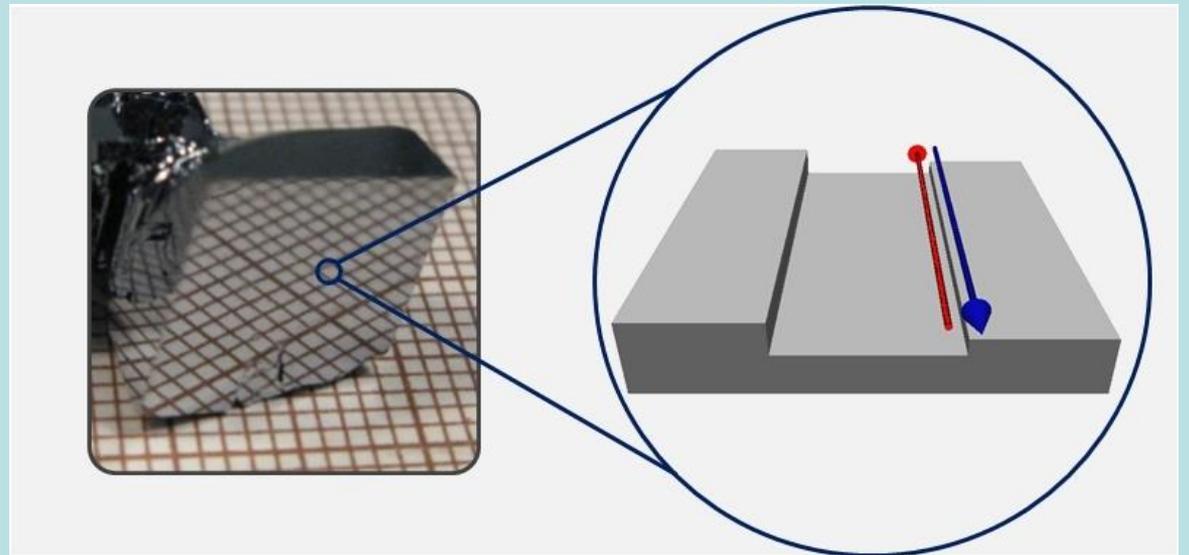
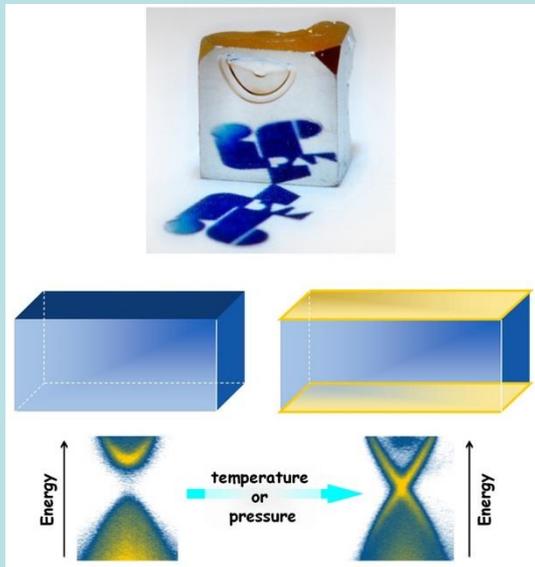


# Topological materials and topological crystalline insulators

Tomasz Story (Institute of Physics PAS, Warsaw)



# Outline

## I. Topological insulators (TI):

- TI concept and key physical factors
- Experimental techniques
- 3D and 2D materials – canonical TI
- Device ideas
- Physical classification and new topological materials

## II. Topological crystalline insulators (TCI)

- IV-VI semiconductors
- Topological protection by crystalline symmetry
- Controlling TCI state (lattice distortion, bandgap engineering)

## III. Atomic steps as new 1D topological systems

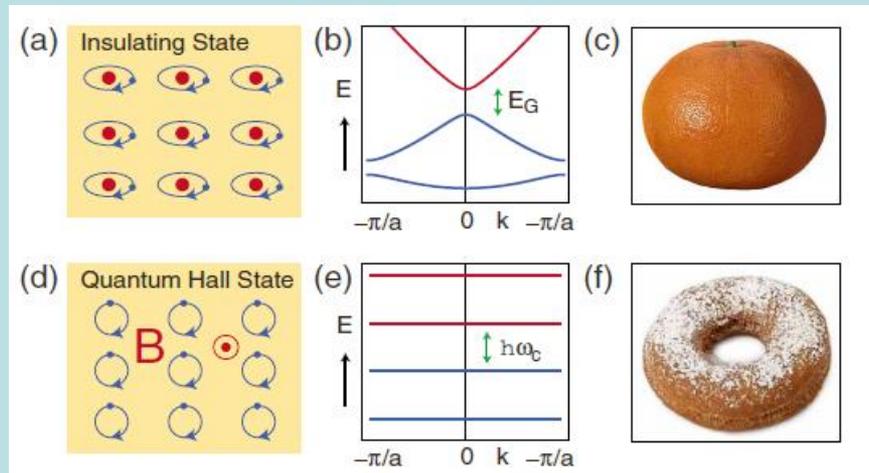
## Summary

# Insulators and metals semiconductors - semimetals

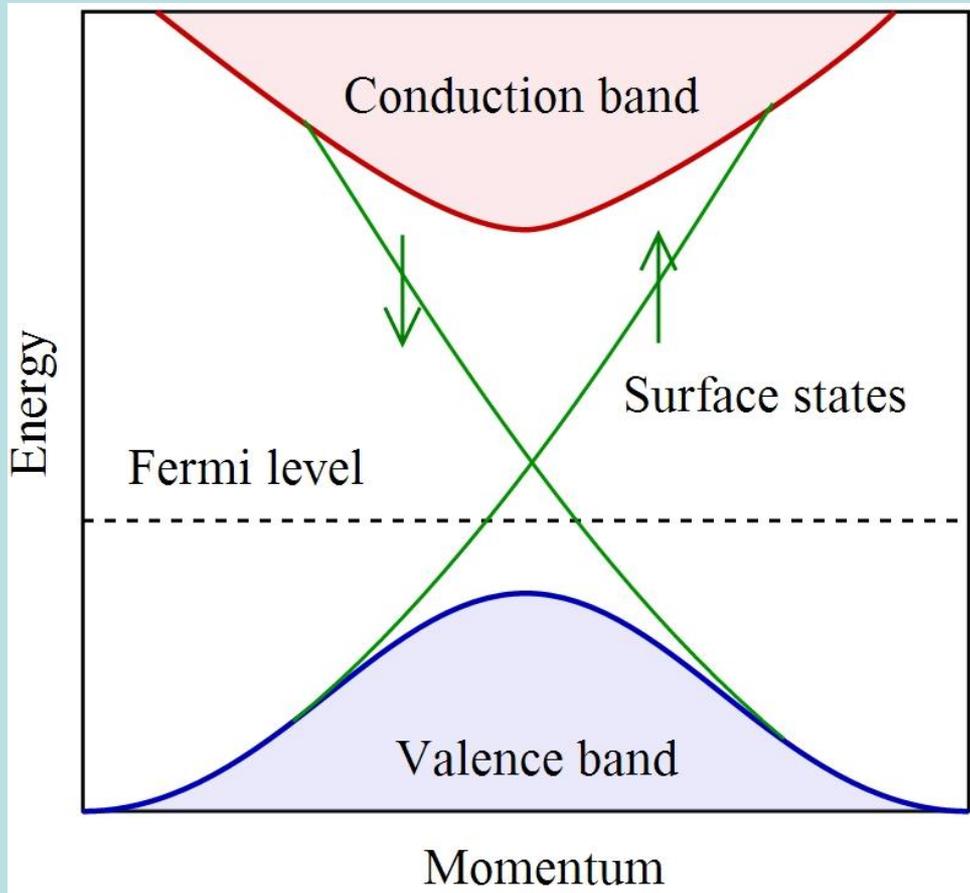
Energy band gap  $E_G$   
Electric conductivity  $\sigma_0 = \sigma(T=0)$

**Insulators:**  $E_G = 0.1-10$  eV;  $\sigma_0=0$

**Metals:**  $E_G = 0$ ;  $\sigma_0$  is finite

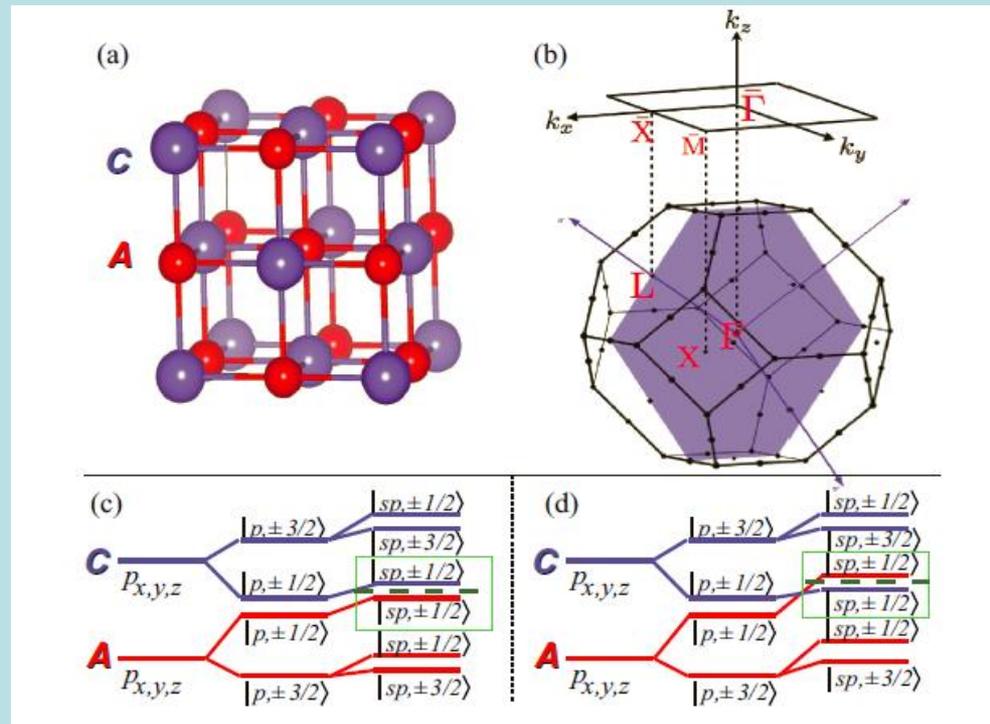


# Topological insulators: physical factors



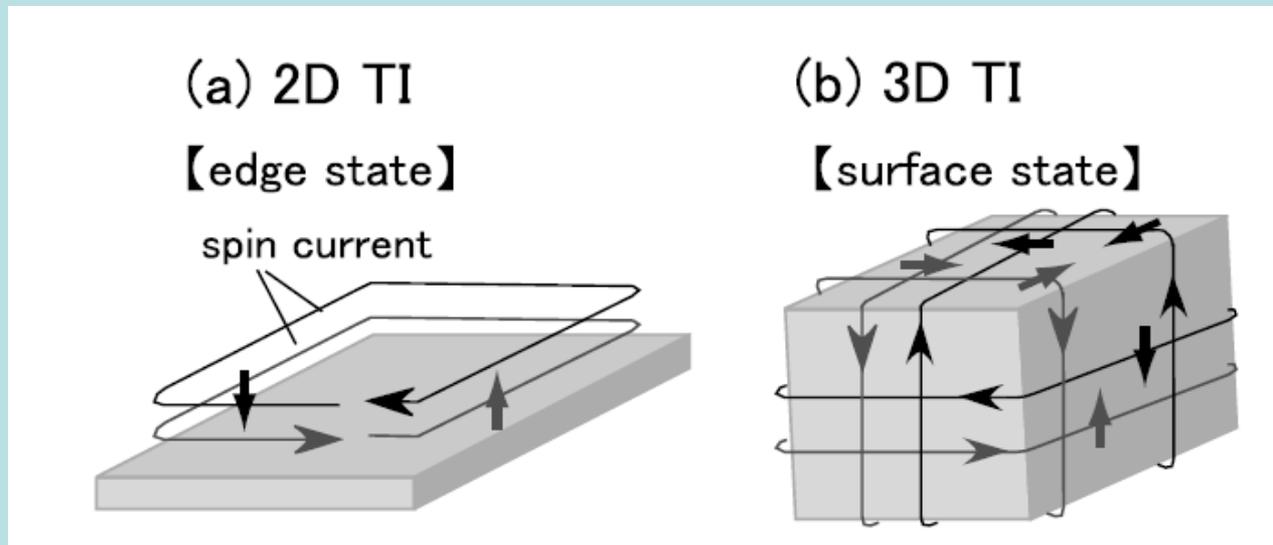
- **Inverted c-band and v-band symmetry**
- **Strong spin-orbit coupling**  
 $E_{so} \approx E_G$
- **Odd number of Dirac cones**
  
- **Metallic, helical Dirac-like electronic surface states**
- **Topological protection by time reversal symmetry**

# Band inversion in semiconductors



# Topological electronic states

Edge states in 2D heterostructures  
Surface states in bulk crystals



# Topological electronic states experimental techniques

Angle- and spin-resolved photoemission spectroscopy (ARPES, SRPES)

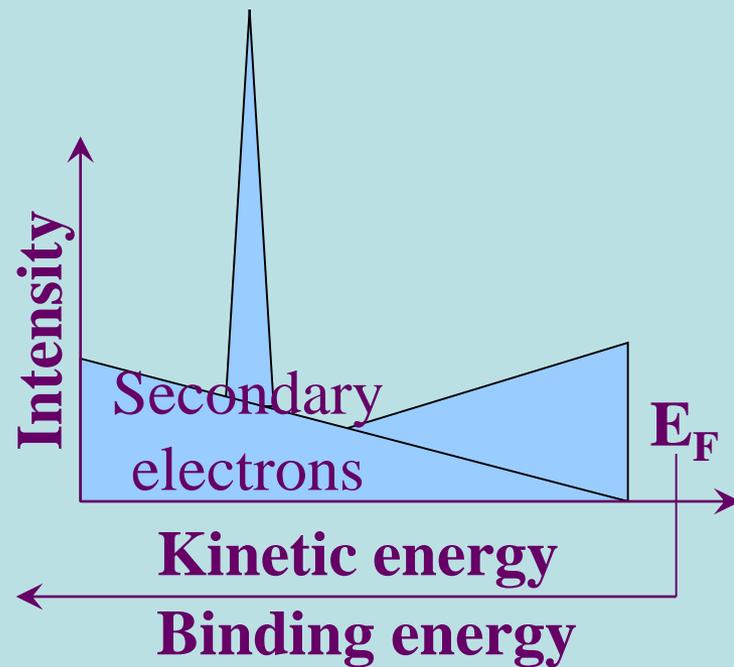
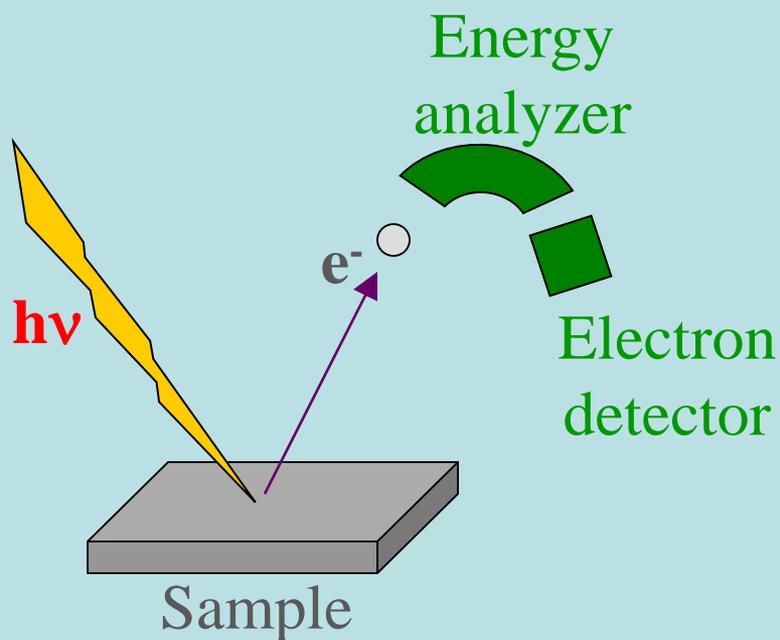
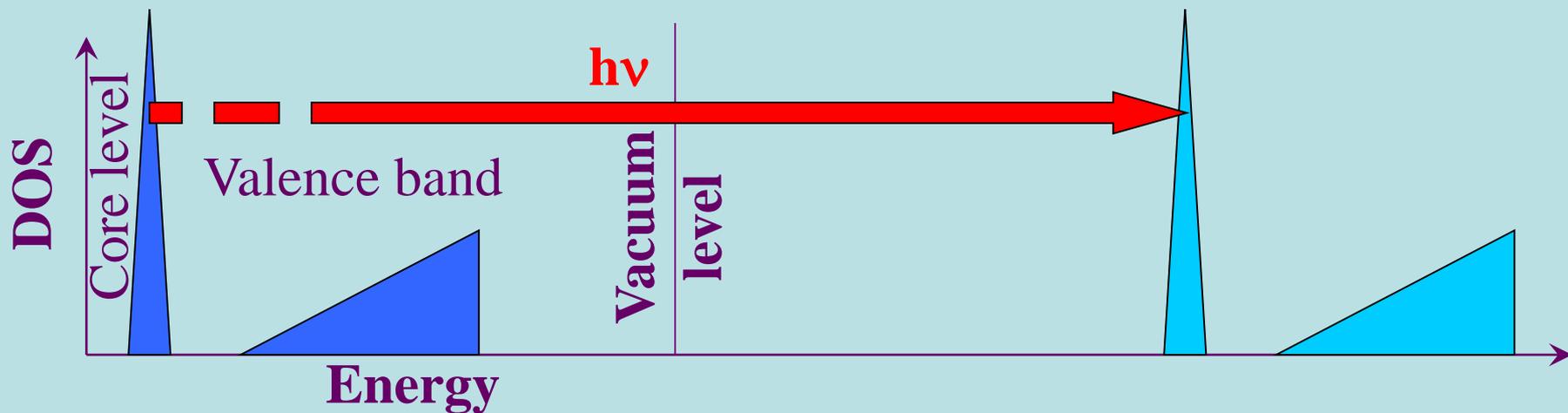
Scanning tunneling microscopy and spectroscopy (STM/STS):  
conductance spectroscopy and quasiparticle interference

Magnetotransport: SdH oscillations, weak antilocalization

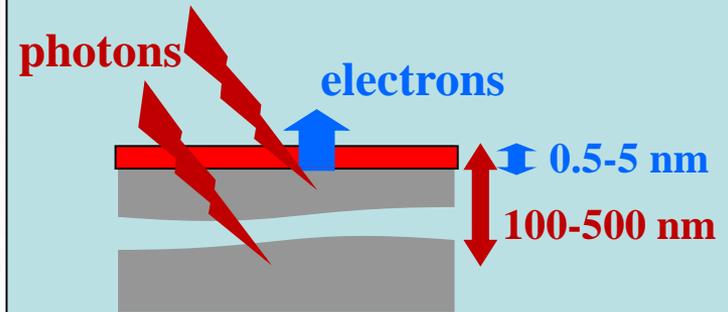
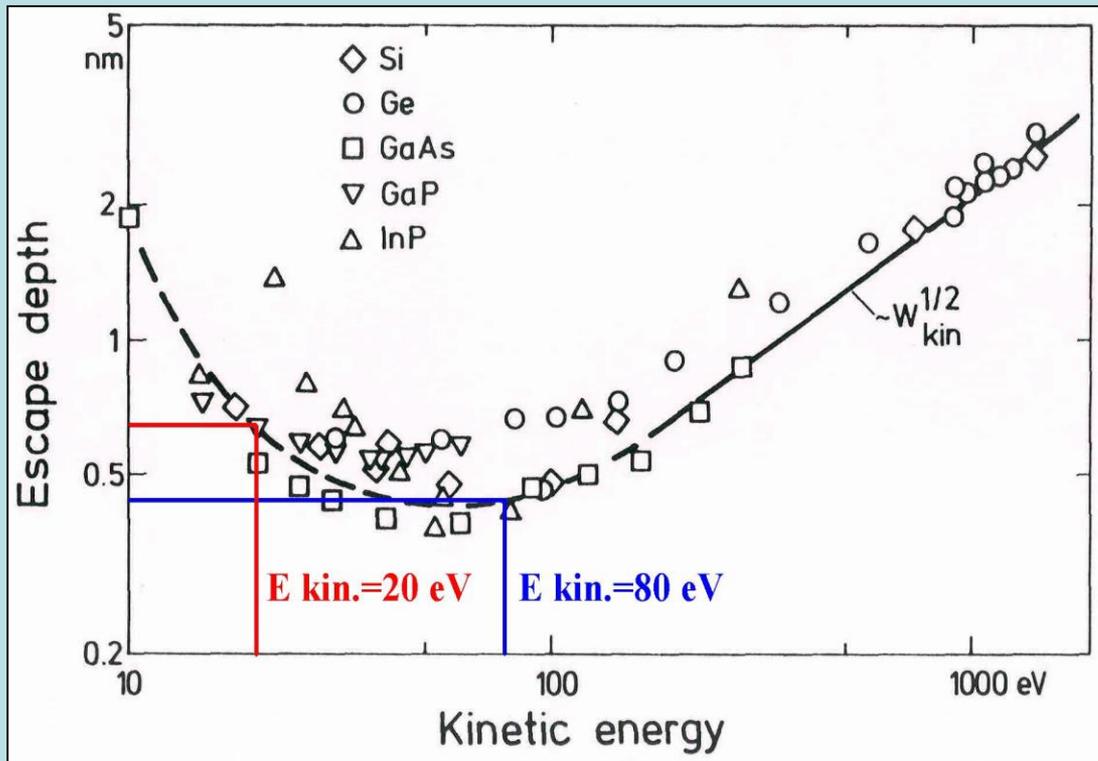
Magnetooptics



# Photoemission electron spectroscopy



# Photoemission – crystal surface sensitive technique



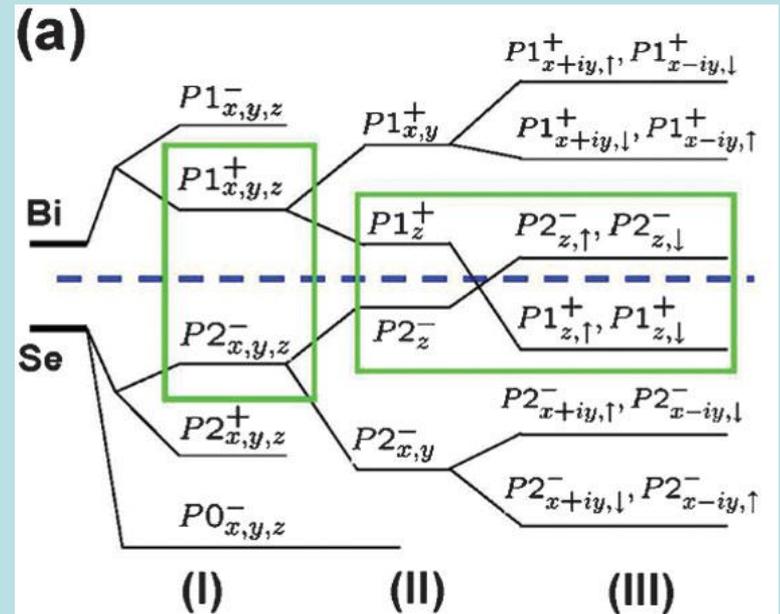
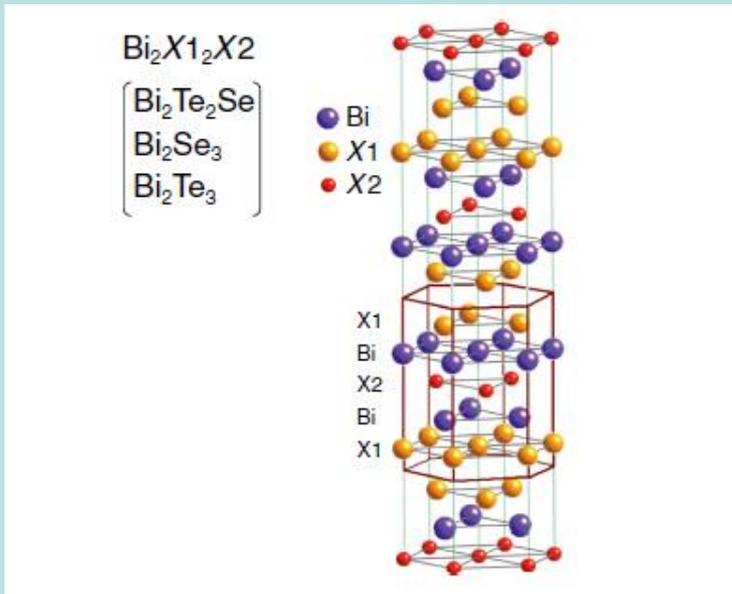
W. Mönch „Semiconductor surfaces and interfaces” 1993

# Topological insulators: key materials

- **Bulk crystals (3D)**
- $\text{Bi}_{1-x}\text{Sb}_x$
- $\text{Bi}_2\text{Se}_3$
- $\text{Bi}_2\text{Te}_3$
- (.....)
  
- **2D electronic systems**
- HgTe/CdTe quantum wells
- InAs-GaSb heterostructures

# 3D topological insulators

$\text{Bi}_2\text{Se}_3$  ,  $\text{Bi}_2\text{Te}_3$  ,  $\text{Sb}_2\text{Te}_3$   
 $\text{Bi}_2\text{Te}_2\text{Se}$



Crystal structure

Chemical bonding

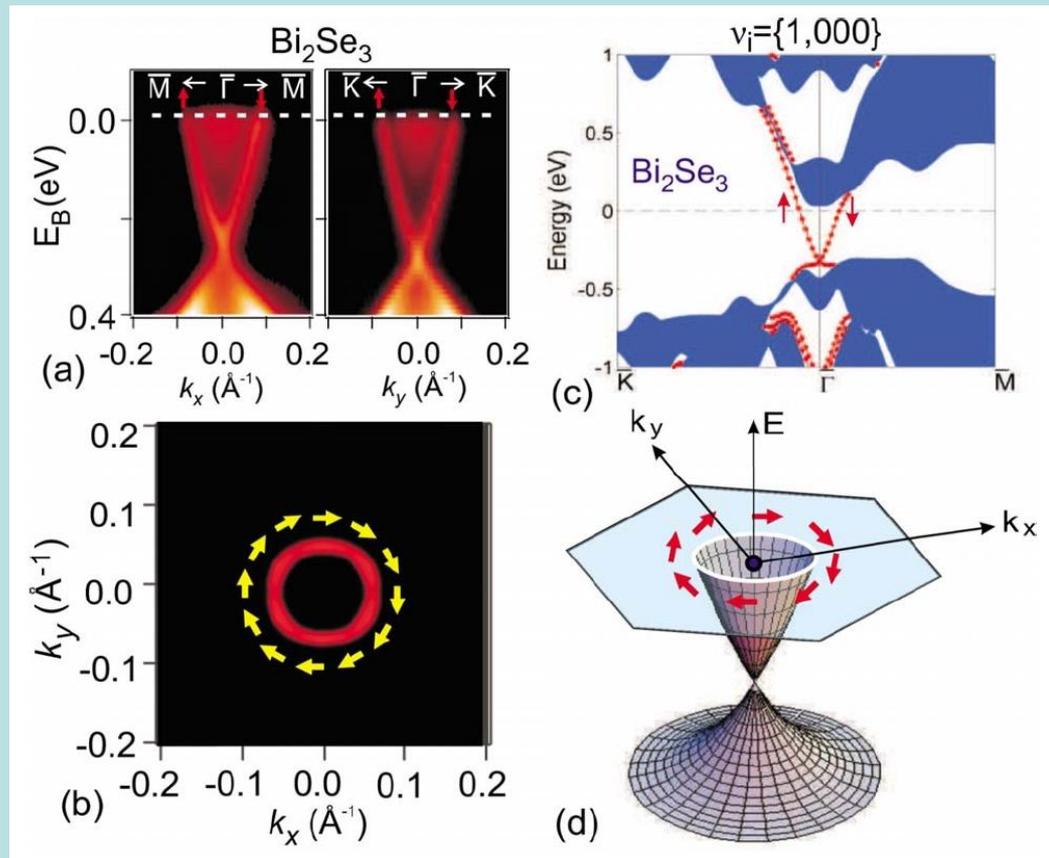
Crystal field splitting

Spin-orbit coupling

H. Zhang et al., Nat. Phys. **5**, 438 (2009)

Electronic structure

# Model topological insulator $\text{Bi}_2\text{Se}_3$

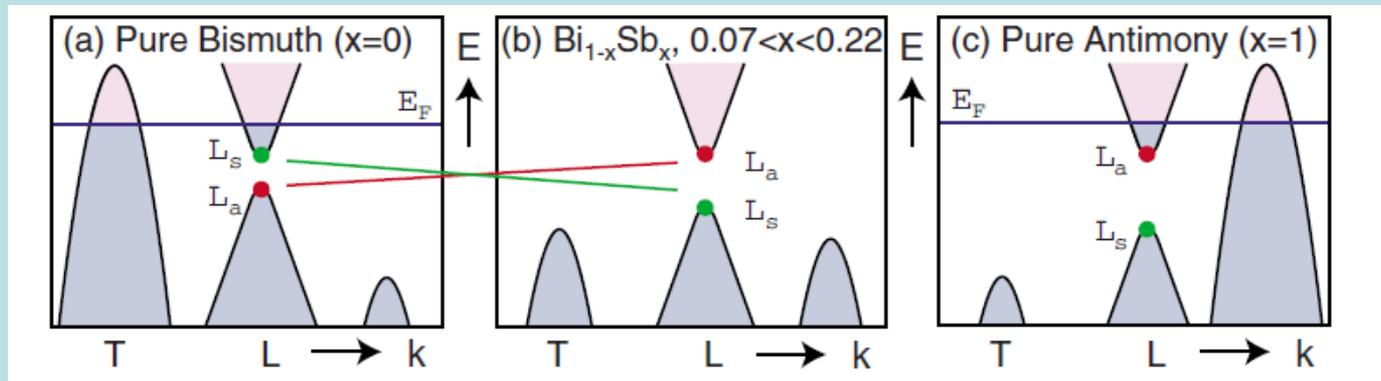


M.Z. Hasan, C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010)

# 3D topological insulators

Bi – semimetal with strong spin-orbit coupling

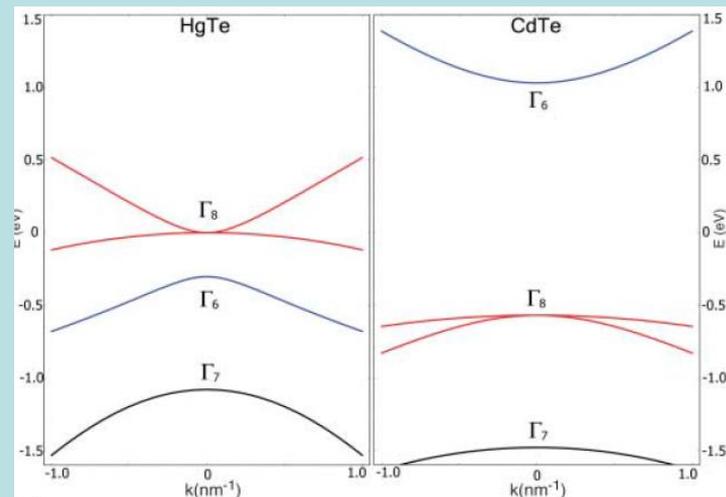
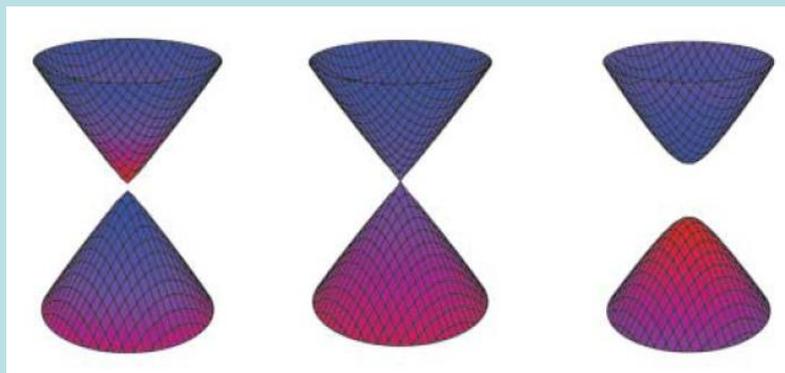
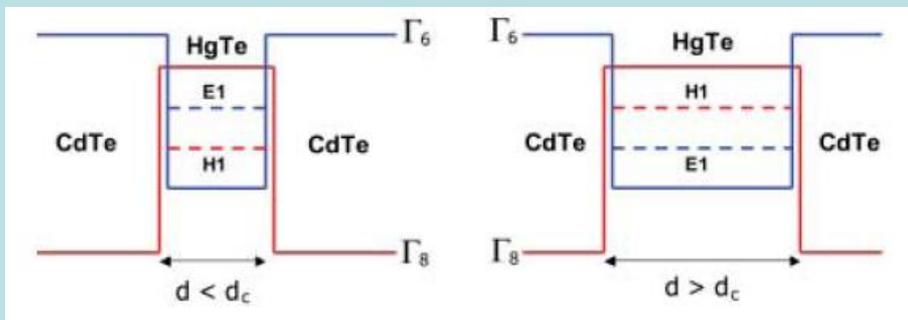
$\text{Bi}_{1-x}\text{Sb}_x$  – semiconductor alloy – thermoelectric material



L. Fu & C. Kane theory for  $\text{Bi}_{1-x}\text{Sb}_x$  (PRB 2007)

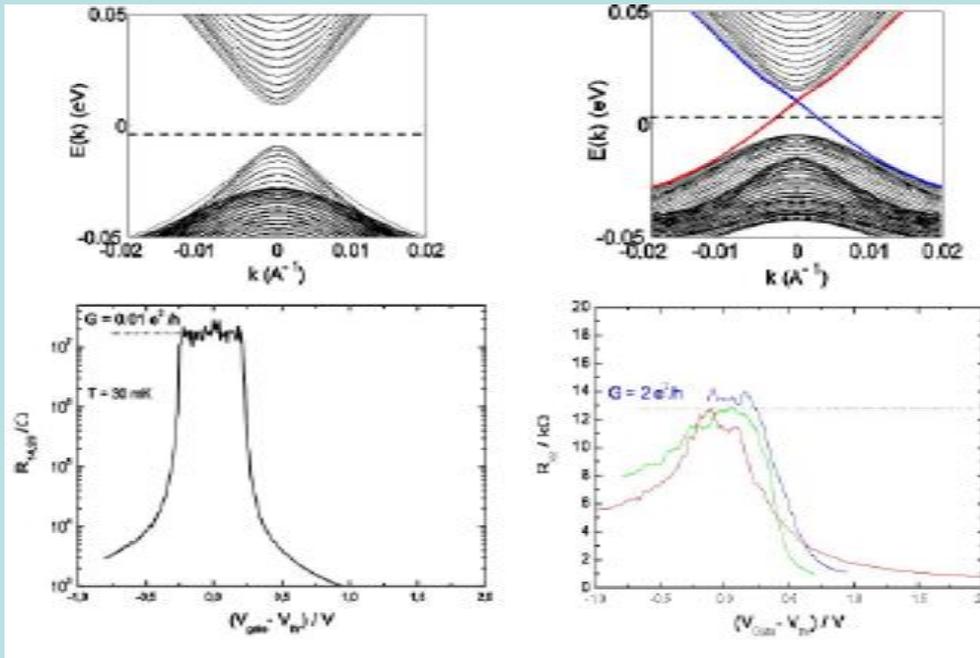
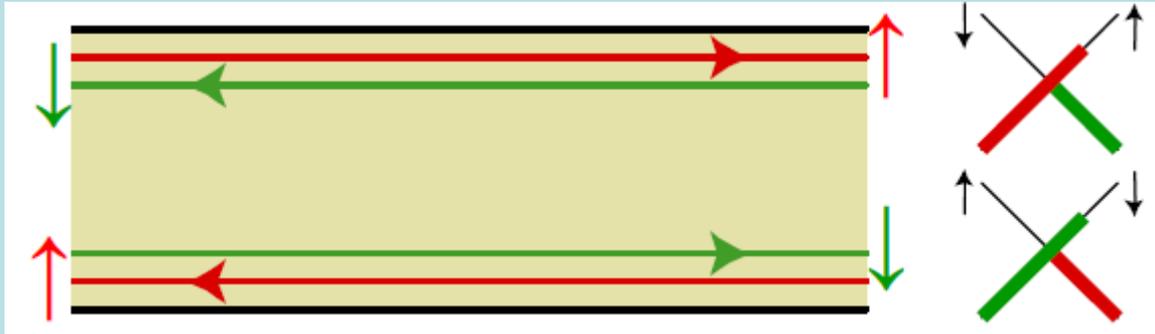
Experimental verification: Hsieh et al., Nature 2008

# HgTe/CdTe quantum wells: 2D topological insulators Quantum spin Hall (QSH) systems



Inversion of band edges determines the topological properties

# Experimental observation of topological edge states in HgTe/CdTe (QSH) (Konig et al, Science 2007)

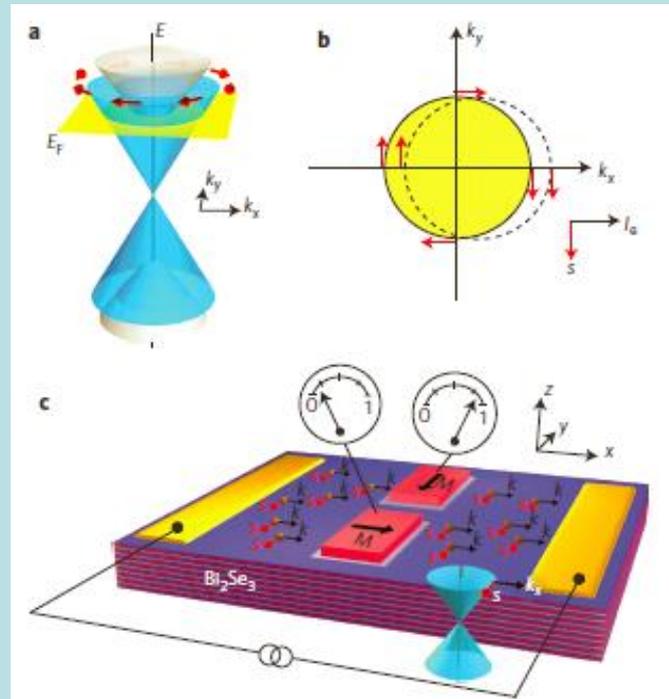


Topological protection of edge states warranted by time reversal symmetry

$$\langle \psi(k, \uparrow) | V | \psi(-k, \downarrow) \rangle = 0$$

# Generation of spin current

## Electrical detection of spin polarization



nature  
nanotechnology

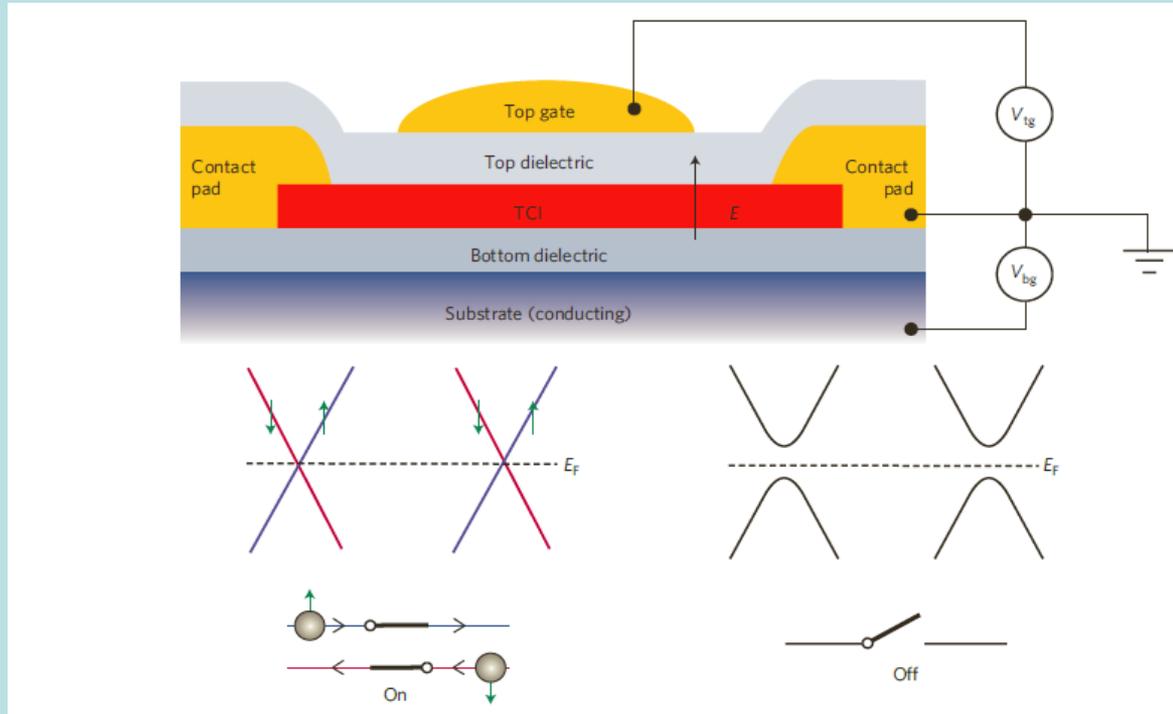
ARTICLES

PUBLISHED ONLINE 23 FEBRUARY 2014 | DOI: 10.1038/NNANO.2014.16

Electrical detection of charge-current-induced spin polarization due to spin-momentum locking in  $\text{Bi}_2\text{Se}_3$

C. H. Li<sup>1\*</sup>, O. M. J. van 't Erve<sup>1</sup>, J. T. Robinson<sup>2</sup>, Y. Liu<sup>3</sup>, L. Li<sup>3</sup> and B. T. Jonker<sup>1\*</sup>

# Topological transistor



ARTICLES

PUBLISHED ONLINE: 22 DECEMBER 2013 | DOI:10.1038/NMAT3828

nature  
materials

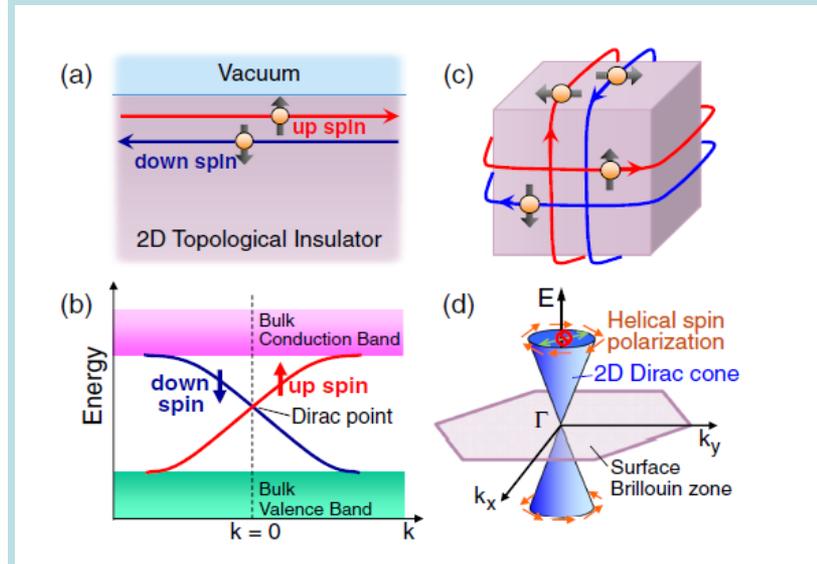
## Spin-filtered edge states with an electrically tunable gap in a two-dimensional topological crystalline insulator

Junwei Liu<sup>1,2</sup>, Timothy H. Hsieh<sup>2</sup>, Peng Wei<sup>2,3</sup>, Wenhui Duan<sup>1</sup>, Jagadeesh Moodera<sup>2,3</sup> and Liang Fu<sup>2\*</sup>

# Topological materials

**Table I.** Summary of topological insulator materials that have been experimentally addressed. The definition of (1;11) etc. is introduced in Sect. 3.7. (In this table, S.S., P.T., and SM stand for surface state, phase transition, and semimetal, respectively.)

Type	Material	Band gap	Bulk transport	Remark	Reference
2D, $\nu = 1$	CdTe/HgTe/CdTe	<10 meV	insulating	high mobility	31
2D, $\nu = 1$	AlSb/InAs/GaSb/AlSb	~4 meV	weakly insulating	gap is too small	73
3D (1;111)	$\text{Bi}_{1-x}\text{Sb}_x$	<30 meV	weakly insulating	complex S.S.	36, 40
3D (1;111)	Sb	semimetal	metallic	complex S.S.	39
3D (1;000)	$\text{Bi}_2\text{Se}_3$	0.3 eV	metallic	simple S.S.	94
3D (1;000)	$\text{Bi}_2\text{Te}_3$	0.17 eV	metallic	distorted S.S.	95, 96
3D (1;000)	$\text{Sb}_2\text{Te}_3$	0.3 eV	metallic	heavily p-type	97
3D (1;000)	$\text{Bi}_2\text{Te}_2\text{Se}$	~0.2 eV	reasonably insulating	$\rho_{xx}$ up to 6 $\Omega\text{cm}$	102, 103, 105
3D (1;000)	$(\text{Bi,Sb})_2\text{Te}_3$	<0.2 eV	moderately insulating	mostly thin films	193
3D (1;000)	$\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$	<0.3 eV	reasonably insulating	Dirac-cone engineering	107, 108, 212
3D (1;000)	$\text{Bi}_2\text{Te}_{1.6}\text{S}_{1.4}$	0.2 eV	metallic	n-type	210
3D (1;000)	$\text{Bi}_{1.1}\text{Sb}_{0.9}\text{Te}_2\text{S}$	0.2 eV	moderately insulating	$\rho_{xx}$ up to 0.1 $\Omega\text{cm}$	210
3D (1;000)	$\text{Sb}_2\text{Te}_2\text{Se}$	?	metallic	heavily p-type	102
3D (1;000)	$\text{Bi}_2(\text{Te,Se})_2(\text{Se,S})$	0.3 eV	semi-metallic	natural Kawazulite	211
3D (1;000)	$\text{TlBiSe}_2$	~0.35 eV	metallic	simple S.S., large gap	110-112
3D (1;000)	$\text{TlBiTe}_2$	~0.2 eV	metallic	distorted S.S.	112
3D (1;000)	$\text{TlBi(S,Se)}_2$	<0.35 eV	metallic	topological P.T.	116, 117
3D (1;000)	$\text{PbBi}_2\text{Te}_4$	~0.2 eV	metallic	S.S. nearly parabolic	121, 124
3D (1;000)	$\text{PbSb}_2\text{Te}_4$	?	metallic	p-type	121
3D (1;000)	$\text{GeBi}_2\text{Te}_4$	0.18 eV	metallic	n-type	102, 119, 120
3D (1;000)	$\text{PbBi}_4\text{Te}_7$	0.2 eV	metallic	heavily n-type	125
3D (1;000)	$\text{GeBi}_{4-x}\text{Sb}_x\text{Te}_7$	0.1-0.2 eV	metallic	n (p) type at $x = 0$ (1)	126
3D (1;000)	$(\text{PbSe})_5(\text{Bi}_2\text{Se}_3)_6$	0.5 eV	metallic	natural heterostructure	130
3D (1;000)	$(\text{Bi}_2)(\text{Bi}_2\text{Se}_2.6\text{S}_{0.4})$	?	metallic	$(\text{Bi}_2)_n(\text{Bi}_2\text{Se}_3)_m$ series	127
3D (1;000)	$(\text{Bi}_2)(\text{Bi}_2\text{Te}_3)_2$	?	?	no data published yet	128
3D TCI	$\text{SnTe}$	0.3 eV (4.2 K)	metallic	Mirror TCI, $n_M = -2$	62
3D TCI	$\text{Pb}_{1-x}\text{Sn}_x\text{Te}$	<0.3 eV	metallic	Mirror TCI, $n_M = -2$	164
3D TCI	$\text{Pb}_{0.77}\text{Sn}_{0.23}\text{Se}$	invert with $T$	metallic	Mirror TCI, $n_M = -2$	162
2D, $\nu = 1$ ?	Bi bilayer	~0.1 eV	?	not stable by itself	82, 83
3D (1;000)?	$\text{Ag}_2\text{Te}$	?	metallic	famous for linear MR	134, 135
3D (1;111)?	$\text{SmB}_6$	20 meV	insulating	possible Kondo TI	140-143
3D (0;001)?	$\text{Bi}_4\text{Rh}_3\text{I}_9$	0.27 eV	metallic	possible weak 3D TI	145
3D (1;000)?	$\text{RBI Pt}$ ( $R = \text{Lu, Dy, Gd}$ )	zero gap	metallic	evidence negative	152
Weyl SM?	$\text{Nd}_2(\text{Ir}_{1-x}\text{Rh}_x)_2\text{O}_7$	zero gap	metallic	too preliminary	158



# Topological materials

## ORIGIN OF BULK BANDGAP:

- **Semiconductor-like**
- **Electron correlations**
- **Superconducting**
- **Magnetic field/magnetization**

- **Topological insulators ( $Z_2$  class – canonical TI)**
- **Topological crystalline insulators**
- **Topological Kondo insulators**
- **Topological superconductors**
- **Quantum Hall effect and Quantum anomalous Hall effect**

• and

- **Topological semimetals (Dirac, Weyl)**

• and

- **Topological photonic, vibronic, atomic and mechanical systems**

## PHYSICAL SYMMETRY:

- **Time reversal symmetry (TRS)**
- **Crystal symmetry**
- **Particle-antiparticle symmetry**

# II. Topological crystalline insulators - TCI

## IV-VI semiconductor family

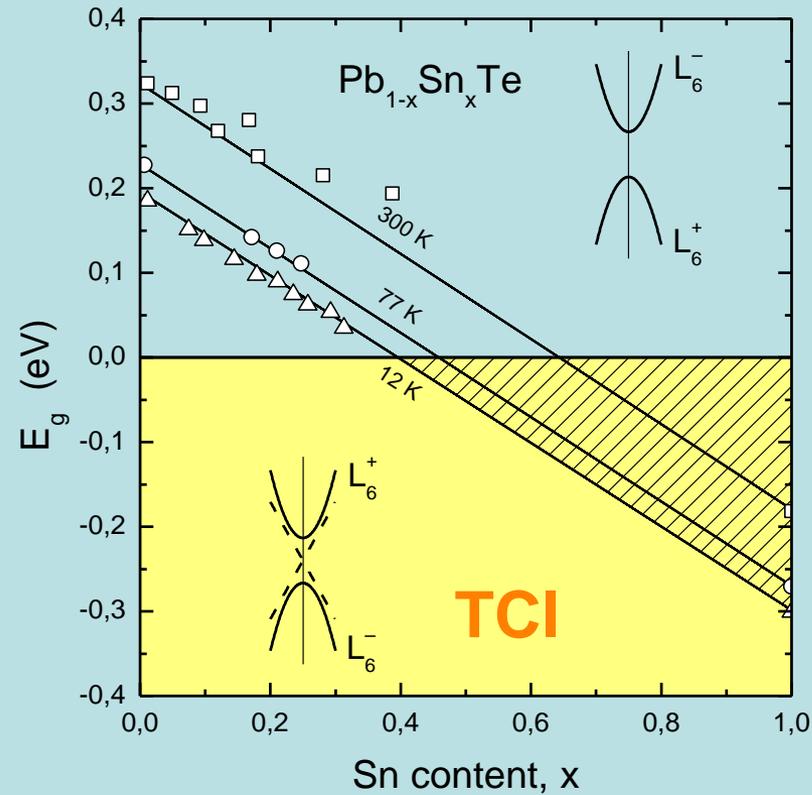
						2 <b>He</b> Helium 4.003
	5 <b>B</b> Boron 10.811	6 <b>C</b> Carbon 12.0107	7 <b>N</b> Nitrogen 14.00674	8 <b>O</b> Oxygen 15.9994	9 <b>F</b> Fluorine 18.9984032	10 <b>Ne</b> Neon 20.1797
	13 <b>Al</b> Aluminum 26.981538	14 <b>Si</b> Silicon 28.0855	15 <b>P</b> Phosphorus 30.973761	16 <b>S</b> Sulfur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

- Binary compounds:
- PbTe, PbSe, PbS, SnTe, GeTe
- Substitutional solid solutions:
- $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ ,  $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$
- Diluted magnetic semiconductors:
- $\text{Sn}_{1-x}\text{Mn}_x\text{Te}$ ,  $\text{Ge}_{1-x}\text{Mn}_x\text{Te}$

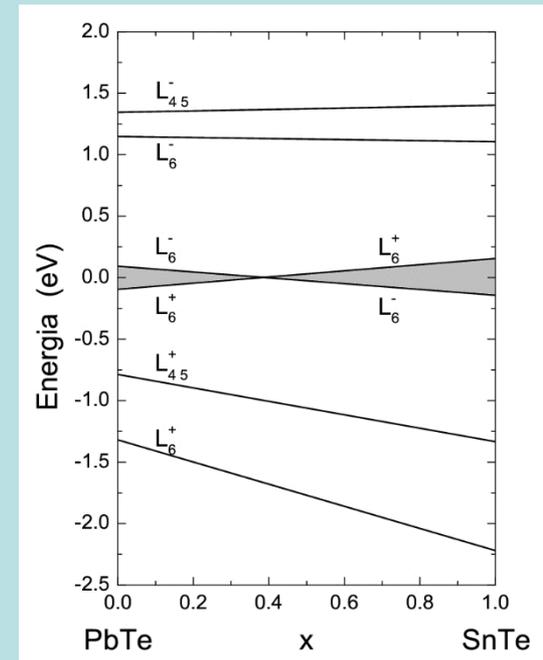
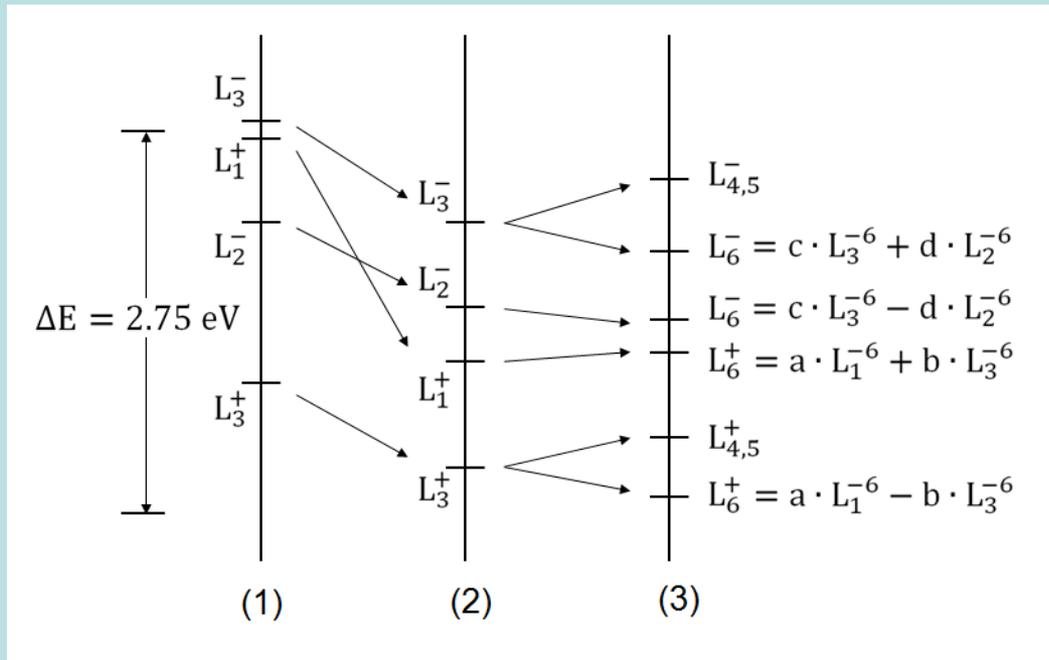


# $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ substitutional solid solutions

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



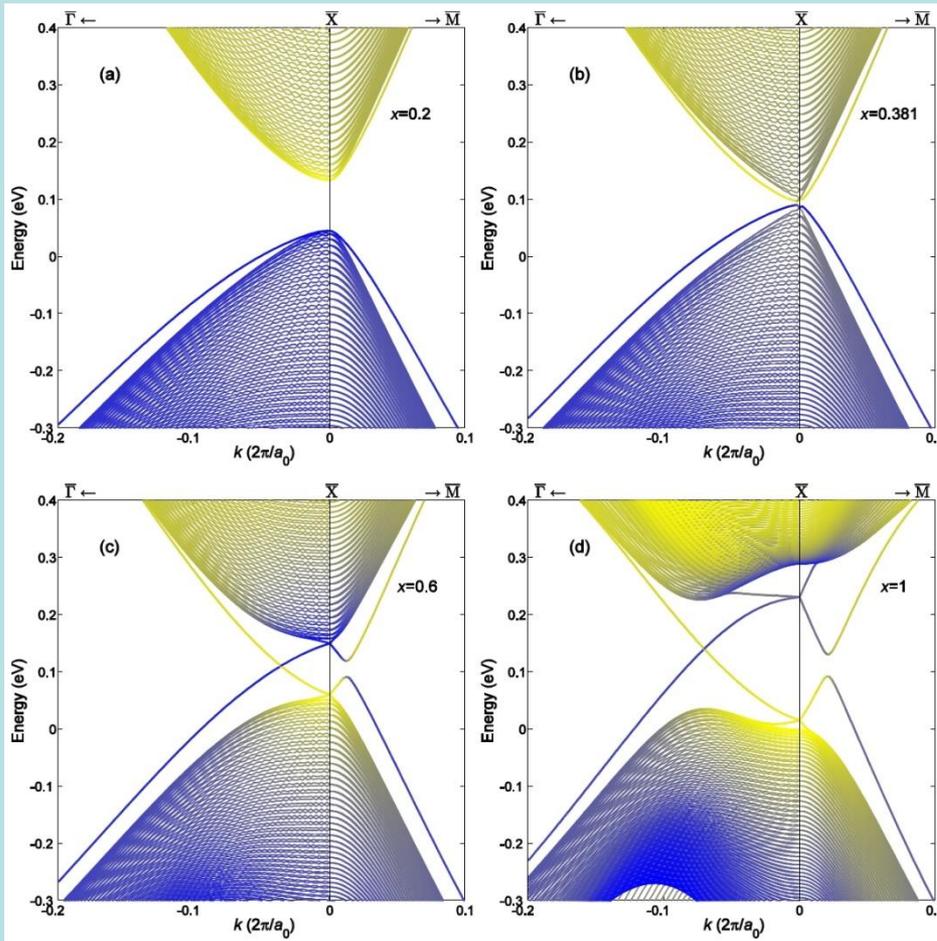
# Electron band structure of IV-VI semiconductors



## Relativistic interactions in $\text{PbTe}$ and $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$

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

# Band structure of $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ : tight binding calculations



- $\text{PbSnTe}$  in band inversion region:
- A) band insulator
- B) zero bulk band gap
- C) inverted gap - TCI
- D) SnTe – TCI

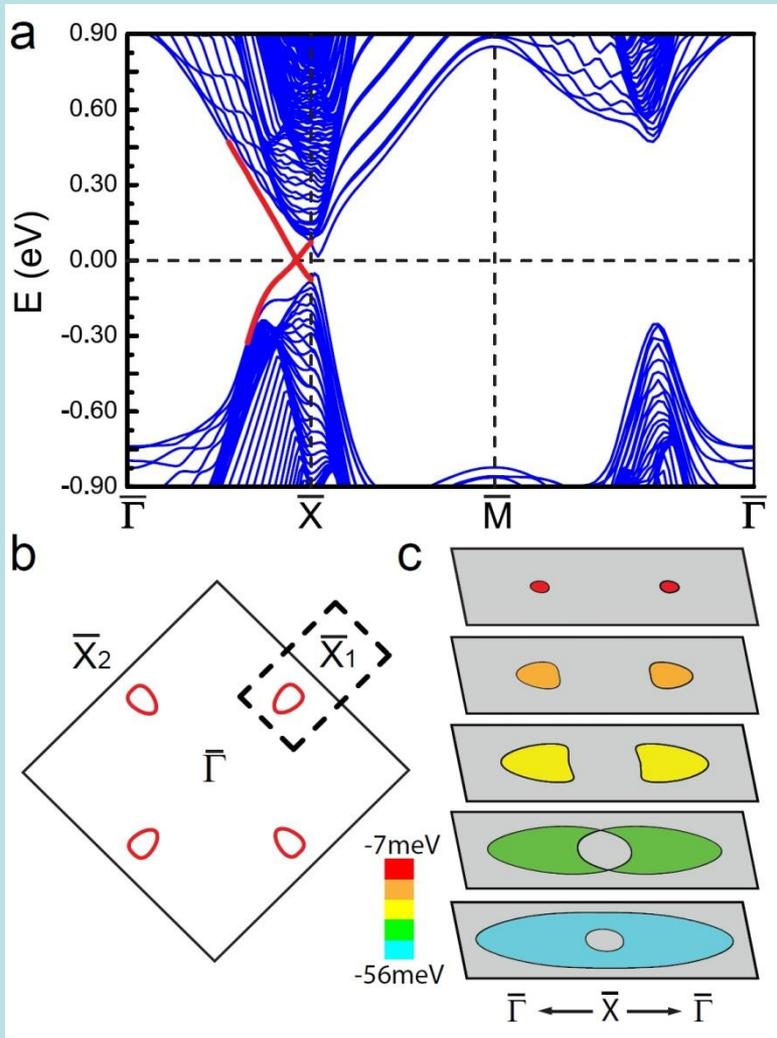
Yellow – p-type cation orbitals  
Blue – p-type anion orbitals

# Topological crystalline insulators

## SnTe - theoretical analysis

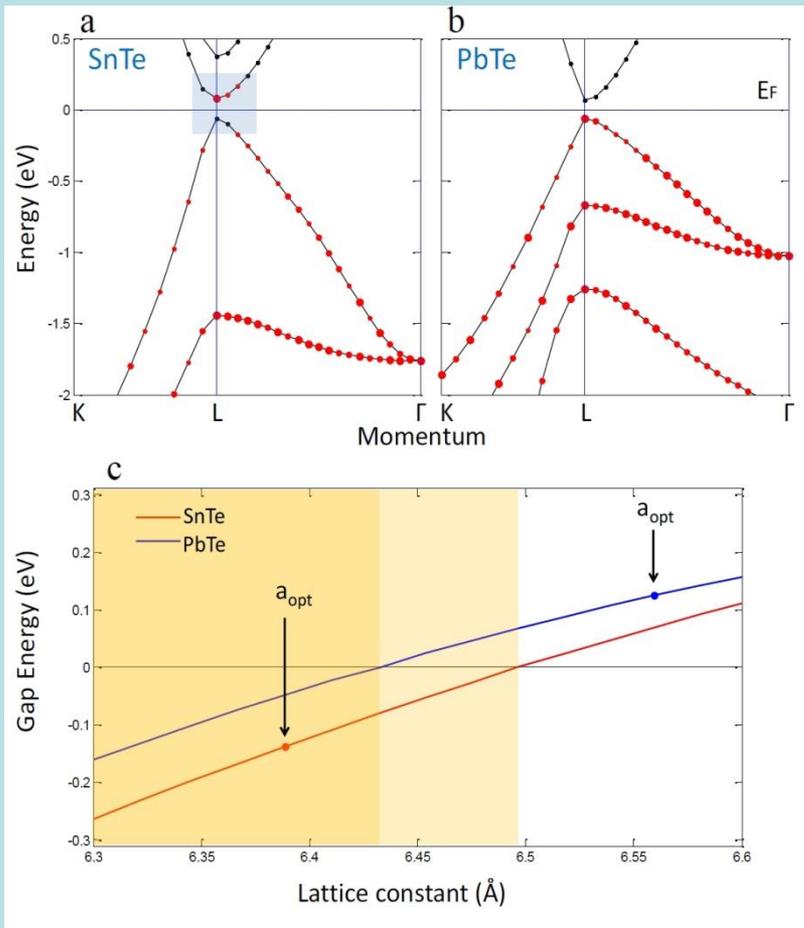
SnTe - TCI states with 4 Dirac cones nearby X-points of the surface Brillouin zone

Lifshitz transition -  
Topological changes of Fermi surface



T.H. Hsieh, H. Lin, J. Liu, W. Duan, A. Bansil, L. Fu,  
Nature Commun. **3**, 982 (2012).

# Topological crystalline insulators: SnTe vs PbTe – theoretical analysis

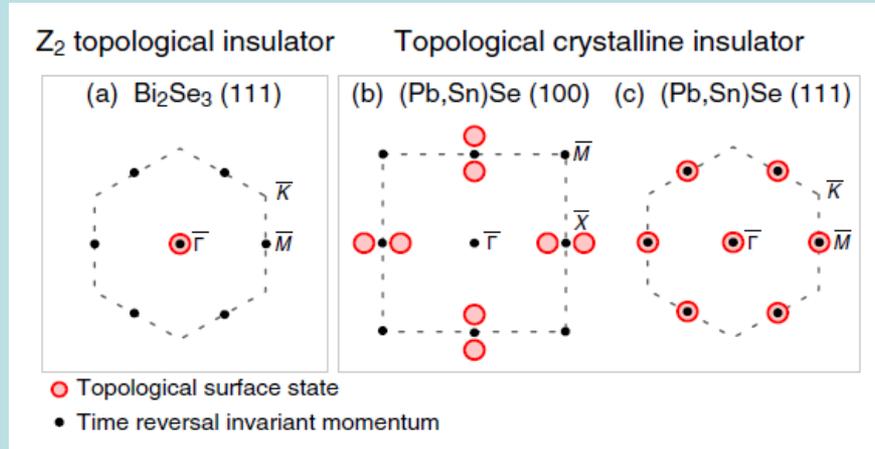


PbTe – trivial band insulator  
 $E_G > 0$

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

T.H. Hsieh, H. Lin, J. Liu, W. Duan, A. Bansil,  
L. Fu, *Nature Commun.* **3**, 982 (2012).

# Topological insulators (TI) vs Topological crystalline insulators (TCI)



**Metallic surface (or edge) states with linear energy dispersion (Dirac-like).  
 Inverted band ordering resulting from relativistic (spin-orbital) effects.  
 Topological protection.  
 Helical spin polarization.**

**Topological protection mechanism (symmetry):**

**Time reversal symmetry (in TI) - mirror-plane crystal symmetry (in TCI)**

**Dirac cones location – odd number at TRIM points of BZ (TI) – even (in TCI)**

**Topological invariant: Chern number, Z<sub>2</sub> (in TI) – mirror Chern number (in TCI)**

## **IV-VI topological materials**

**Crystal growth: A. Szczerbakow**

**Structural and chemical characterization:**

**J. Domagała, W. Domuchowski, E. Łusakowska, R. Minikayev,  
A. Reszka**

**Magneto-transport and magnetic studies – K. Dybko, W. Knoff,  
M. Szot**

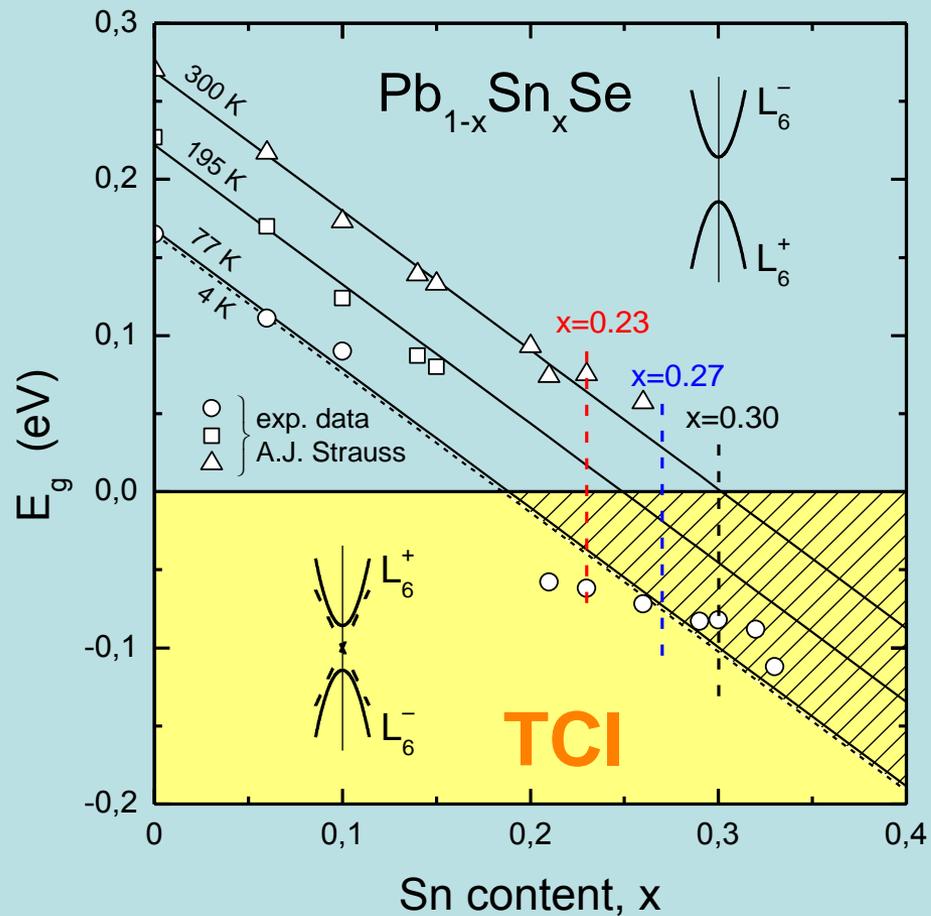
**Band structure calculations – R. Buczko, M. Galicka, P. Kacman,  
S. Safaei**

**Photoemission measurements at Lund University (synchrotron  
facility) and KTH Stockholm (laser facility):**

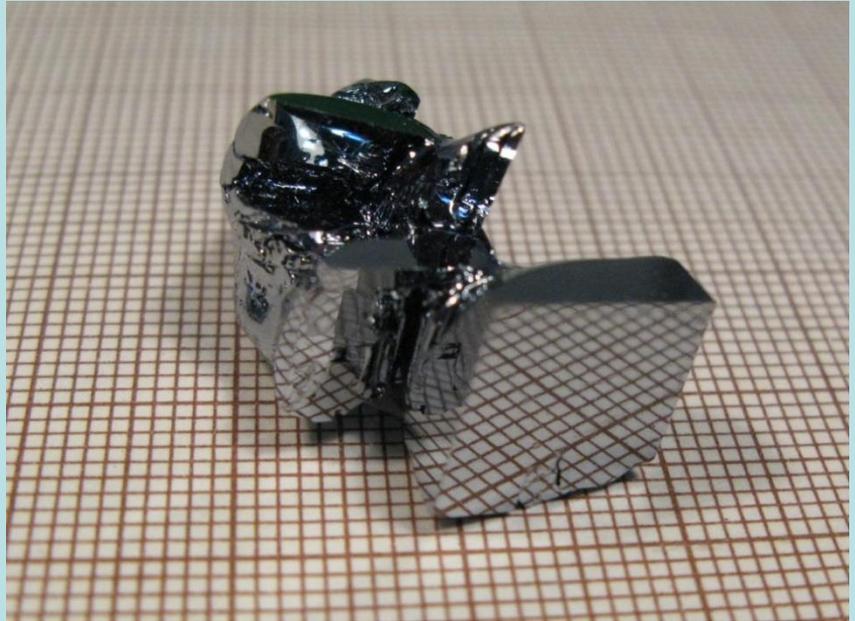
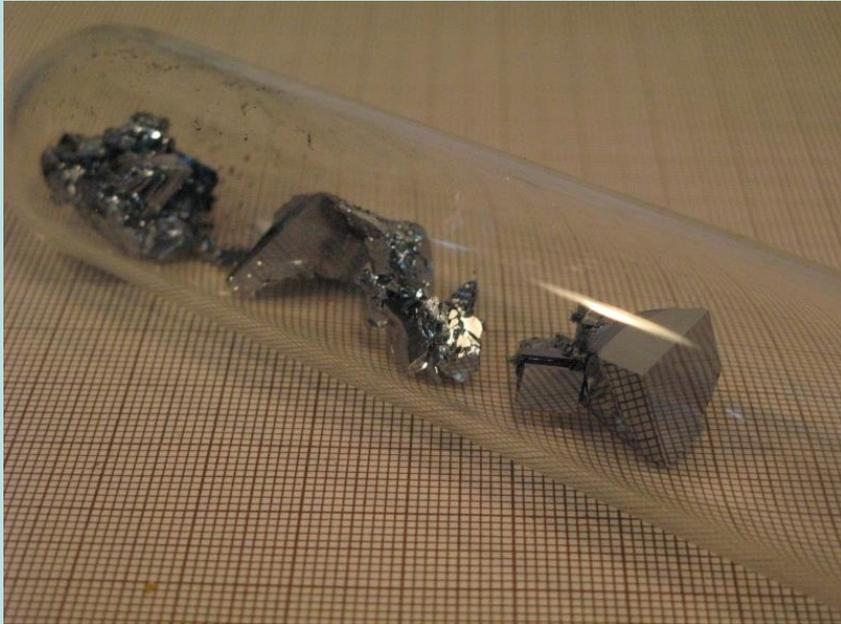
**P. Dziawa, B.J. Kowalski (IP PAS), T. Balasubramanian, C.M. Polley  
(Lund), M.H. Berntsen, O. Tjernberg, B.M. Wojek (KTH)**

**TS**

# $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ substitutional solid solutions



# $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ monocrystals grown by self-selecting vapor growth



**Natural (001) crystal facets – cleavage planes**  
**Stoichiometry control of n – and p-type conductivity**  
**Highly homogeneous chemical composition of solid solutions**

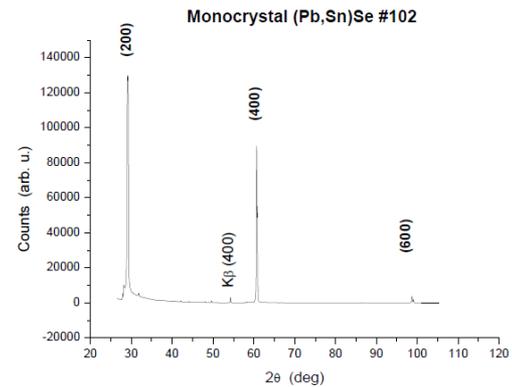
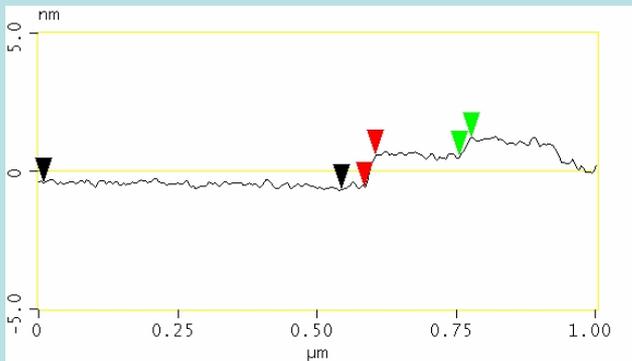
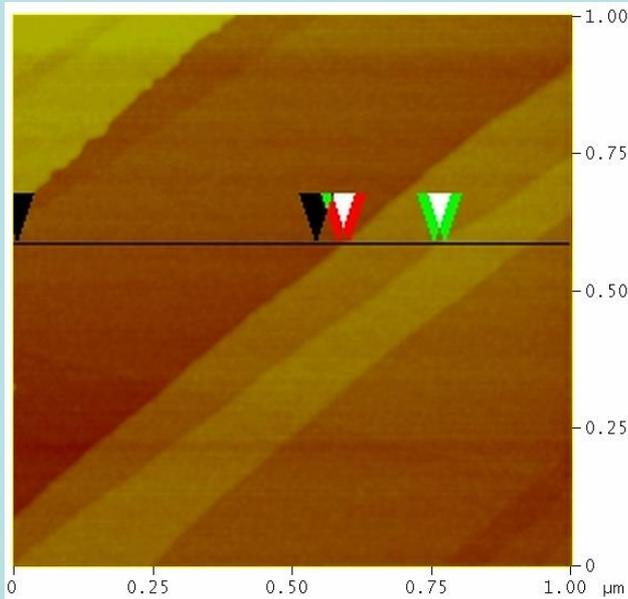
**A. Szczerbakow - IF PAN: J. Cryst. Growth 139, 172 (1994);**

# Structural and chemical characterization

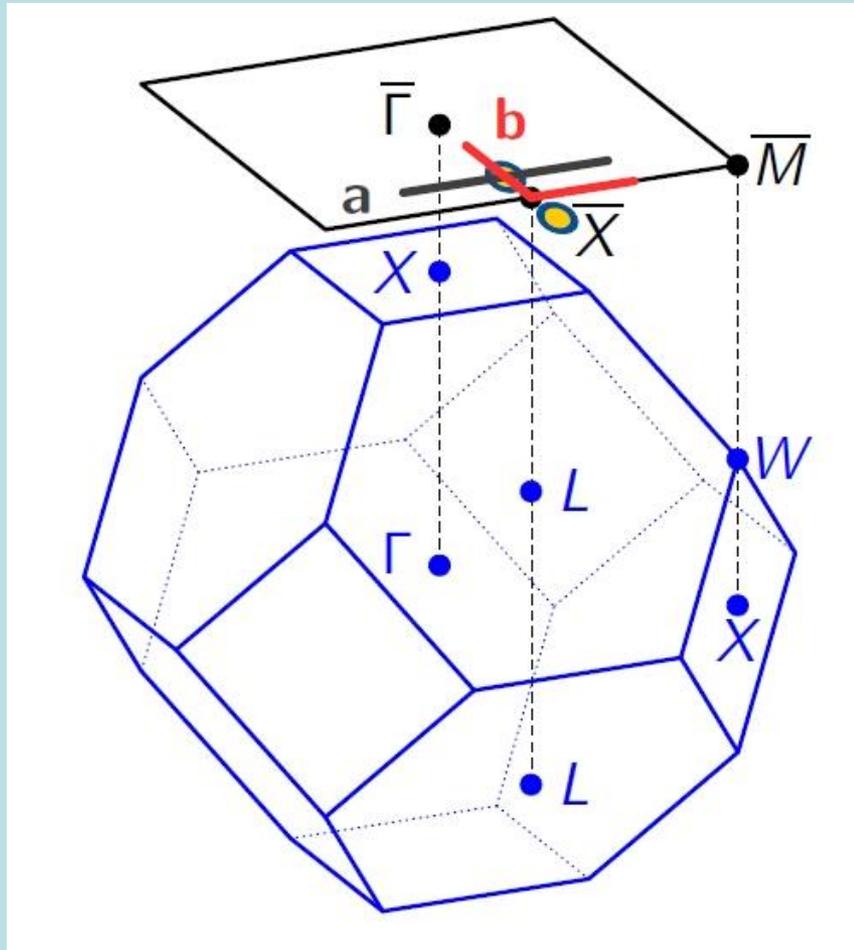
X-ray diffraction (XRD)

EDX chemical analysis

Surface morphology analysis  
by AFM microscopy

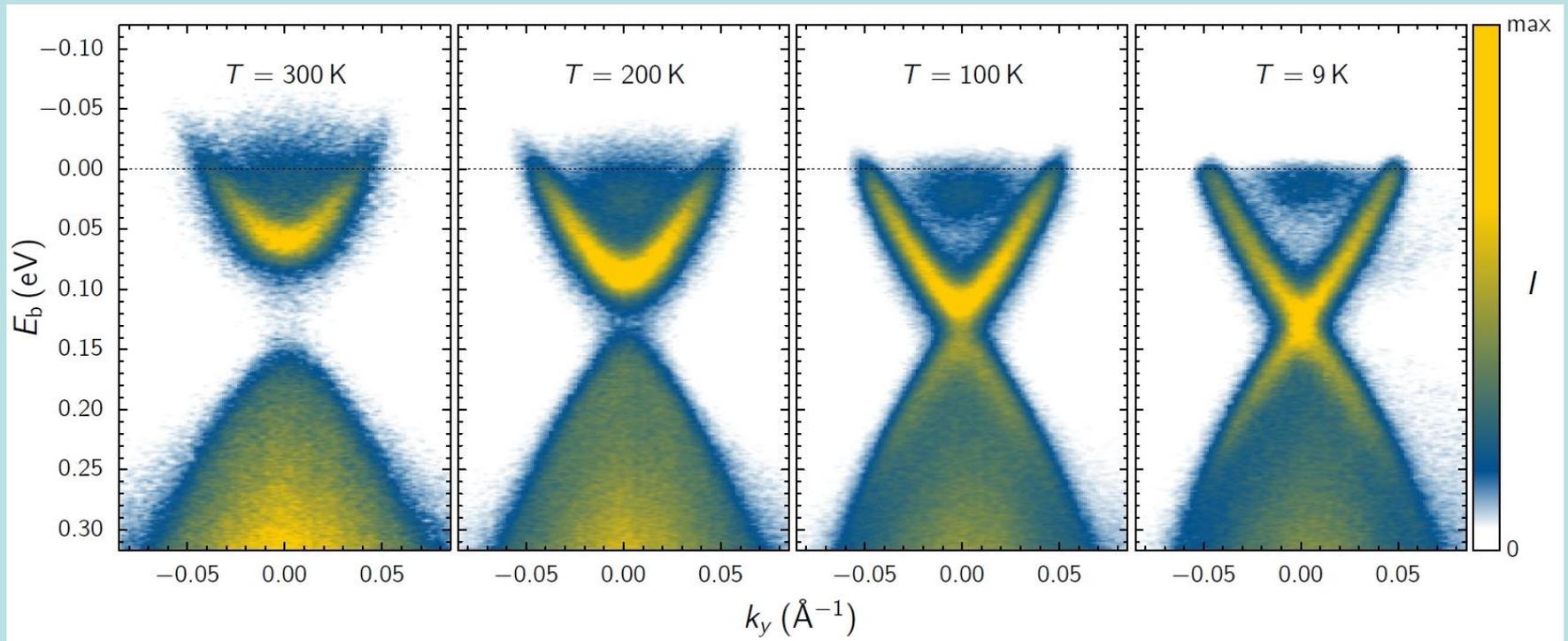


# Brillouin zone for (001) surface



# Electron band structure of $\text{Pb}_{0.77}\text{Sn}_{0.23}\text{Se}$

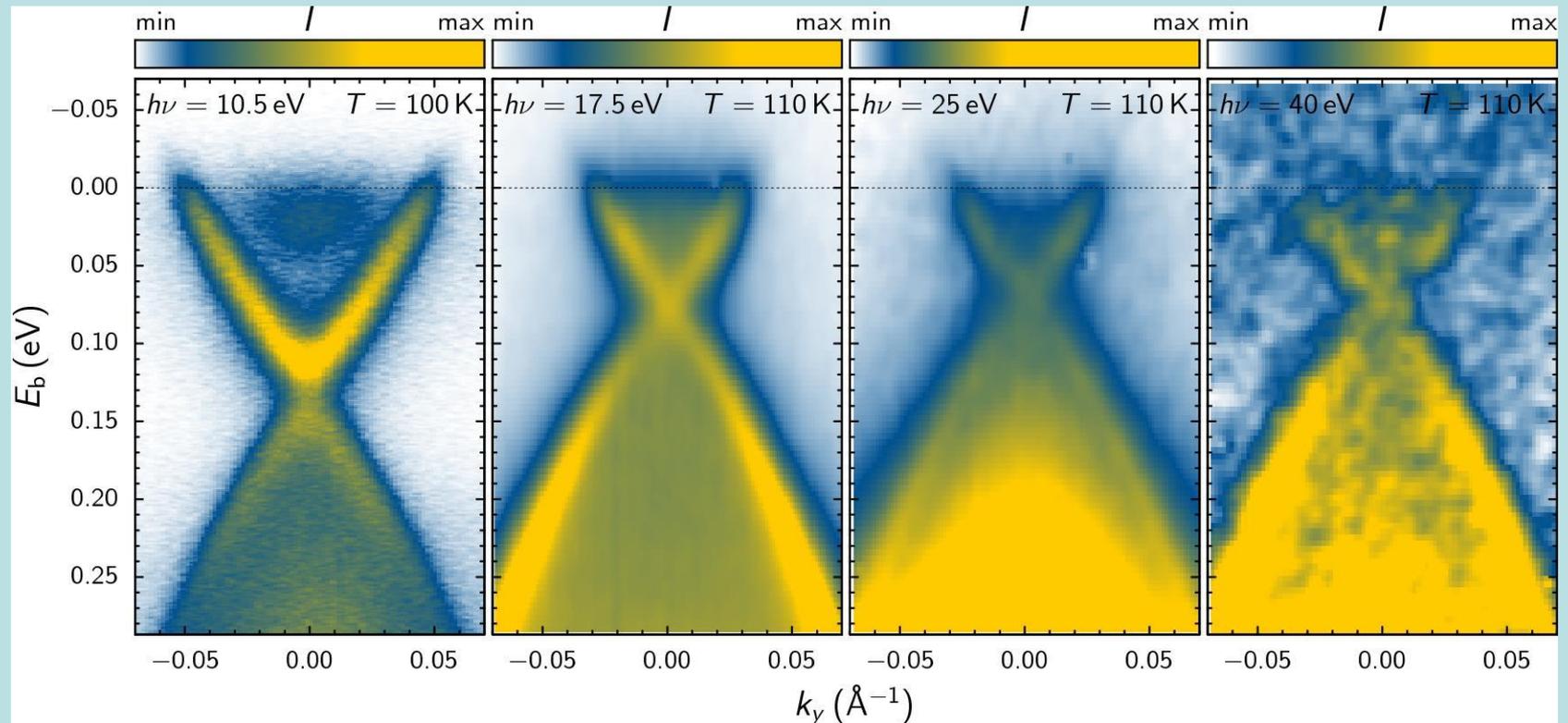
## ARPES experimental studies



- **Energy dispersion relation for temperature varying across band inversion point**
- P. Dziawa, B.J. Kowalski, K. Dybko, R. Buczko, A. Szczerbakow, et al. *Nature Materials* **11**, 1023 (2012)

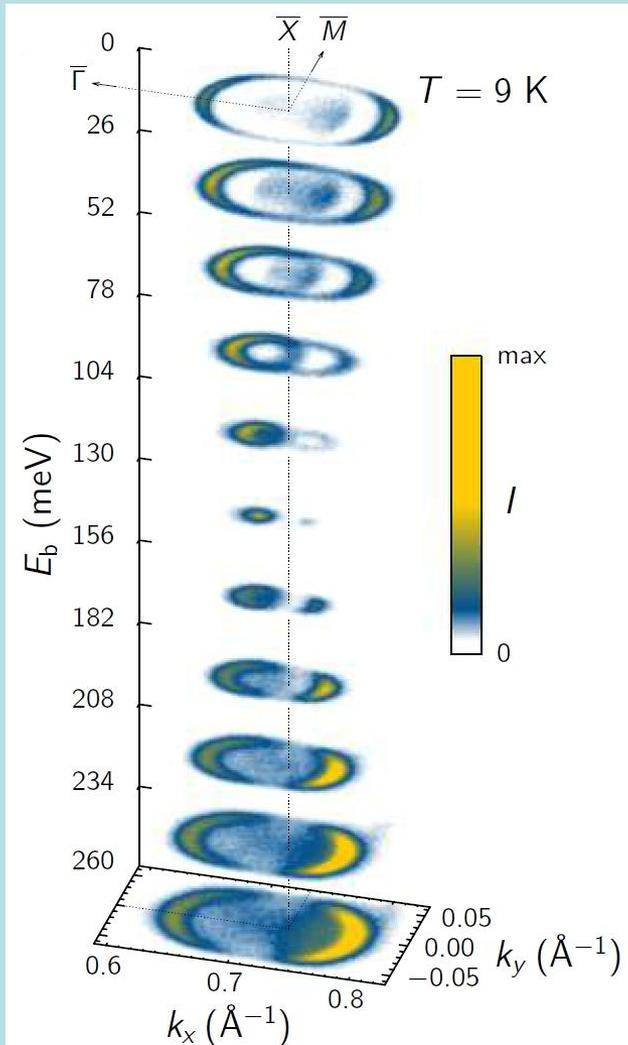
# Electron band structure of $\text{Pb}_{0.77}\text{Sn}_{0.23}\text{Se}$

## ARPES experimental studies



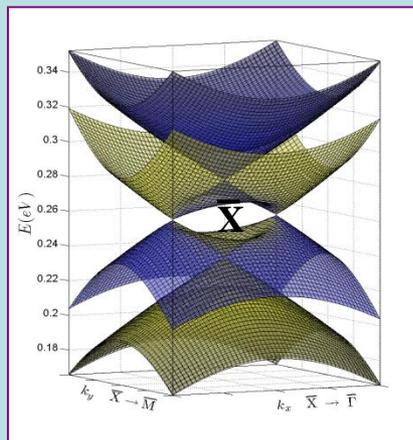
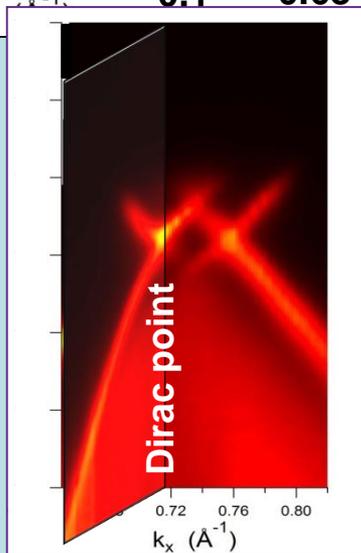
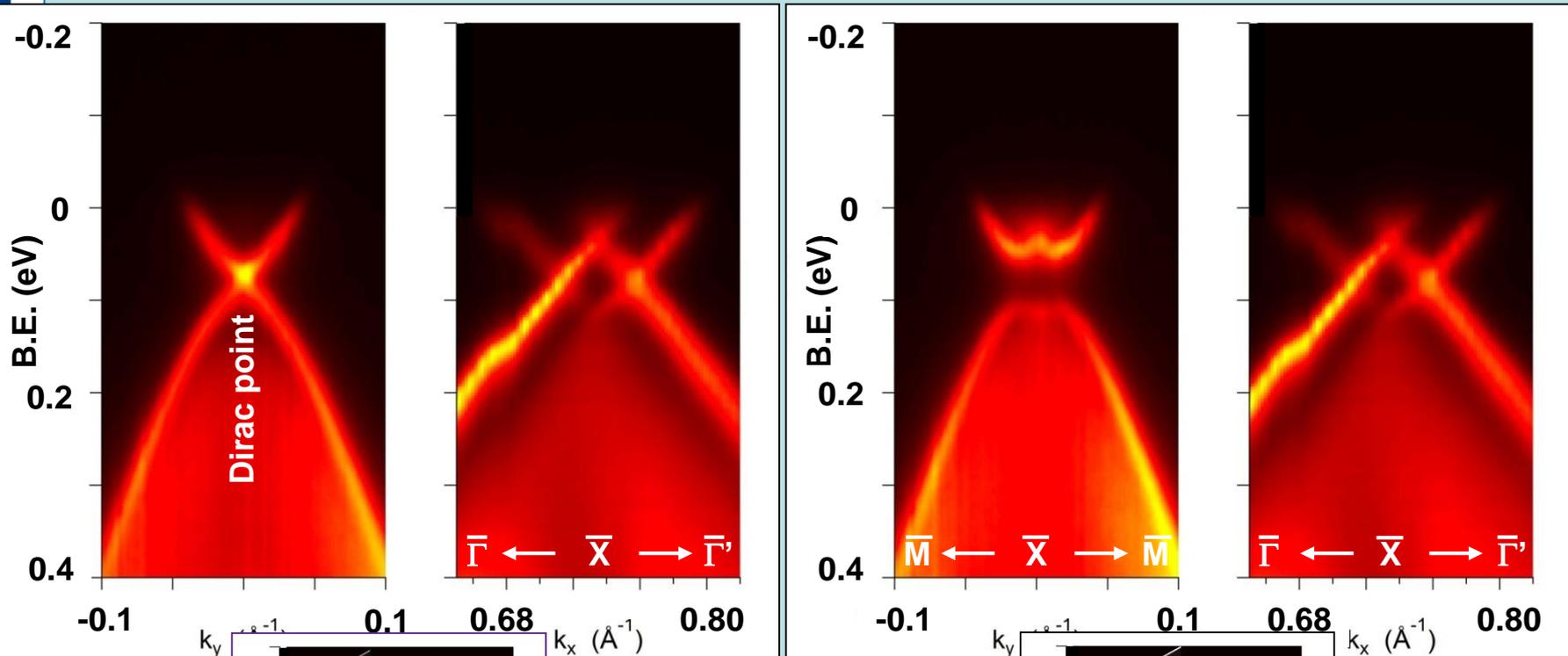
Energy dispersion  $E(k_y)$  for varying photon energy

# Electronic structure - ARPES

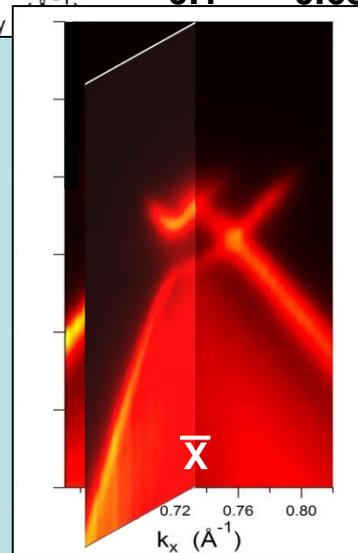


- Fermi surface  $E(k_x, k_y)$  for various binding energies  $E_b$

# Pb<sub>0.67</sub>Sn<sub>0.33</sub>Se, T=87 K, hν=18.5 eV



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



# Trivial insulator (PbSe) vs topological crystalline insulator (Pb<sub>1-x</sub>Sn<sub>x</sub>Se)

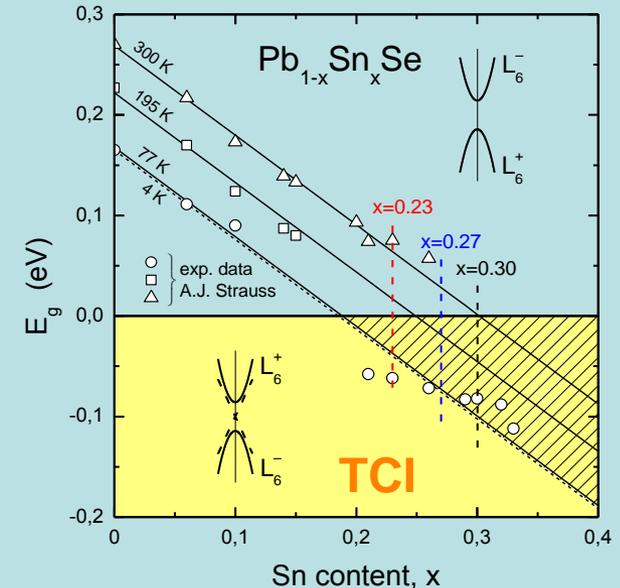
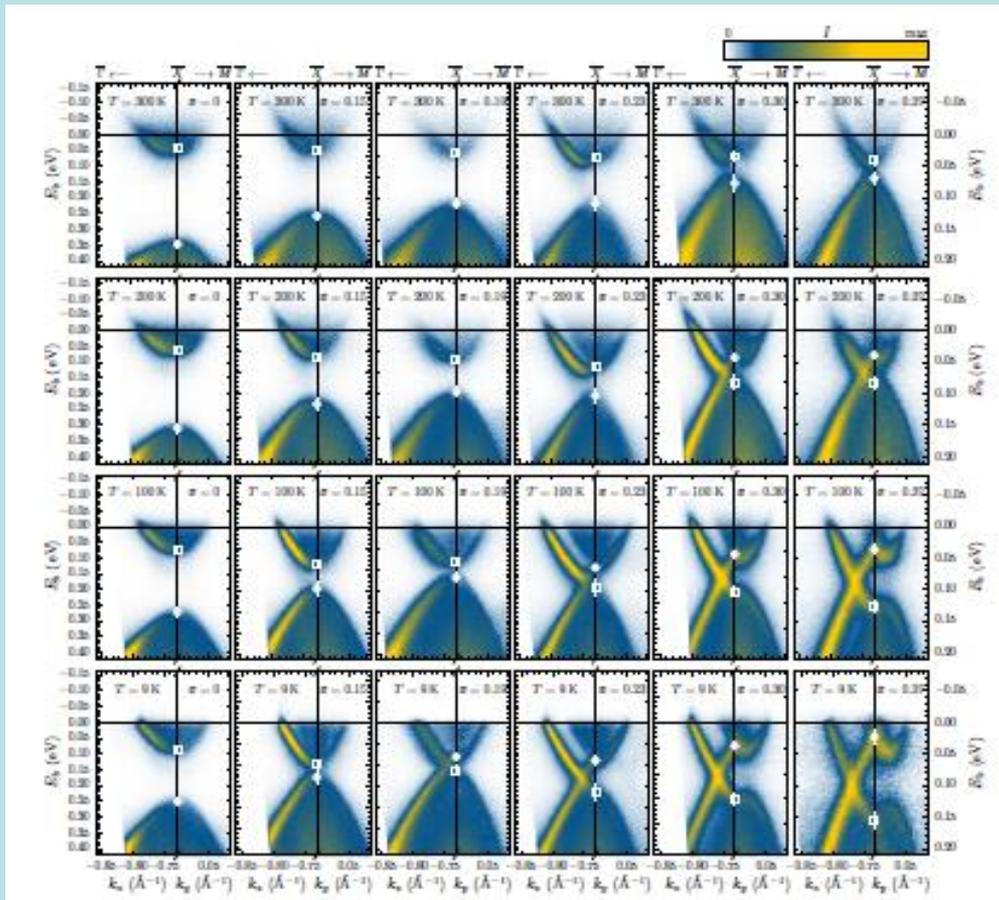
**x=0, 0.15, 0.19, 0.23, 0.30, 0.37**

T=300 K

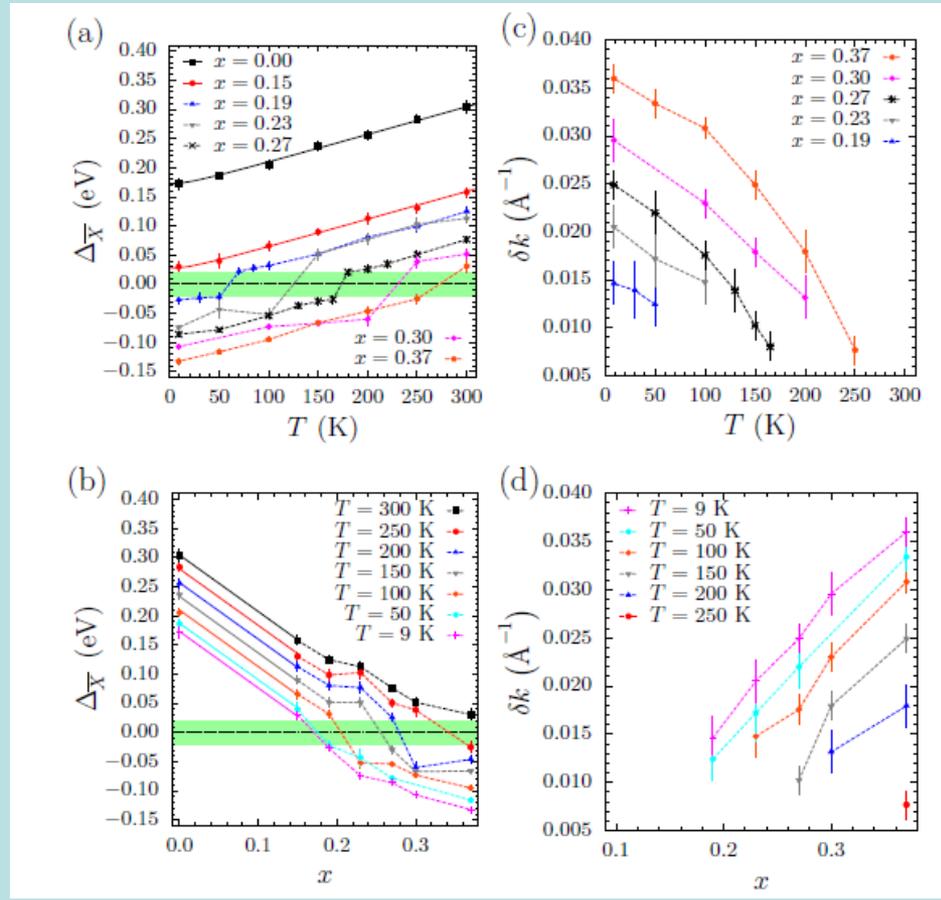
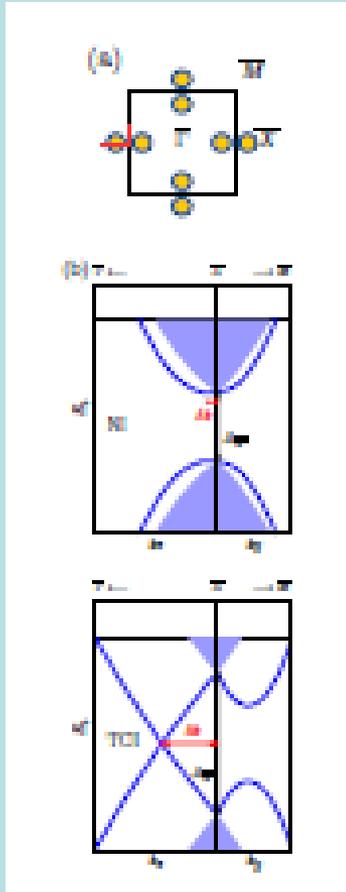
T= 200 K

T=100 K

T=9 K

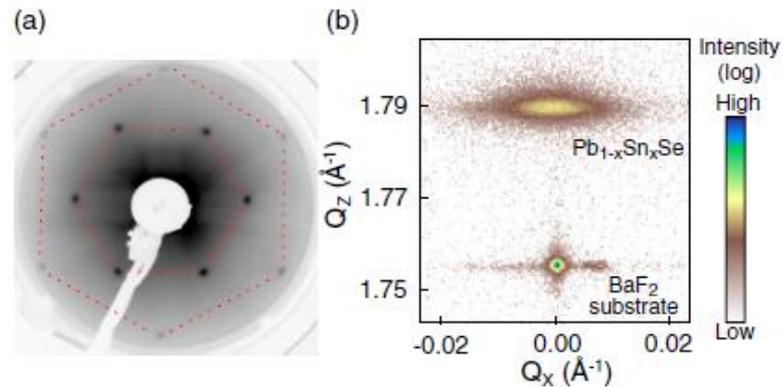
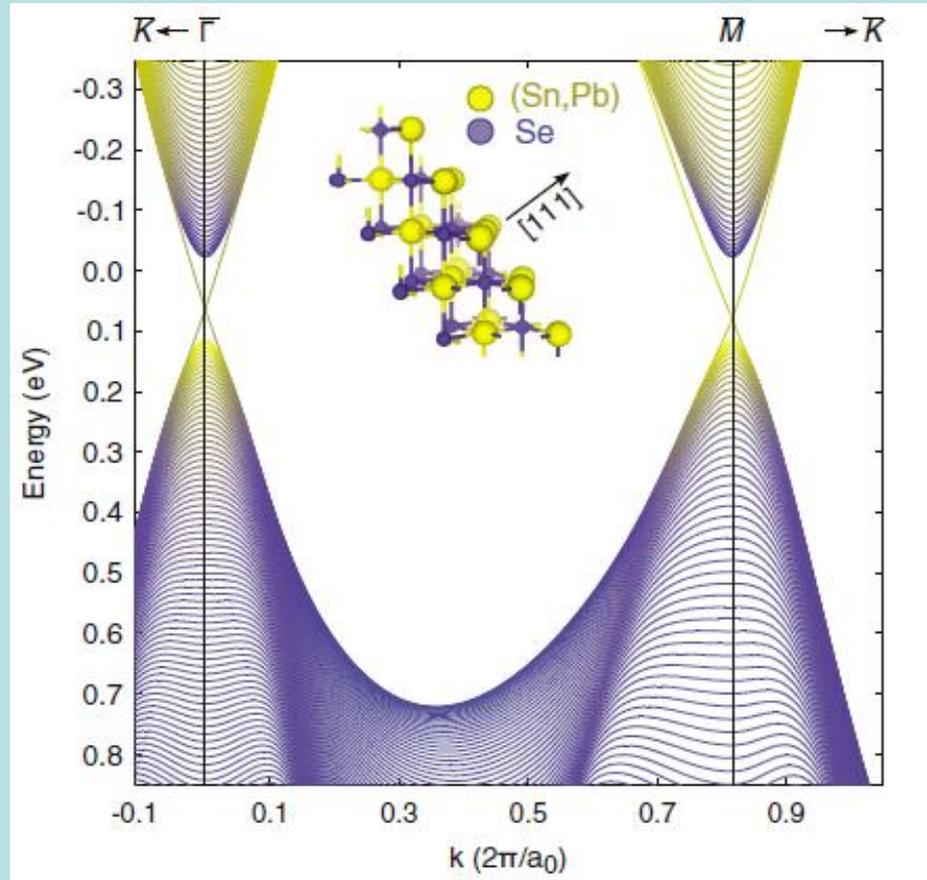
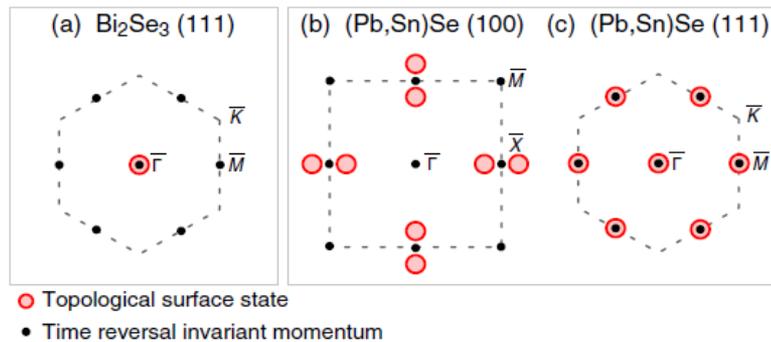


# Pb<sub>1-x</sub>Sn<sub>x</sub>Se: Topological T-x phase diagram

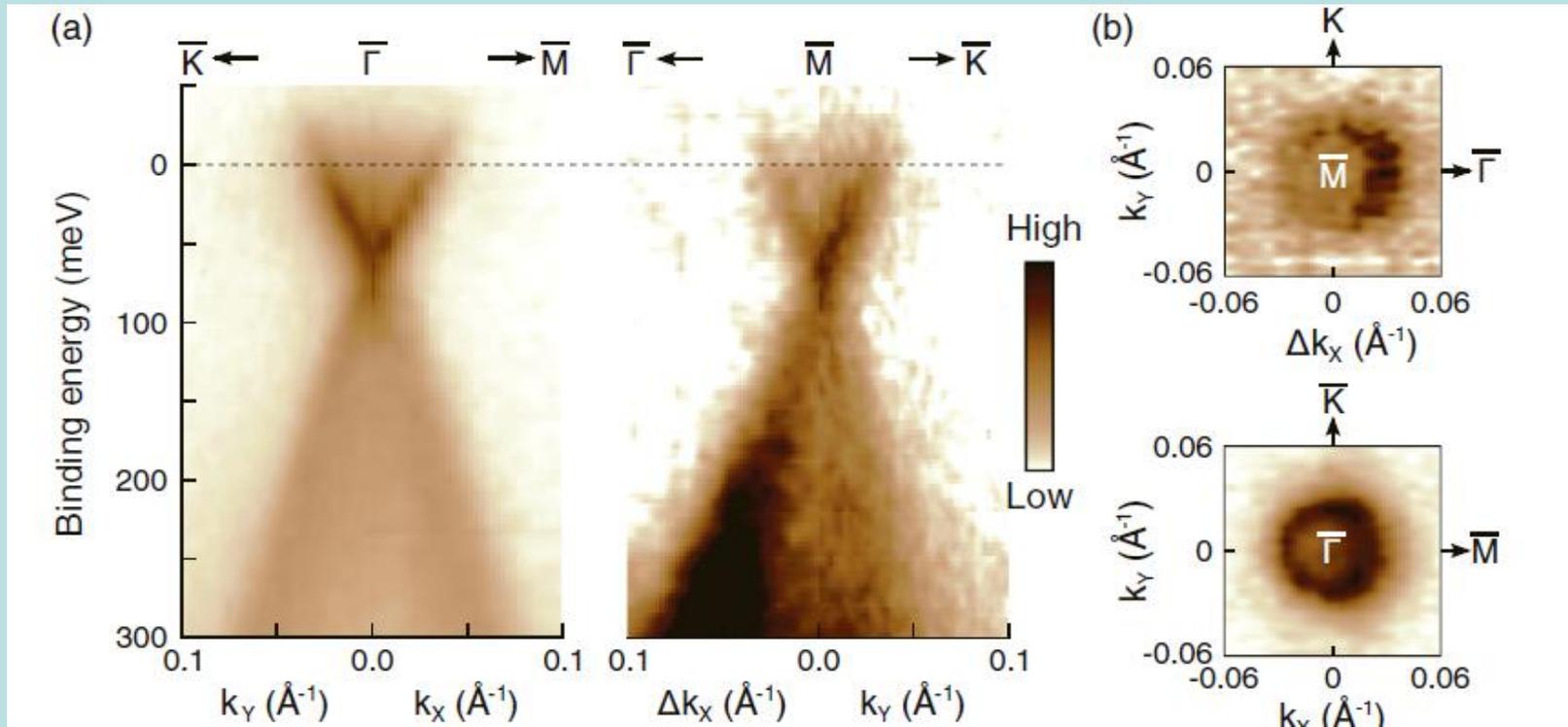


# Pb<sub>1-x</sub>Sn<sub>x</sub>Se/BaF<sub>2</sub> (111) – thin layers

Z<sub>2</sub> topological insulator      Topological crystalline insulator



# $\text{Pb}_{1-x}\text{Sn}_x\text{Se}/\text{BaF}_2$ (111) layers

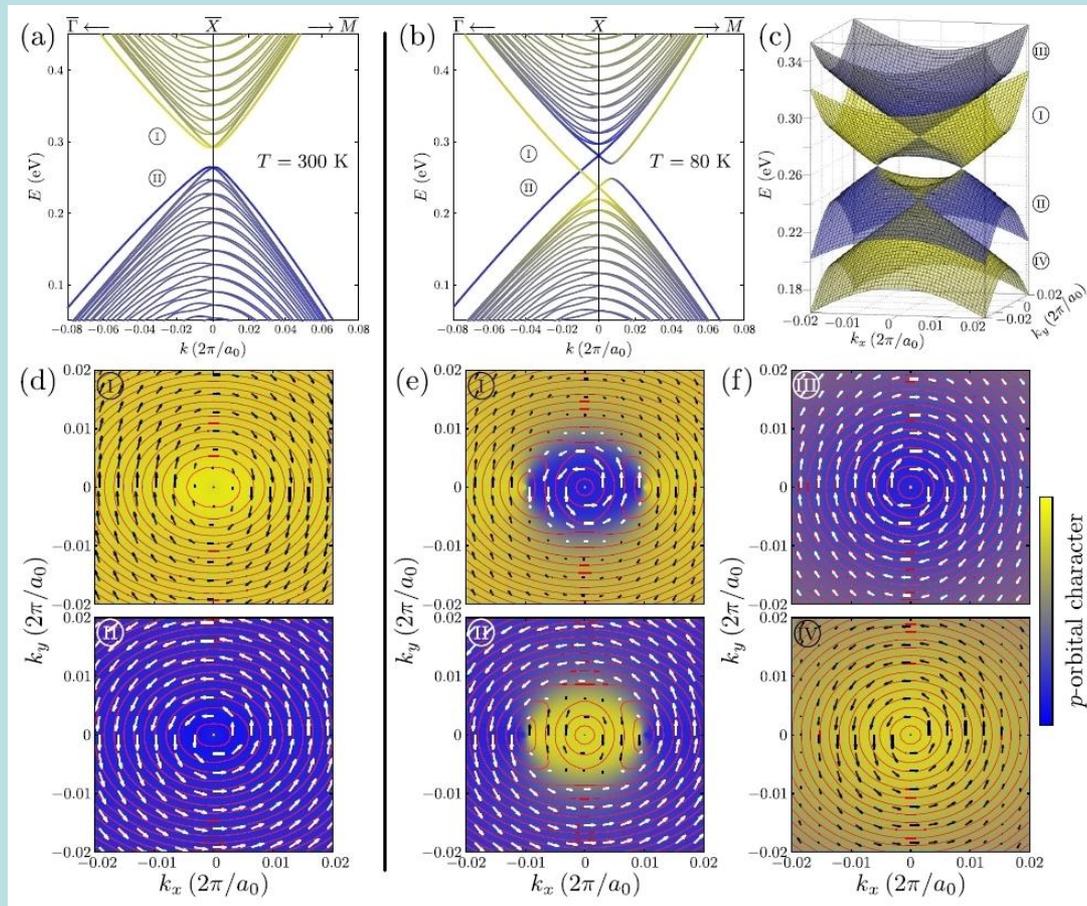


PHYSICAL REVIEW B 89, 075317 (2014)

## Observation of topological crystalline insulator surface states on (111)-oriented $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ films

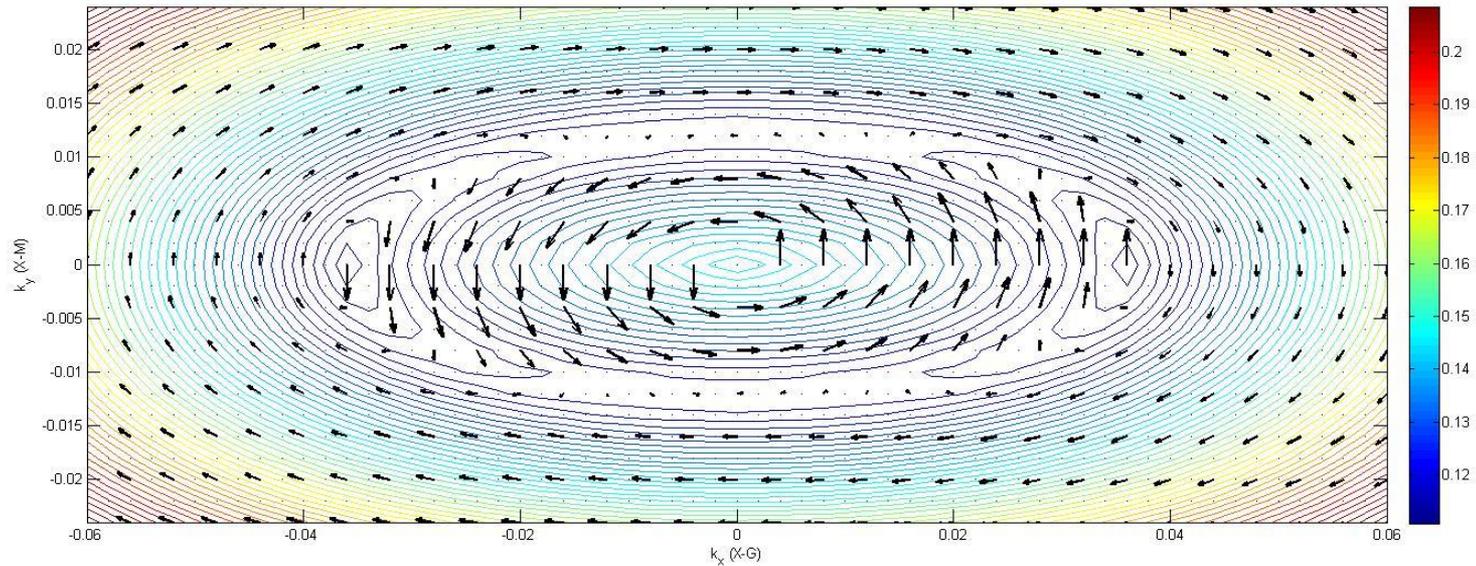
C. M. Polley,<sup>1,\*</sup> P. Dziawa,<sup>2</sup> A. Reszka,<sup>2</sup> A. Szczerbakow,<sup>2</sup> R. Minikayev,<sup>2</sup> J. Z. Domagala,<sup>2</sup> S. Safaei,<sup>2</sup> P. Kacman,<sup>2</sup> R. Buczko,<sup>2</sup> J. Adell,<sup>1</sup> M. H. Berntsen,<sup>3,†</sup> B. M. Wojek,<sup>3</sup> O. Tjernberg,<sup>3</sup> B. J. Kowalski,<sup>2</sup> T. Story,<sup>2</sup> and T. Balasubramanian<sup>1</sup>

# Spin polarization of TCI states: tight binding model – $\text{Pb}_{0.76}\text{Sn}_{0.24}\text{Se}$



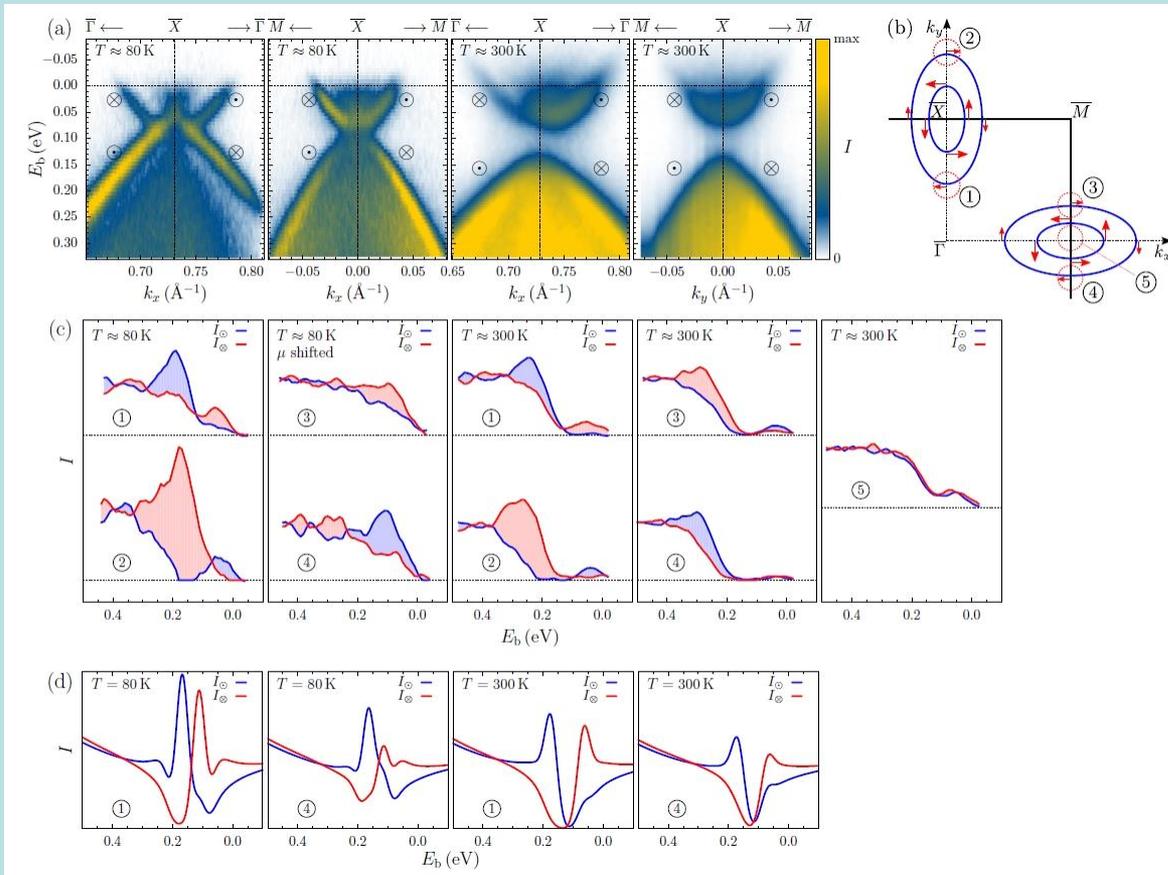
B.M. Wojek, R. Buczko et al. Phys. Rev. B 87, 115105 (2013)

# Spin polarization of TCI states in SnTe

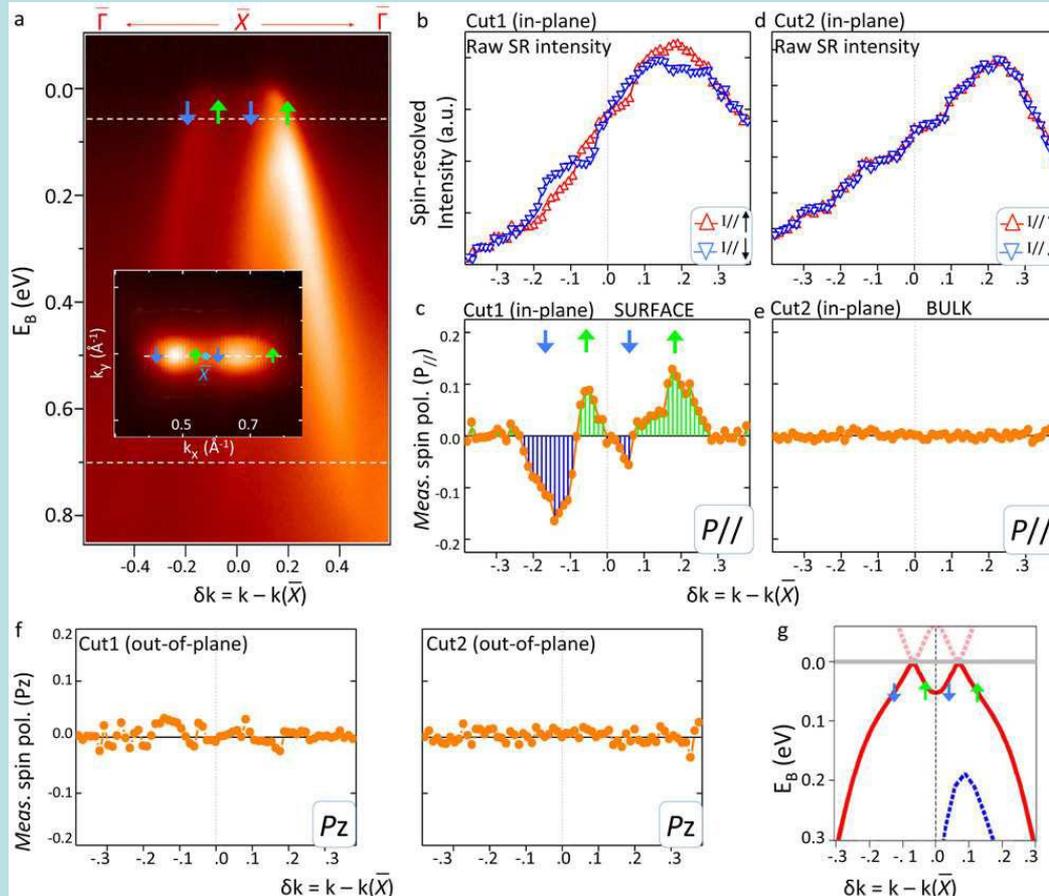


S. Safaei, P. Kacman, R. Buczko, Phys. Rev. B 88, 045305 (2013)  
tight binding calculations

# Spin polarization of TCI states: SRPES experiment – $\text{Pb}_{0.76}\text{Sn}_{0.24}\text{Se}$

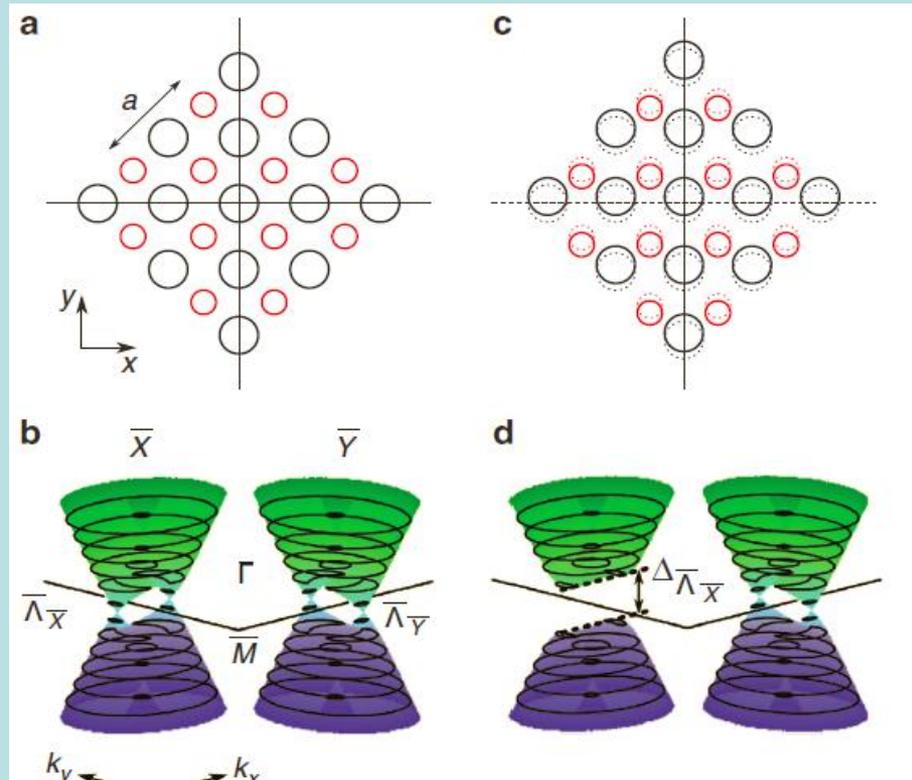


# Spin polarization in TCI: SRPES – $\text{Pb}_{0.6}\text{Sn}_{0.4}\text{Te}$



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

# Topological surface states in distorted PbSnSe crystal lattice



ARTICLE

Received 13 May 2015 | Accepted 23 Aug 2015 | Published 13 Oct 2015

DOI: 10.1038/ncomms9463

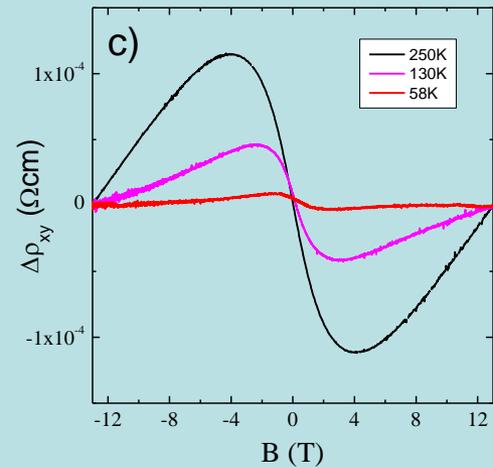
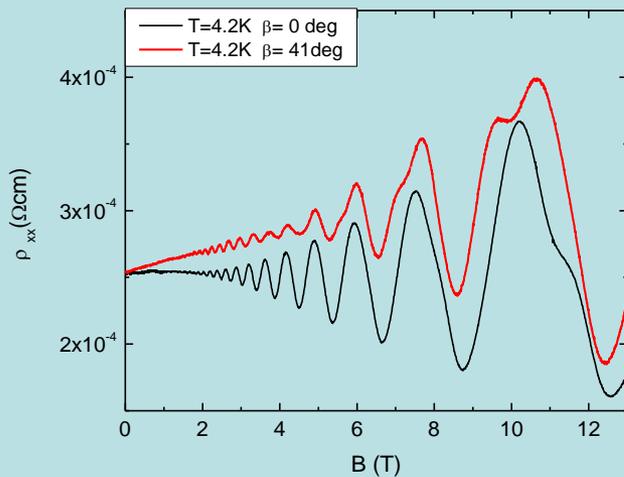
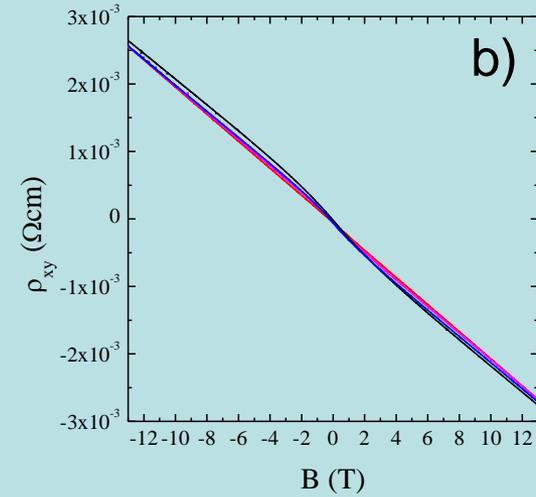
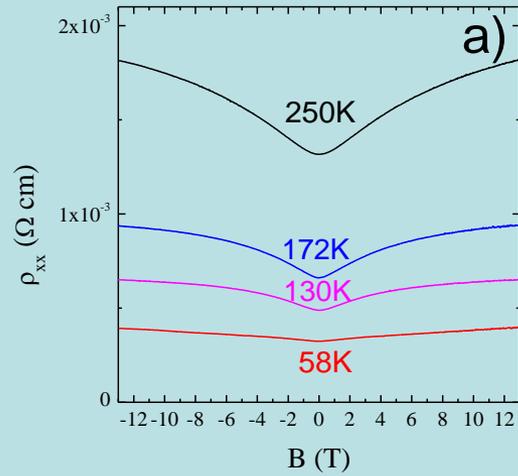
OPEN

Direct observation and temperature control of the surface Dirac gap in a topological crystalline insulator

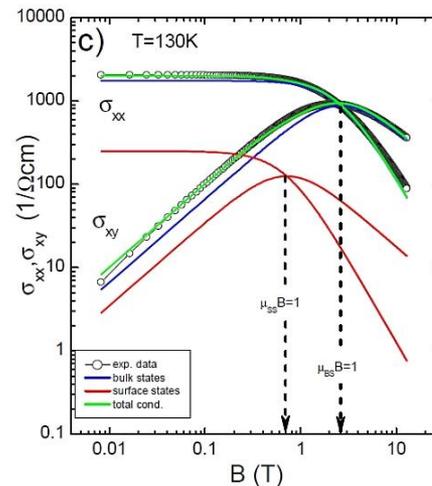
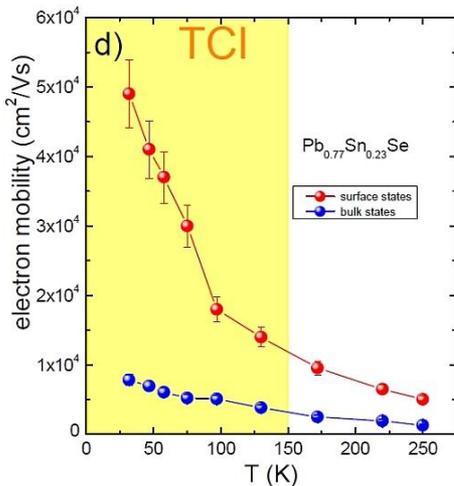
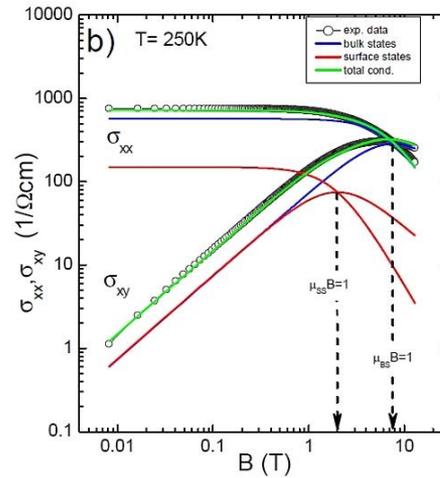
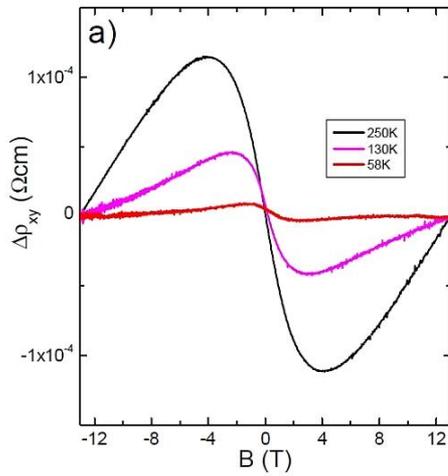
B.M. Wojek<sup>1</sup>, M.H. Berntsen<sup>1</sup>, V. Jonsson<sup>1,2</sup>, A. Szczerbakow<sup>3</sup>, P. Dziawa<sup>3</sup>, B.J. Kowalski<sup>3</sup>, T. Story<sup>3</sup> & O. Tjernberg<sup>1,2</sup>



# $\text{Pb}_{0.77}\text{Sn}_{0.23}\text{Se}$ : magneto-transport



# Pb<sub>0.77</sub>Sn<sub>0.23</sub>Se: magneto-transport



Drude model for magneto-conductivity

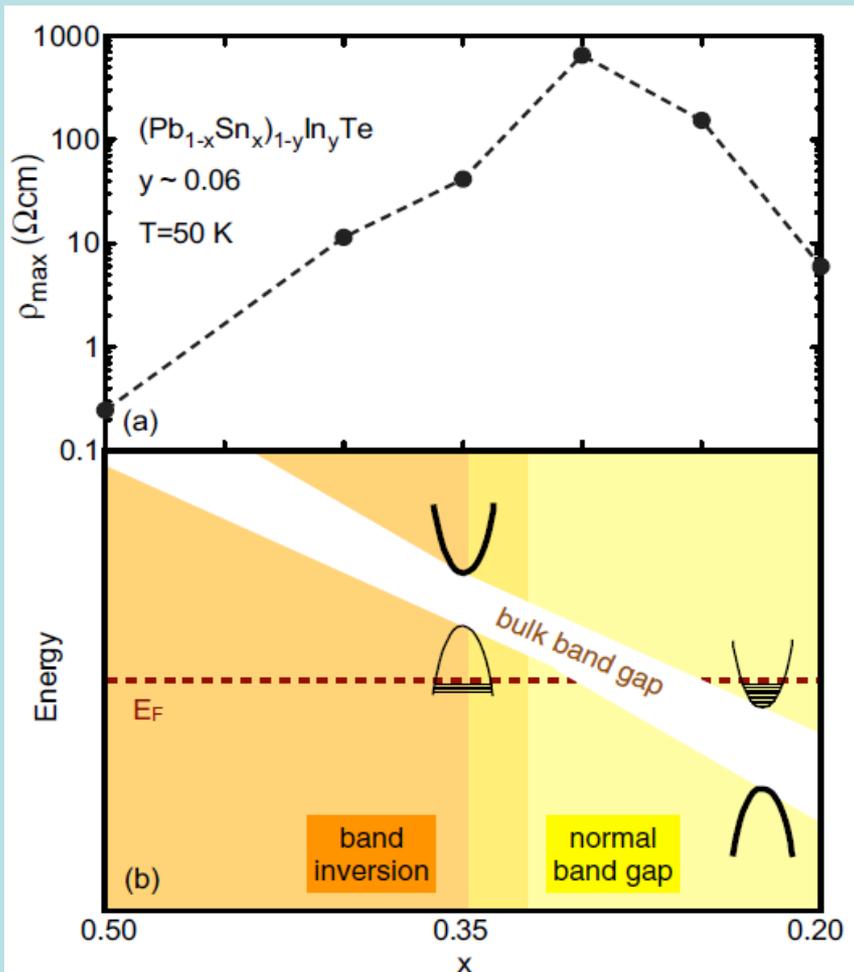
Two parallel conduction channels

Fitting of electron transport parameters

$\sigma_{BS}$ ,  $\mu_{BS}$ ,  $\sigma_{SS}$ ,  $\mu_{SS}$   
for bulk crystal and surface channels

K. Dybko et al.

# Controlling electrical properties of TCI materials



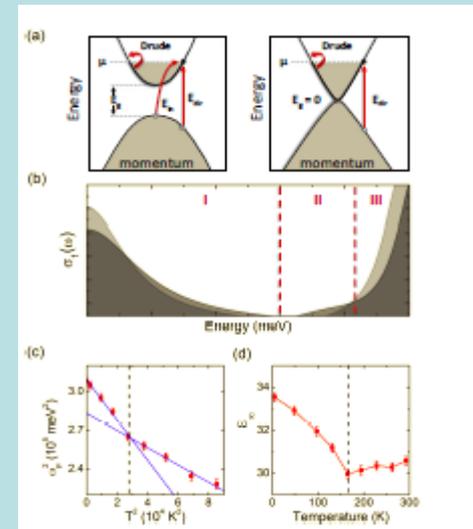
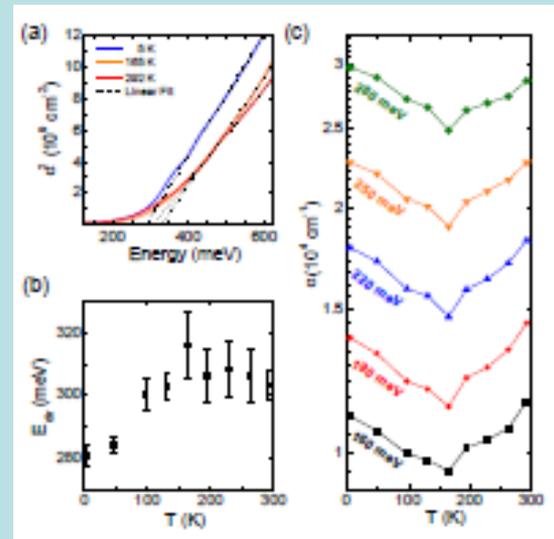
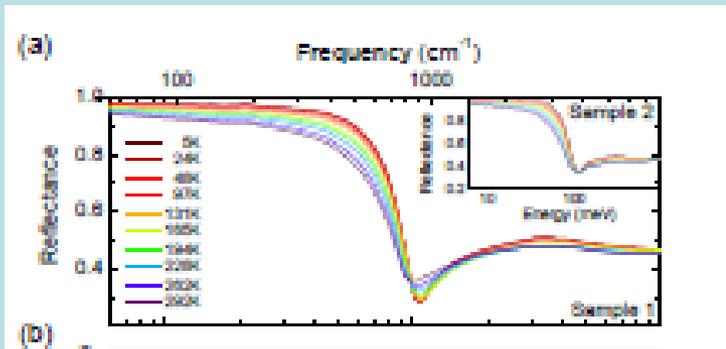
Deep mid-gap doping centers:

group III: In

Transition metals (V, Mo)

R. Zhong et al., Phys. Rev. B 91, 195321 (2015)

# Pb<sub>1-x</sub>Sn<sub>x</sub>Se: infrared optical studies

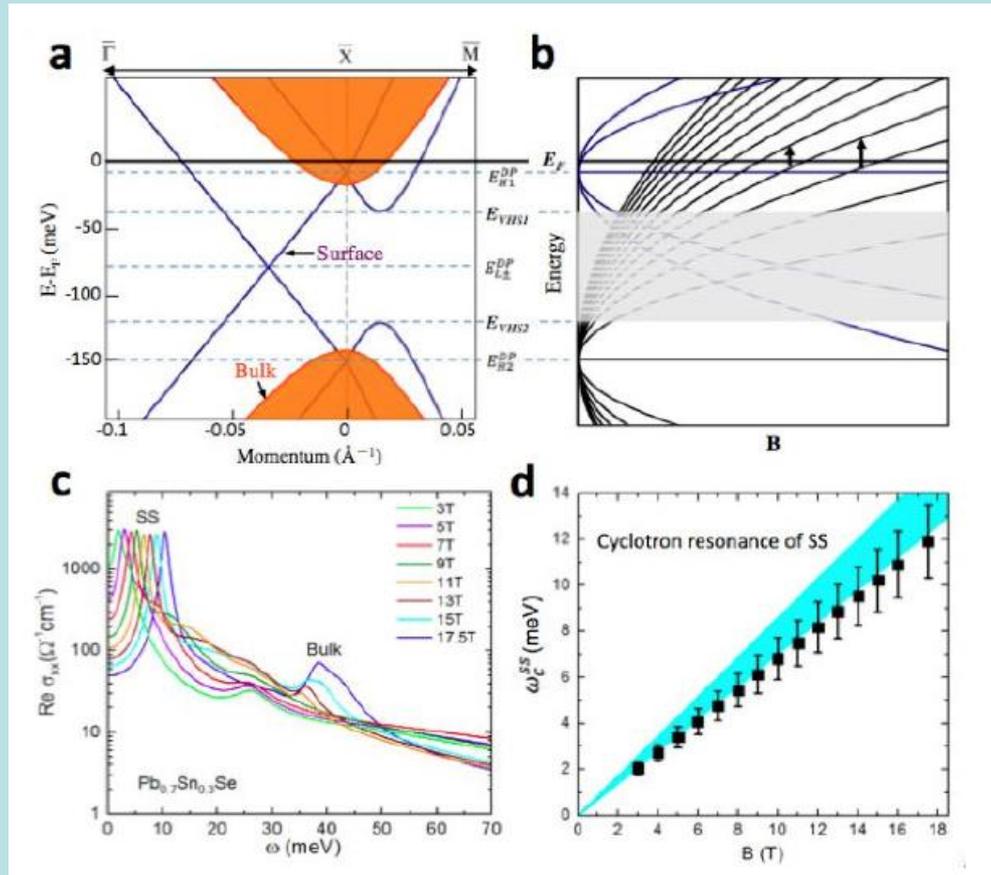


A. Reijnders et al., Phys. Rev B 90, 235144 (2014)

N. Anand et al., Phys. Rev. B 90, 235143 (2014)

X. Xi et al., Phys. Rev. Lett. 113, 096401 (2014)

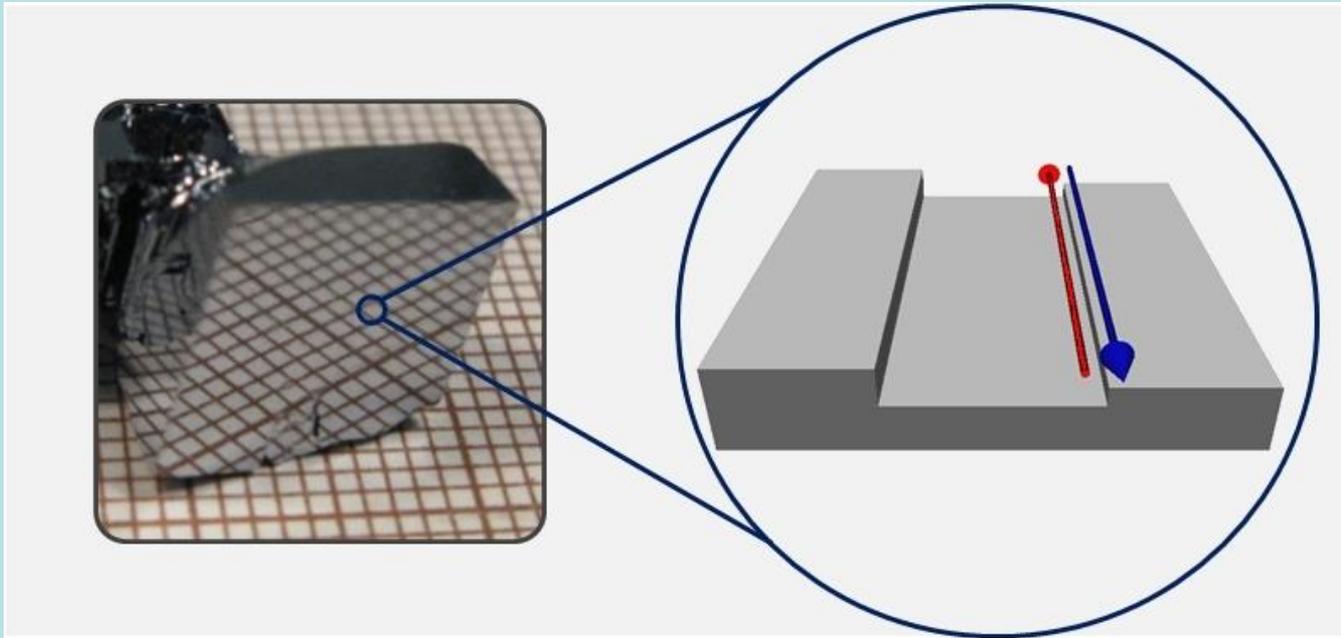
# $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ : infrared magneto-optical studies



[Y. Wang et al., arXiv 1611.04302](#)

[B.A. Assaf et al., Sci. Rep. 6, 20323 \(2016\)](#)

# III. Atomic steps as new 1D topological systems



# Atomic steps as new 1D topological systems

RESEARCH | REPORTS

TOPOLOGICAL MATTER

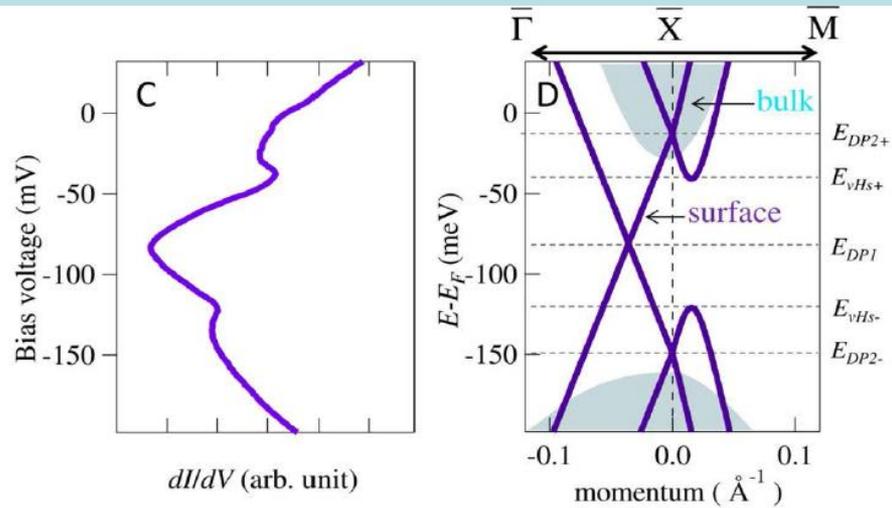
## Robust spin-polarized midgap states at step edges of topological crystalline insulators

Paolo Sessi,<sup>1\*</sup> Domenico Di Sante,<sup>2</sup> Andrzej Szcerbakow,<sup>3</sup> Florian Glott,<sup>1</sup> Stefan Wilfert,<sup>1</sup> Henrik Schmidt,<sup>1</sup> Thomas Bathon,<sup>1</sup> Piotr Dziawa,<sup>3</sup> Martin Greiter,<sup>2</sup> Titus Neupert,<sup>4</sup> Giorgio Sangiovanni,<sup>2</sup> Tomasz Story,<sup>3</sup> Ronny Thomale,<sup>2</sup> Matthias Bode<sup>1,5</sup>

P. Sessi et al., *Science* **354** (6317), 1269 (2016)

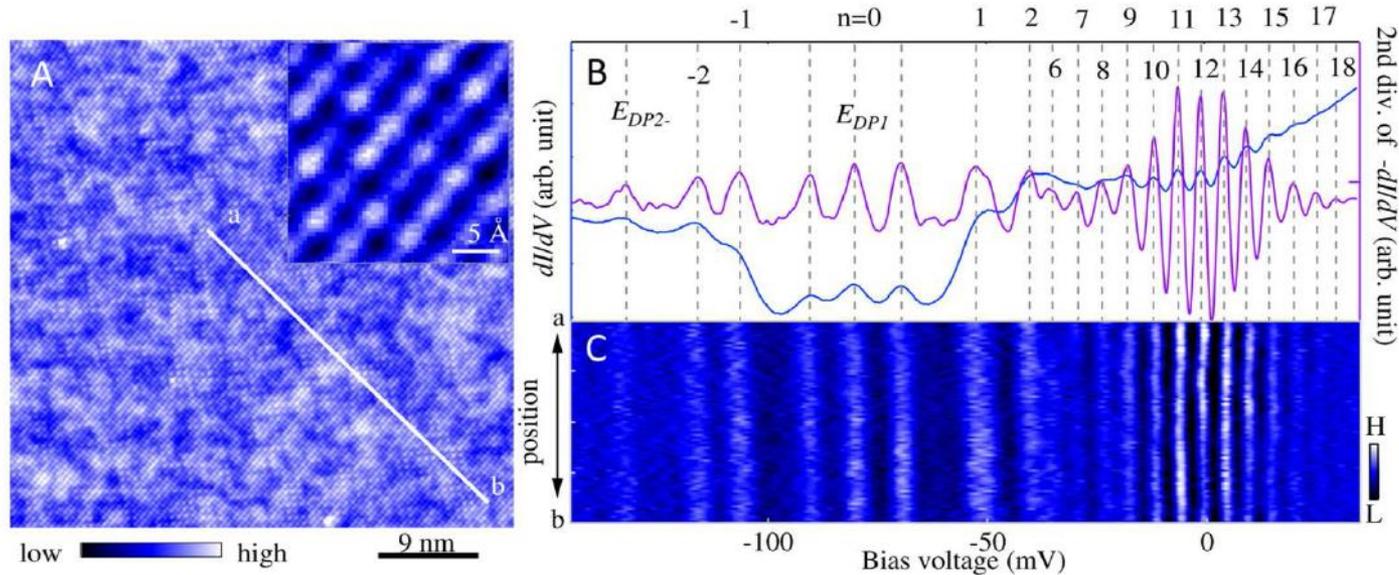
- **Experiment STM/STS:** Würzburg University (EP2)
- **Theory:** Würzburg University (TP1) and Zürich University
- **Monocrystals** (growth and characterization): IP PAS, Warsaw

# STM – conductance spectroscopy

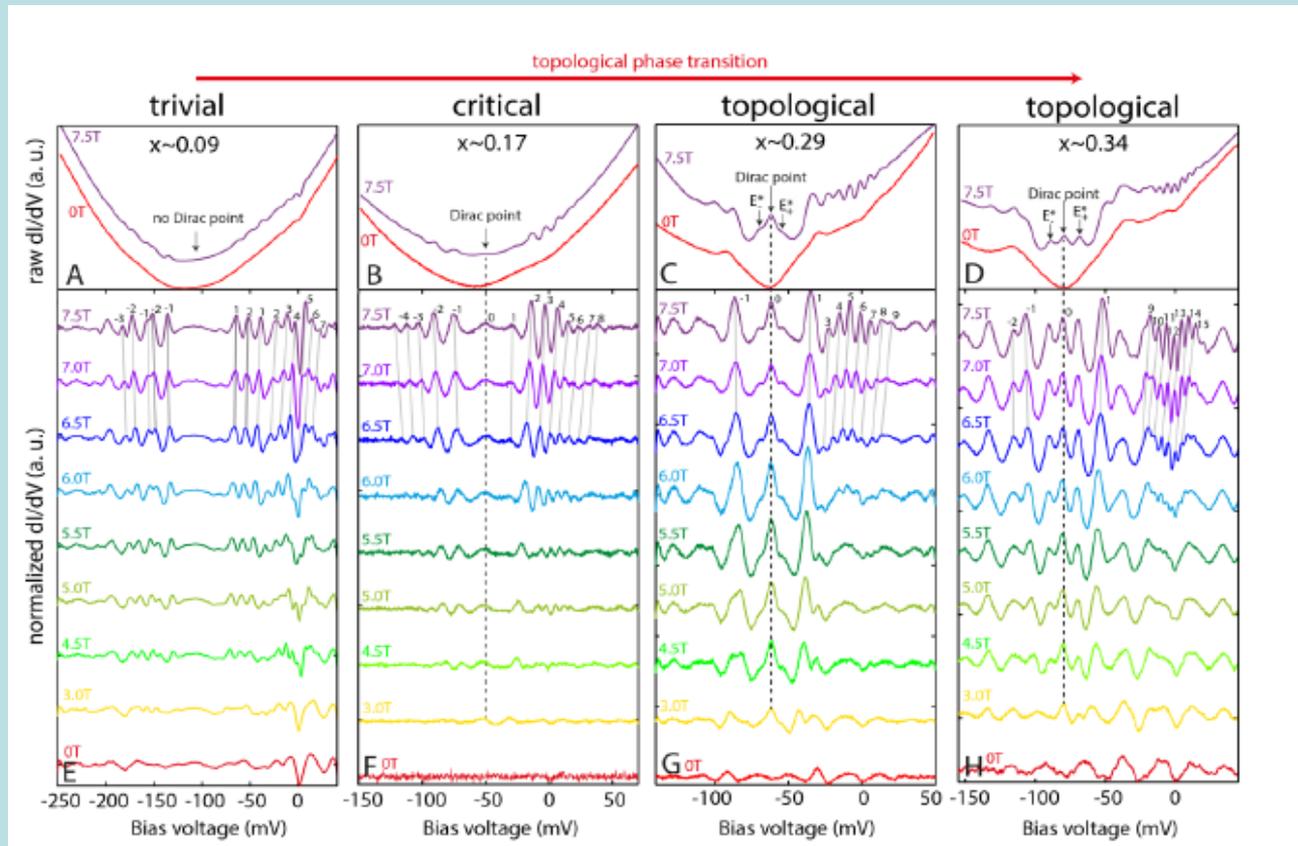


**Pb<sub>1-x</sub>Sn<sub>x</sub>Se**

Y. Okada et al.,  
Science 341, 1496 (2013)

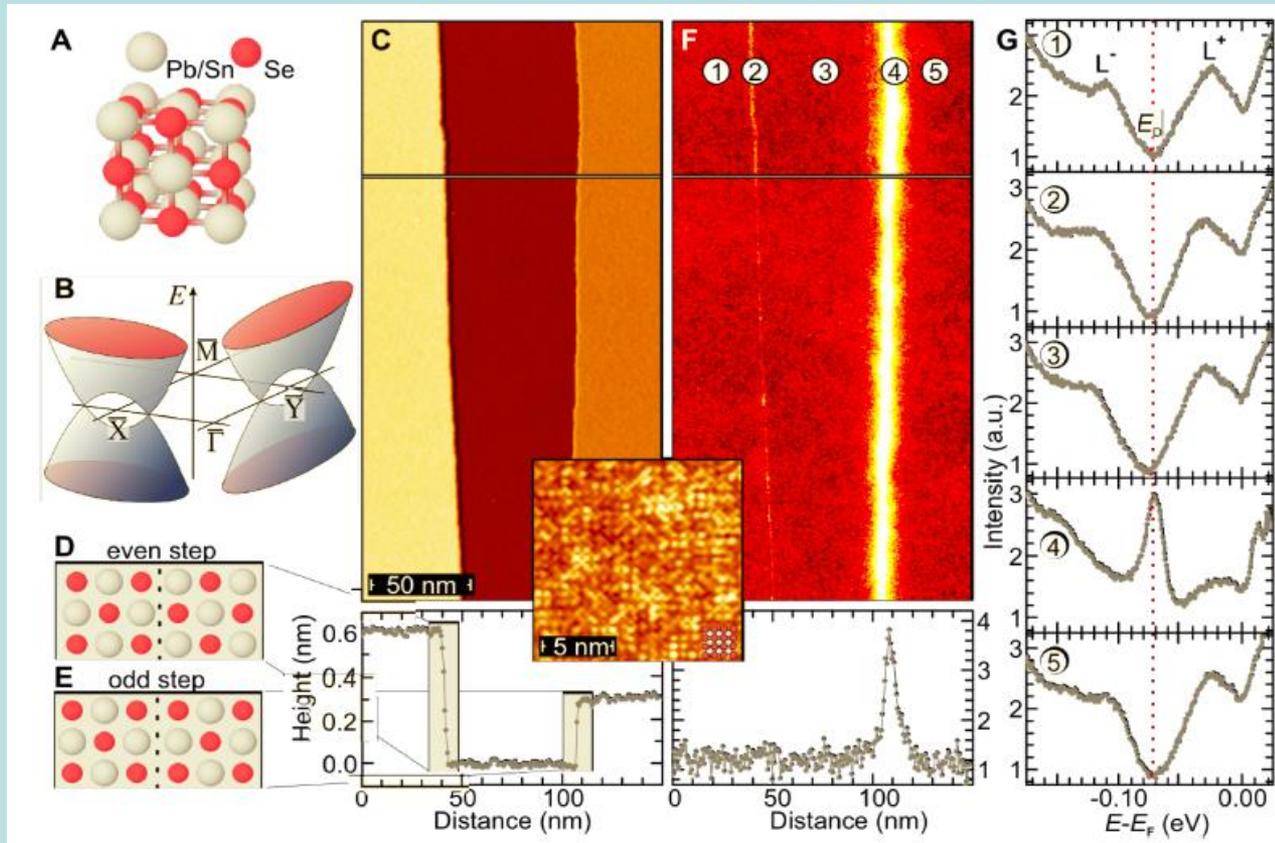


# $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ - STM spectroscopy Landau quantization



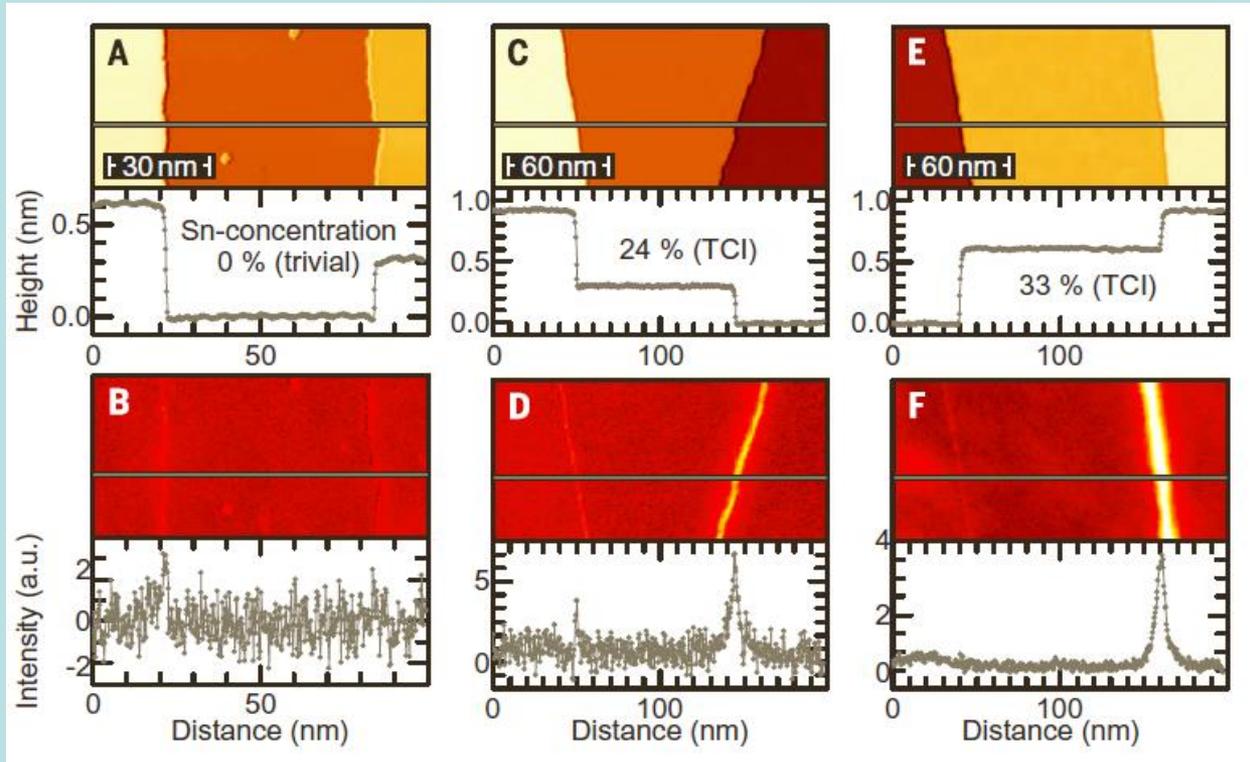
I. Zeljkovic, ...V. Madhavan, Nature Physics 10, 572 (2014);

# STM/STS spectroscopy in $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ : topological 1D states



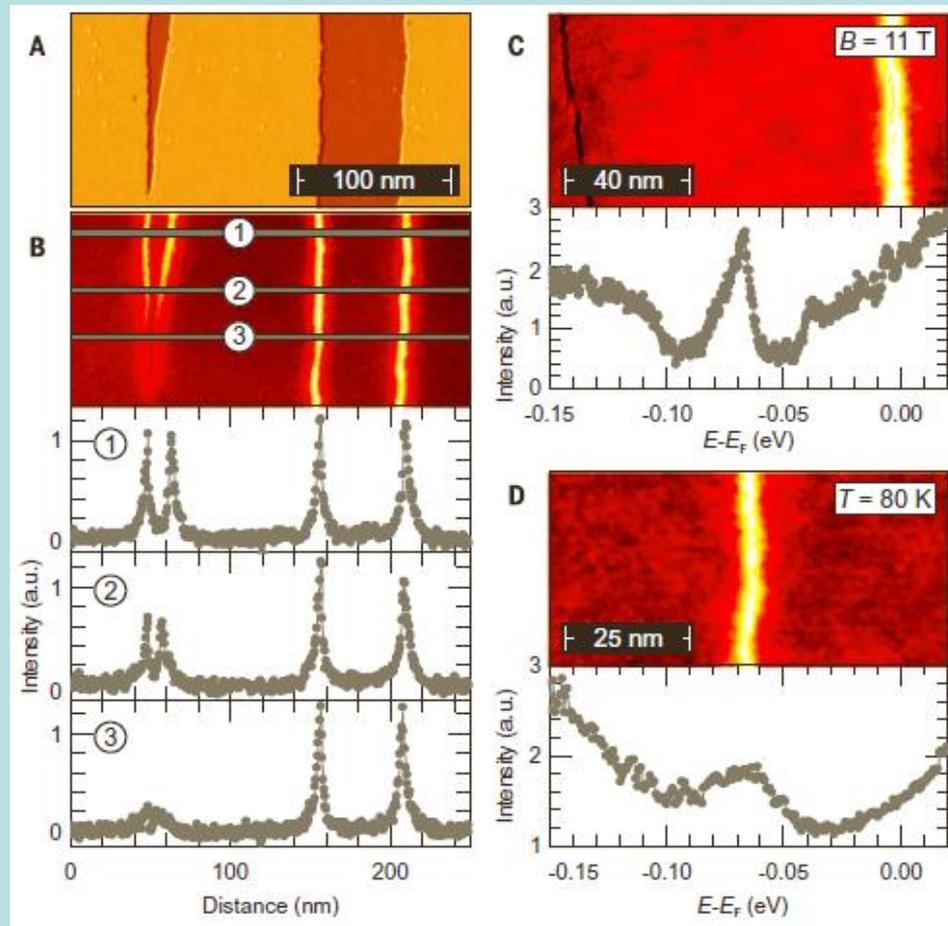
P. Sessi et al., *Science* **354** (6317), 1269 (2016)

# STM/STS spectroscopy in $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ : topological 1D states

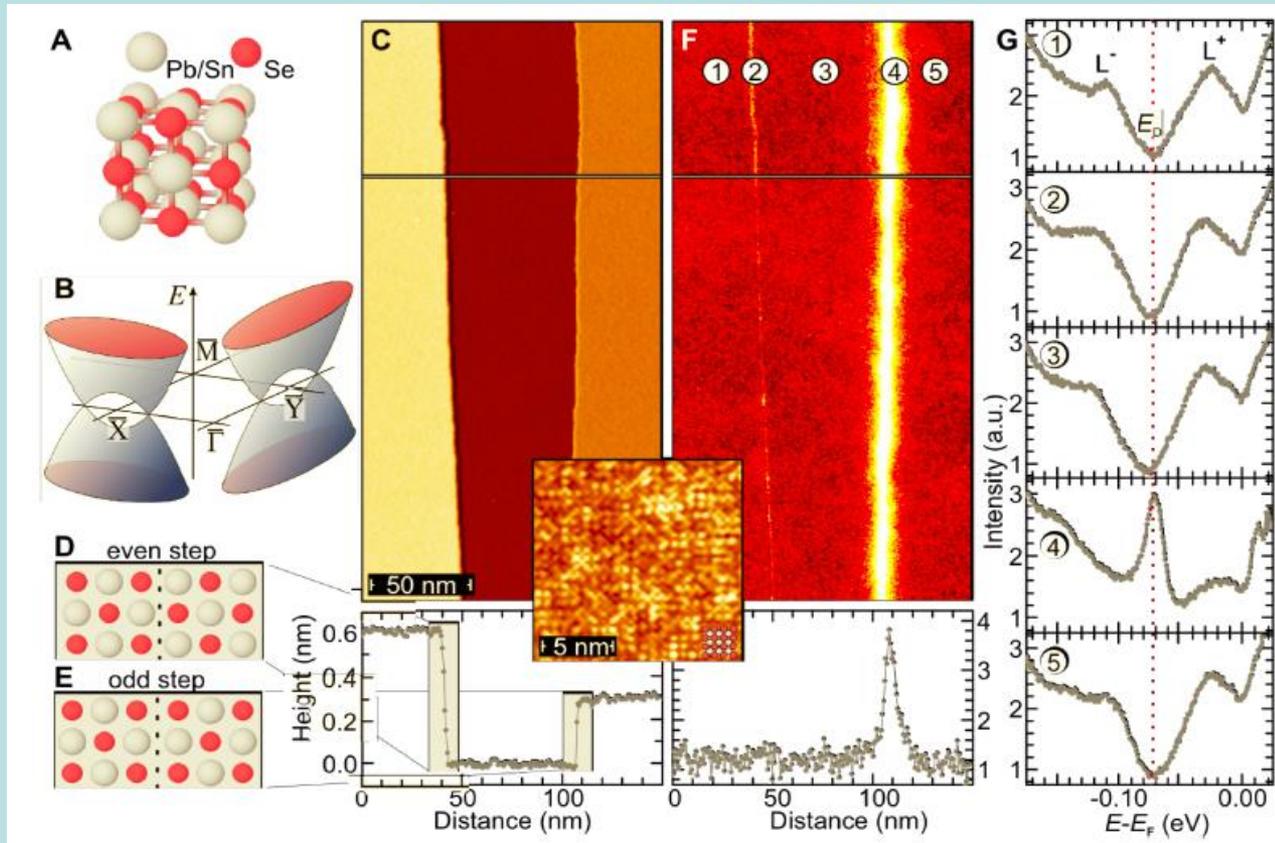


P. Sessi et al., *Science* **354** (6317), 1269 (2016)

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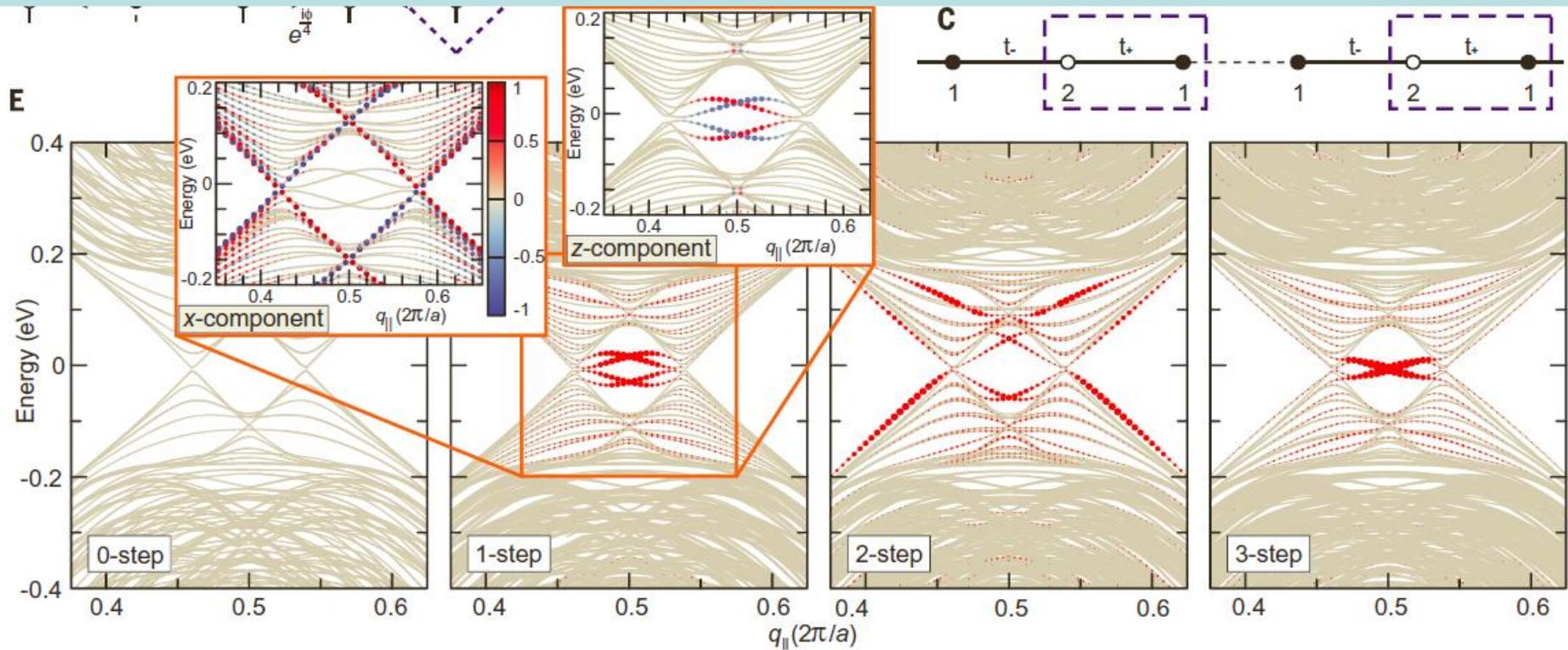


# STM/STS spectroscopy in $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ : topological 1D states

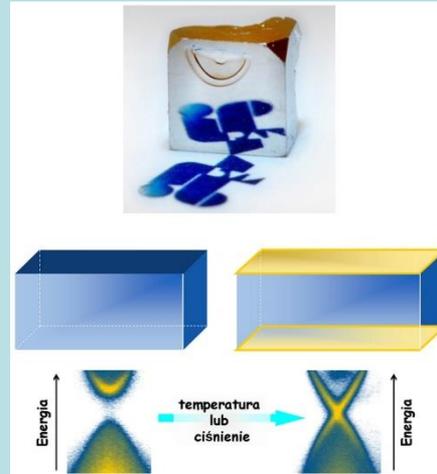


P. Sessi et al., *Science* **354** (6317), 1269 (2016)

# Electronic structure of $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ (001) with atomic steps



# Topological materials - summary



- Metallic surface (or edge) states with linear energy dispersion (massless Dirac fermions).
- Inverted band structure: relativistic effects (spin-orbit coupling, Darwin term).
- Topological protection, suppression of backscattering.
- Spin polarization, helical states, spin-momentum locking.
  
- Bandgap origin and symmetry protection based classification:
- topological insulators (TRS),
- topological crystalline insulators (mirror-plane symmetry):  
IV-VI semiconductors SnTe , (Pb,Sn)Te and (Pb,Sn)Se