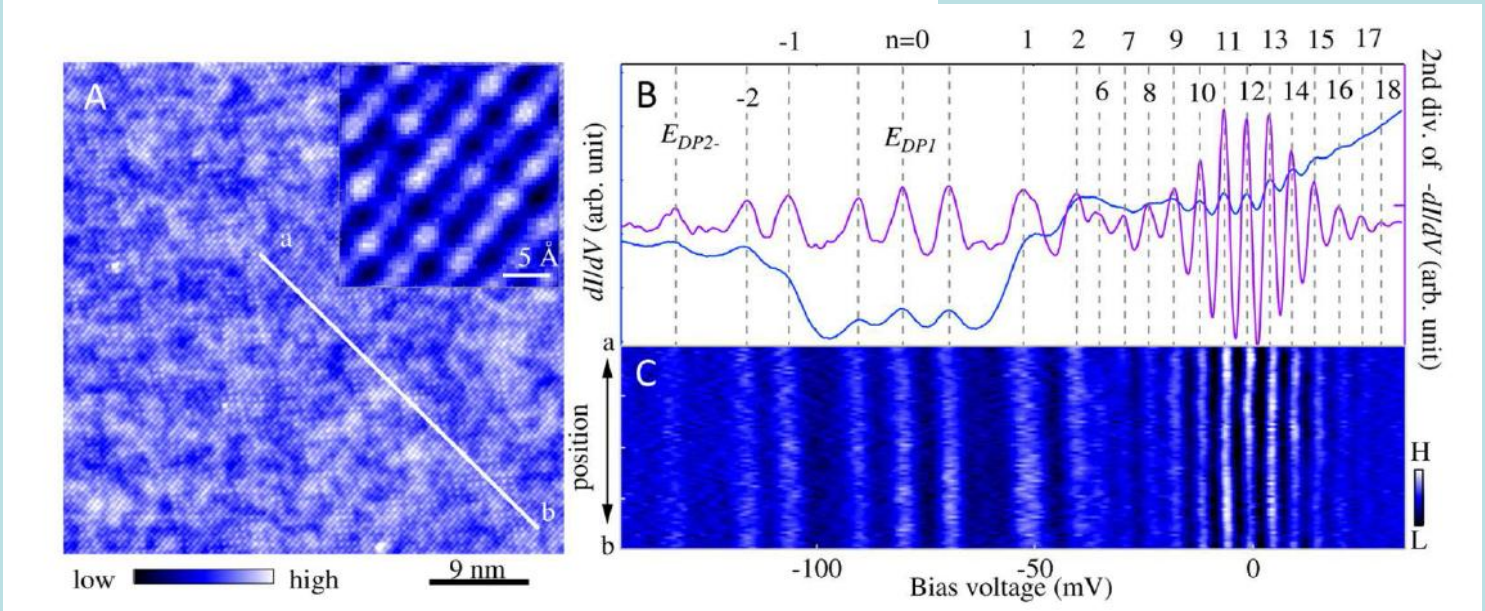
σ_{BS} , μ_{BS} , σ_{SS} , μ_{SS}
for bulk crystal and surface channels

K. Dybko et al. 2012

STM $Pb_{1-x}Sn_xSe$



Y. Okada et al., Science 2013



TCI - materials

nature materials

LETTERS

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Topological crystalline insulator states in $Pb_{1-x}Sn_xSe$

P. Dziawa[1], B. J. Kowalski[1], K. Dybko[1], R. Buczko[1], A. Szczerbakow[1], M. Szot[1], E. Łusakowska[1], T. Balasubramanian[2], B. M. Wojek[3], M. H. Berntsen[3], O. Tjernberg[3]* and T. Story[1]*

nature physics

LETTERS

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Experimental realization of a topological crystalline insulator in SnTe

Y. Tanaka[1], Zhi Ren[2], T. Sato[1]*, K. Nakayama[1], S. Souma[3], T. Takahashi[1,3], Kouji Segawa[2] and Yoichi Ando[2]*

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ARTICLE

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Observation of a topological crystalline insulator phase and topological phase transition in $Pb_{1-x}Sn_xTe$

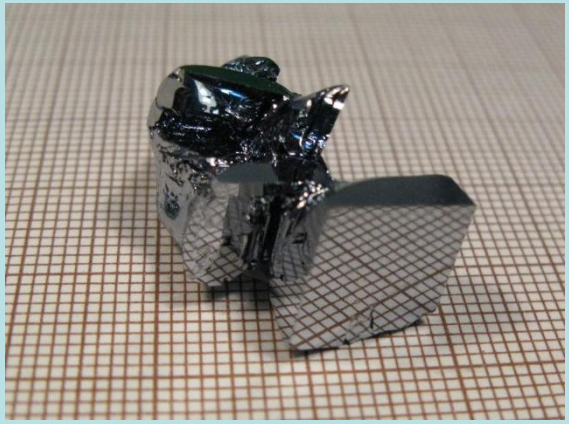
Su-Yang Xu[1], Chang Liu[1], N. Alidoust[1], M. Neupane[1], D. Qian[1,2], I. Belopolski[1], J.D. Denlinger[3], Y.J. Wang[4], H. Lin[4], L.A. Wray[1,3], G. Landolt[5,6], B. Slomski[5,6], J.H. Dil[5,6], A. Marcinkova[7], E. Morosan[7], Q. Gibson[8], R. Sankar[9], F.C. Chou[9], R.J. Cava[8], A. Bansil[4] & M.Z. Hasan[1,10]

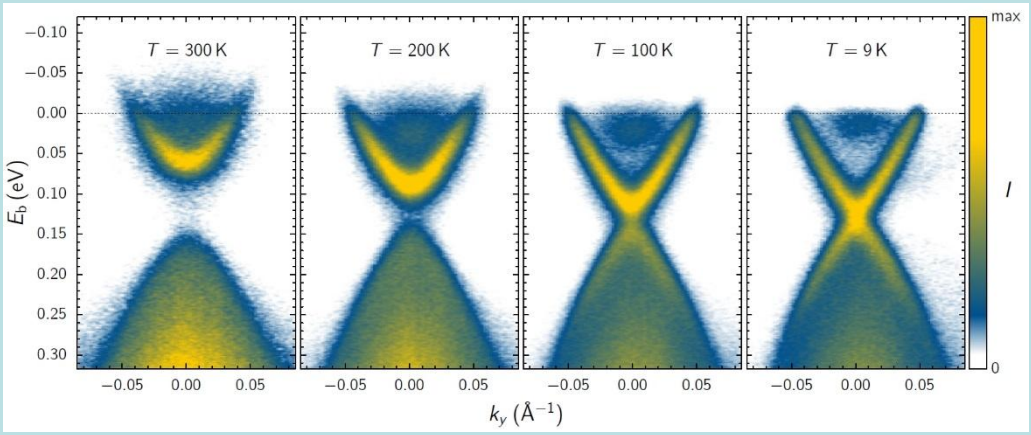
Summary

- **Topological crystalline insulators (TCIs) are a new class of quantum materials in which the topological protection of metallic surface states is warranted not by time-reversal symmetry as in TI but by specific crystalline symmetries.**

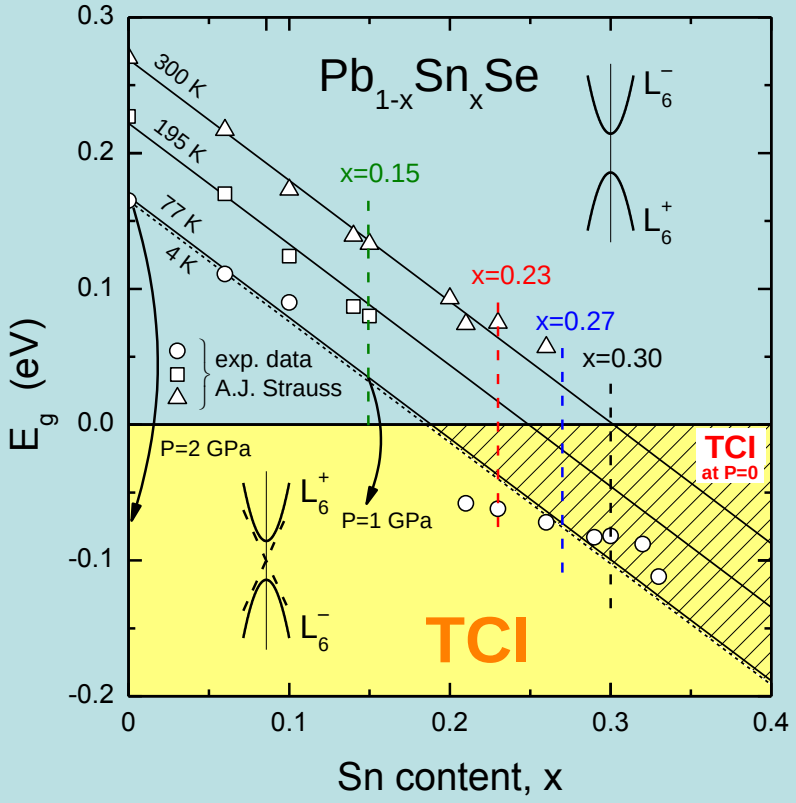
- **$Pb_{1-x}Sn_xSe$ – IV-VI narrow–gap semiconductor is a TCI, in which a temperature-driven topological phase transition is observed from a trivial insulator to a TCI due to band inversion.**

- **We discussed growth of monocrystals, electronic band structure investigations by angle- and spin-resolved photoemission spectroscopy (ARPES, SRPES), magneto-transport studies, and electronic band structure calculations of $Pb_{1-x}Sn_xSe$ ($x \leq 0.4$) .**





Future outlook



Topological phase diagram study: $Pb_{1-x}Sn_xSe$ i $Pb_{1-x}Sn_xTe$ – (T, P)

Controlling electrical and optical properties

Other surface sensitive experimental methods - STM

Co-existence of ferromagnetism and TCI state in $Sn_{1-x}Mn_xTe$?

TCI/ferromagnet and TCI/superconductor heterostructures

Influence of lattice distorsion on TCI