

Relaxation dynamics in topological insulators

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Collaborators

➤ *ARPES Experiments*

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➤ *Synchrotron Beam Line Assistance*

S.-K. Mo, J. D. Denlinger, A. Fedorov : **Advanced Light Source, LBNL; Stanford Synchrotron Radiation Lightsource, Stanford, CA; Swiss Light Source, PSI**

Laser based TR-ARPES

T. Kondo, Y. Ishida, S. Shin (ISSP, University of Tokyo, Japan)

➤ *Crystal Growth*

Robert Cava (Princeton University, Chemistry), E. D. Bauer (Los Alamos National Laboratory)

D. Kaczorowski (Polish Academy of Science), N. Samarth (Penn State)

F.C. Chou (Taiwan), D.J. Kim, Z. Fisk (University of California at Irvine)

➤ *Theory and Calculations*

T. Rahman group (University of Central Florida), **Jianxin Zhu** (LANL), T.-R. Chang, T.-H. Jeng (National Tsing Hua University, Taiwan), **H. Lin** (NUS), **A. Bansil** (Northeastern University)

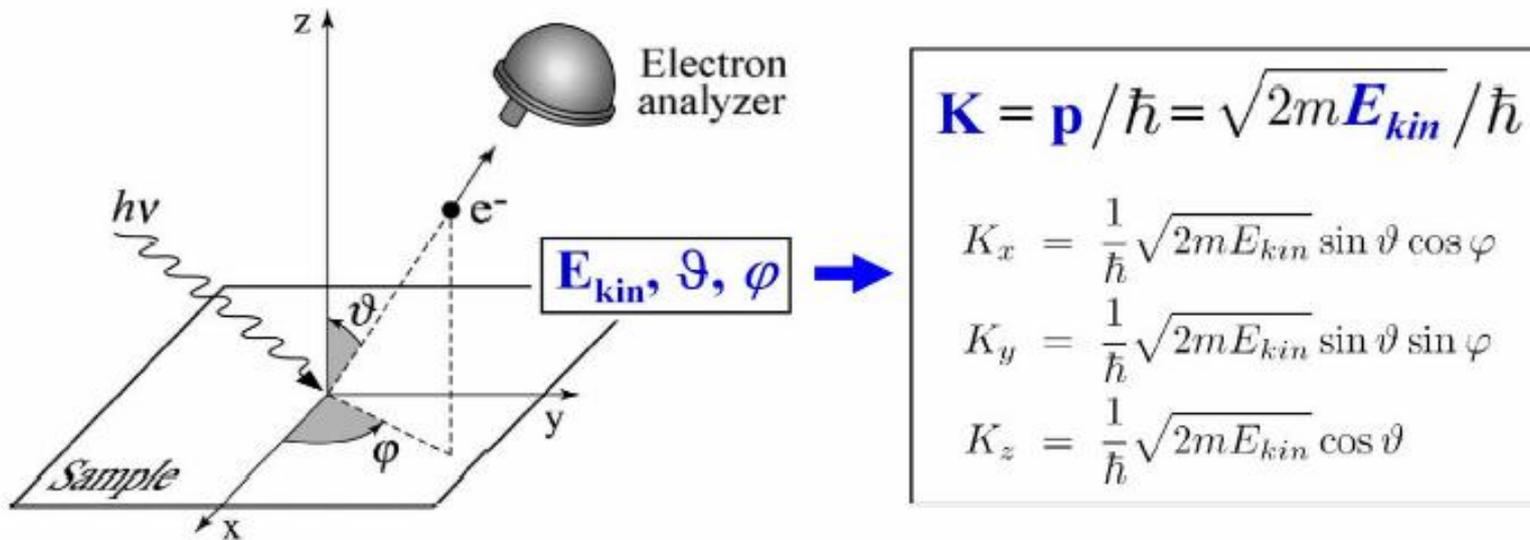
Outline

Photoemission studies of topological insulators and beyond

- Introduction: Photoemission & topological insulators
- Binary and ternary topological insulators – time-resolved phenomena
- New topological phases – 3D Dirac, Weyl and nodal phases

Technique: Photoemission

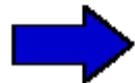
Angle-resolved Photoemission Spectroscopy (ARPES)



Vacuum

$$E_{kin}$$

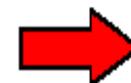
$$\vec{K}$$



Conservation laws

$$E_{kin} = h\nu - |E_B| - \Phi$$

$$\vec{K} = \vec{k} + \cancel{\vec{k}_{photon}}$$



Solid

$$E_B$$

$$\vec{k}$$

momentum conservation

ARPES “sees” electrons

ARPES measures spectral function

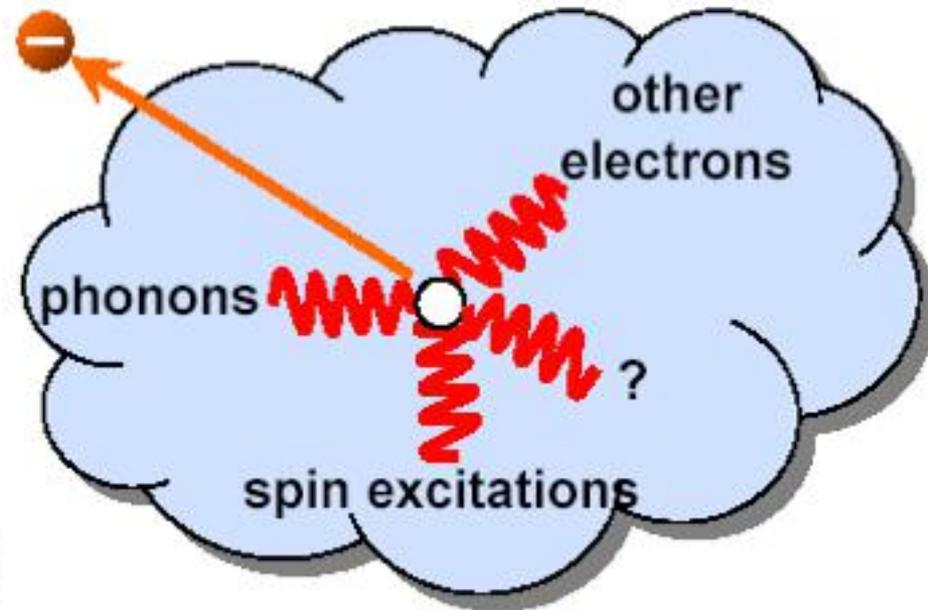
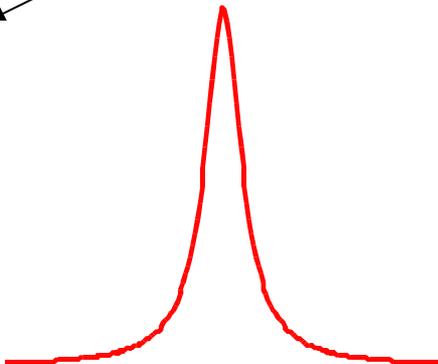
$$I(\vec{k}, \omega) = I_0(\vec{k}, \nu, \vec{A}) f(\omega) A(\vec{k}, \omega)$$

$$A(k, \omega) = \frac{1}{\pi} \text{Im}(G(k, \omega))$$

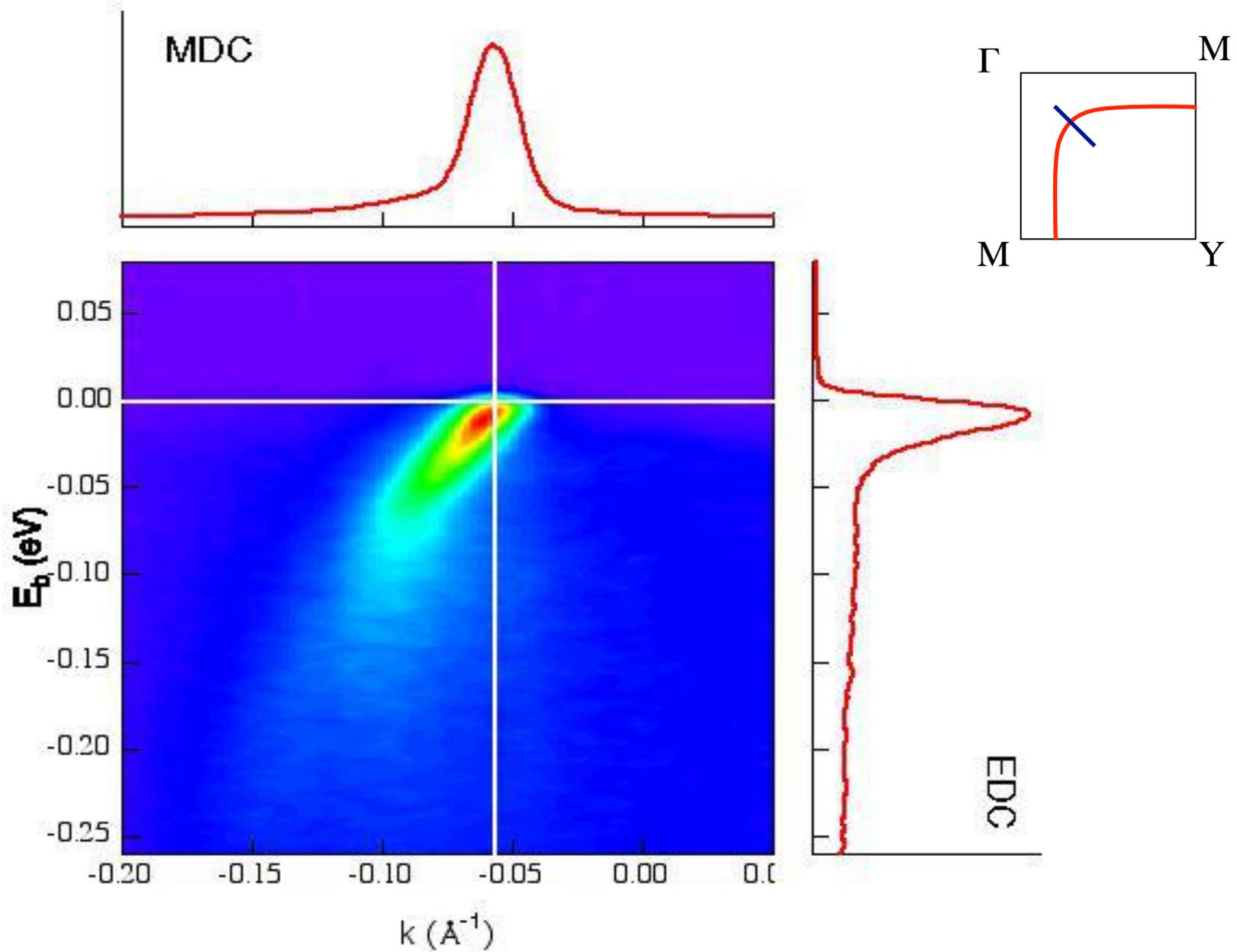
$$G(k, \omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(k, \omega)} \quad \leftarrow \text{self energy}$$

$$A(k, \omega) = \frac{1}{\pi} \frac{\Sigma''(k, \omega)}{[\omega - \varepsilon_k - \Sigma'(k, \omega)]^2 + [\Sigma''(k, \omega)]^2}$$

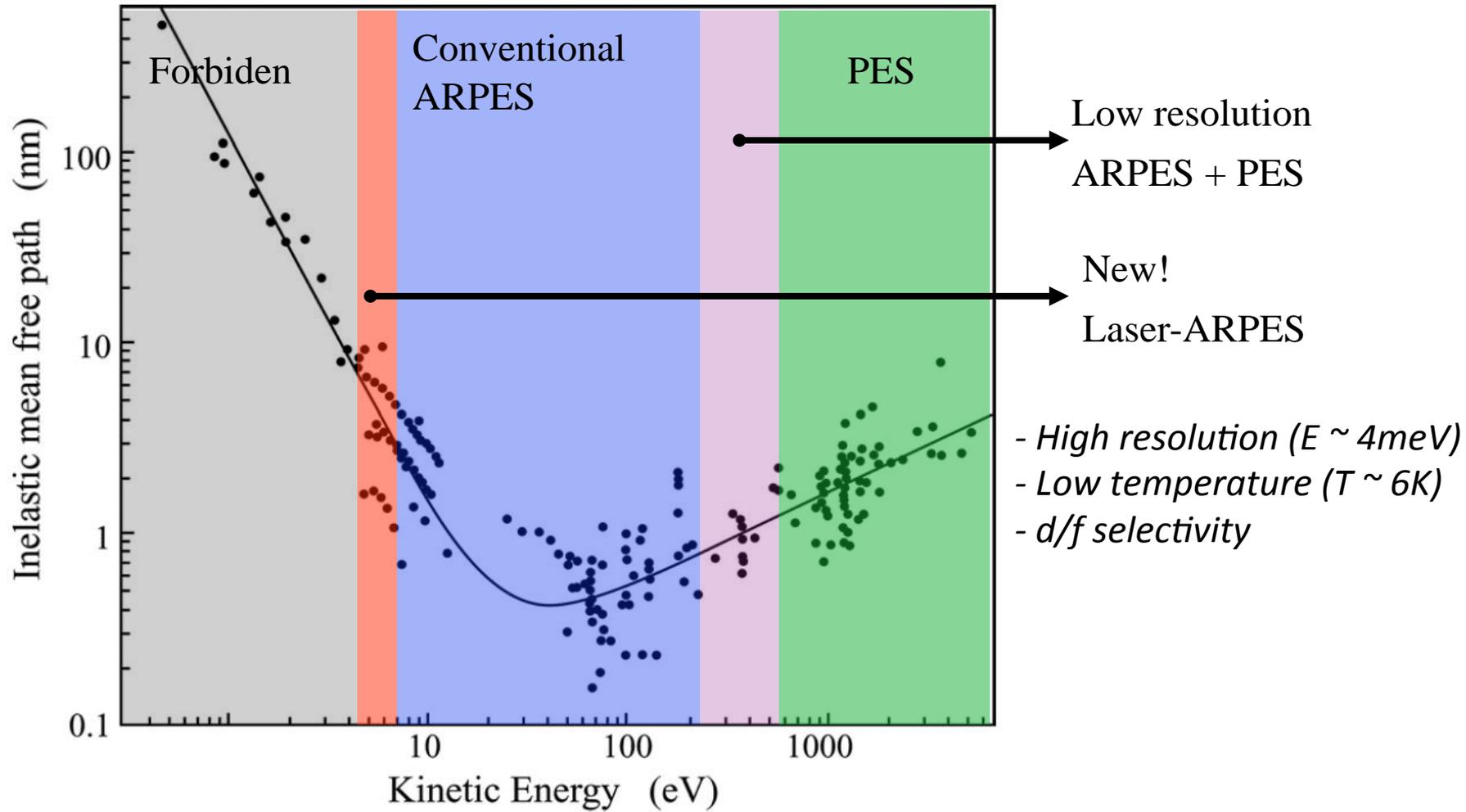
Γ



ARPES SPECTRA

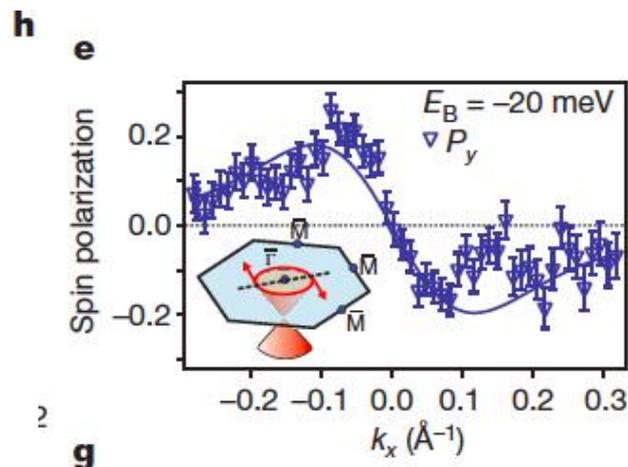
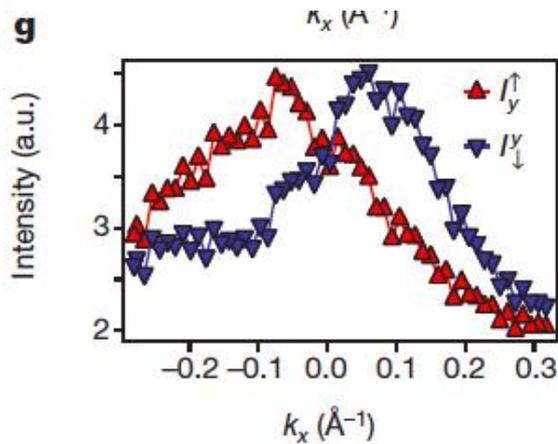
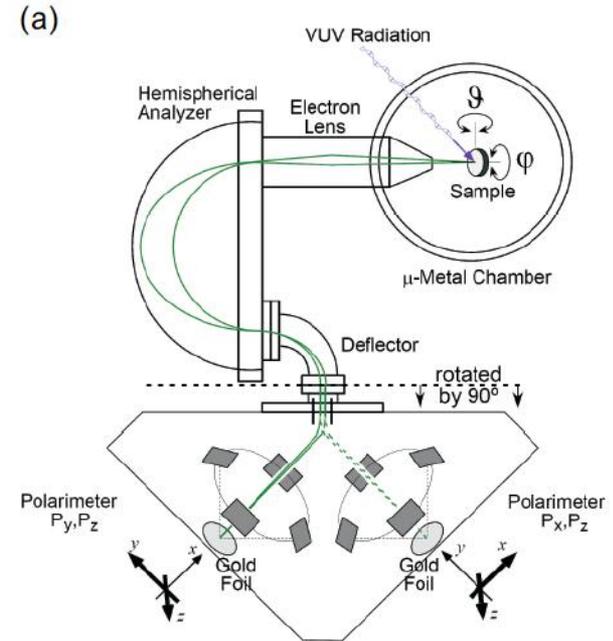
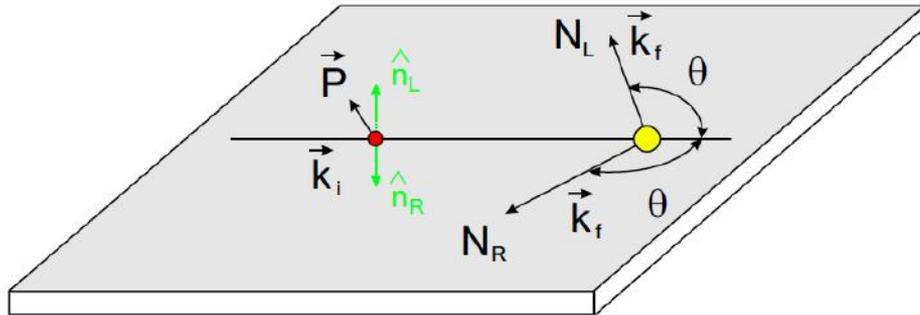


Surface probe



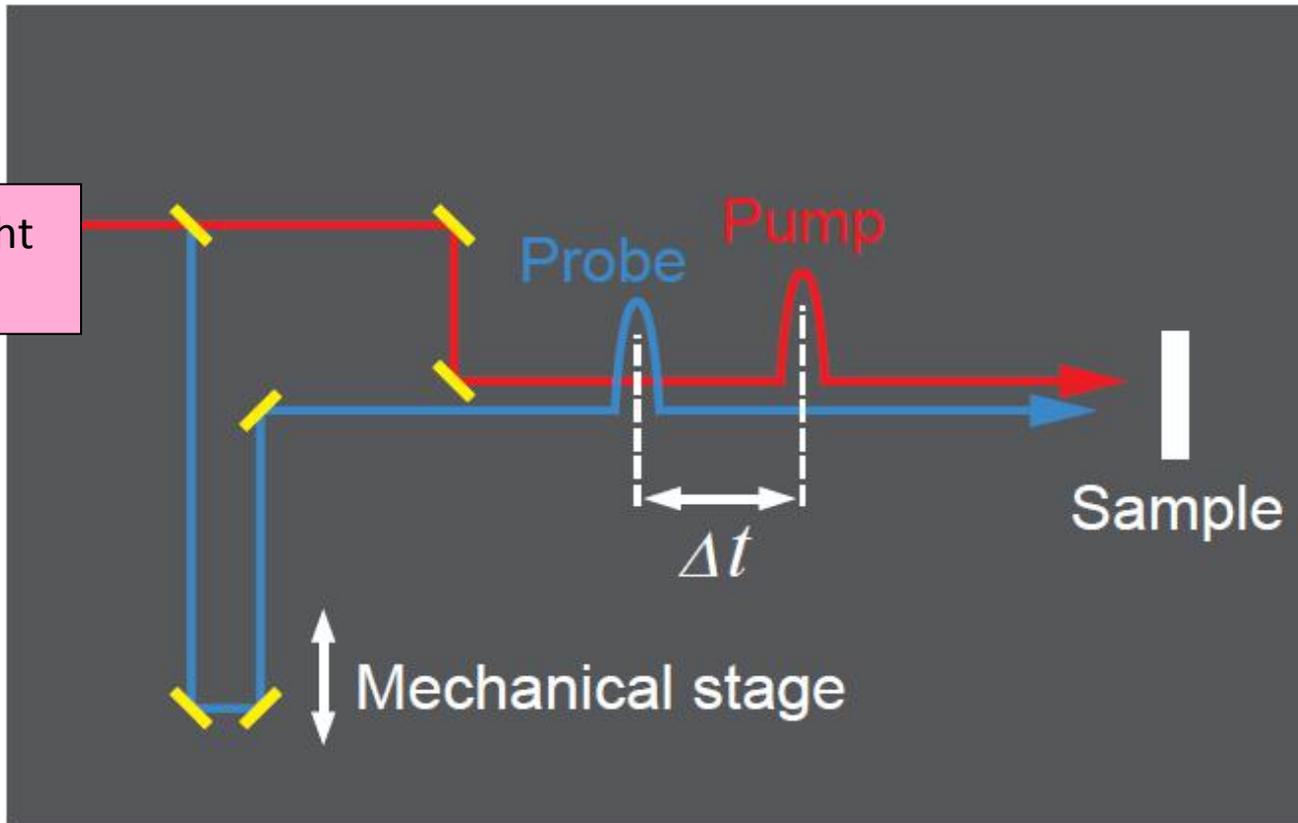
Seah *et al.*, Surf. Interface Anal. **1**, 2 (1979).

Spin-resolved ARPES



Time-resolved spectroscopy

Pulsed light source

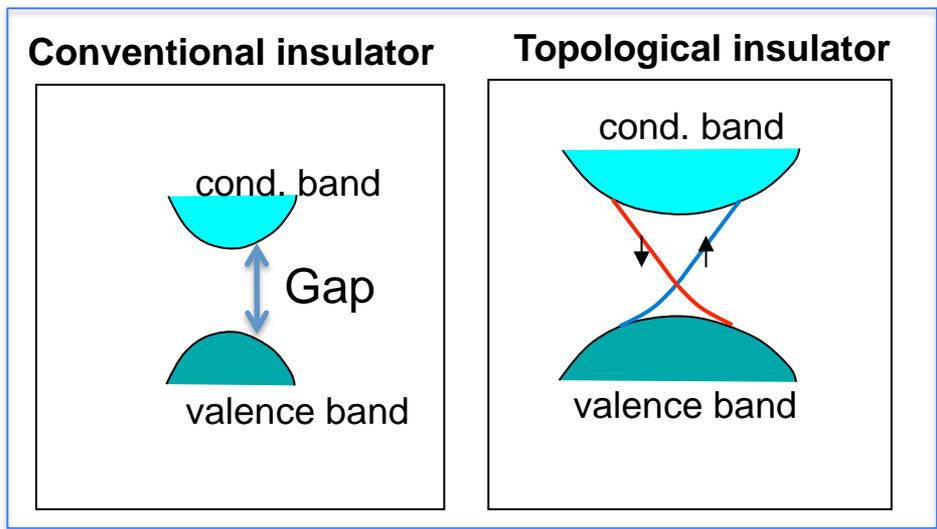


Pump-probe spectroscopy:

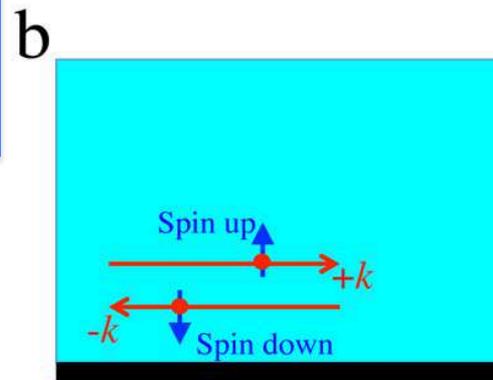
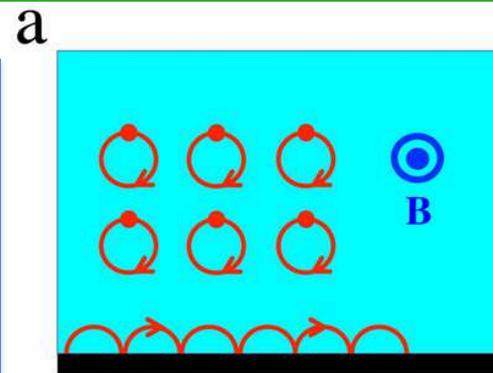
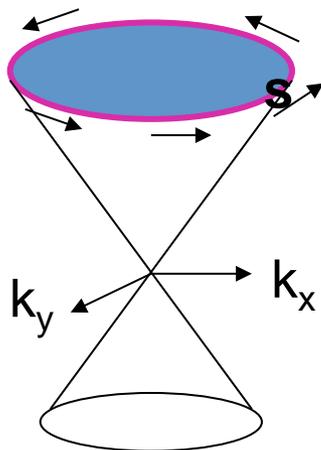
Pump pulse initiates the dynamics, and probe pulse snapshots the transient.

New class of insulator

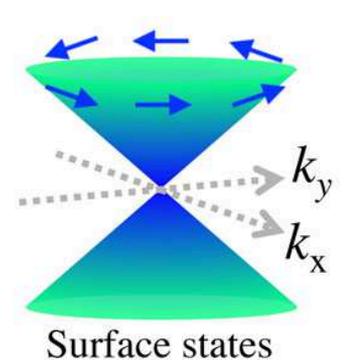
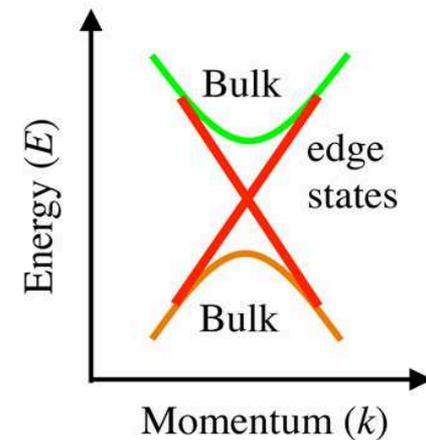
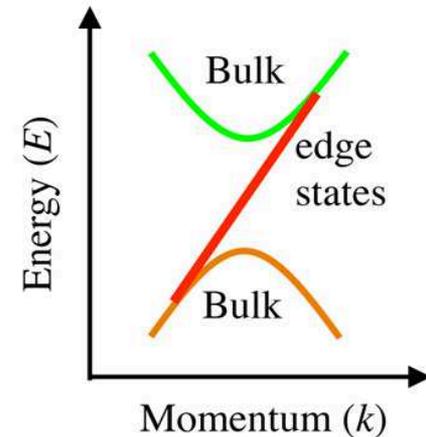
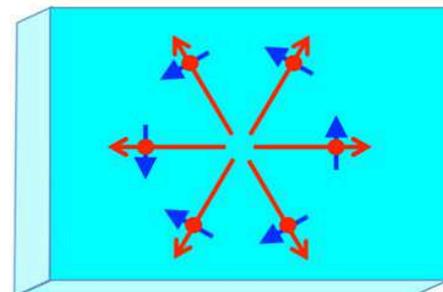
Fu, Kane '06
 Zhang et al. '06
 Moore Balents '06
 Xi, Hughes, Zhang '09



Surface state has Dirac dispersion



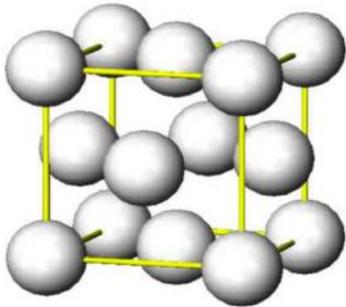
c Topological Surface States



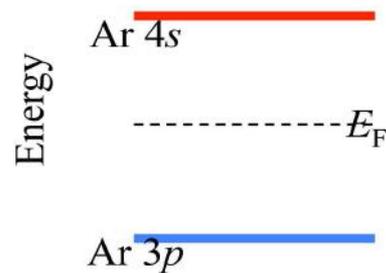
New class of insulator: TI

Conventional Band Insulator – Solid argon Ar

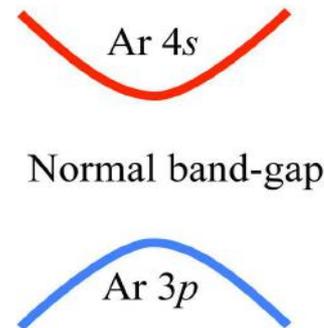
(a) Crystal Structure
Lattice constant = a



(b) Atomic limit
($a \rightarrow \infty$)

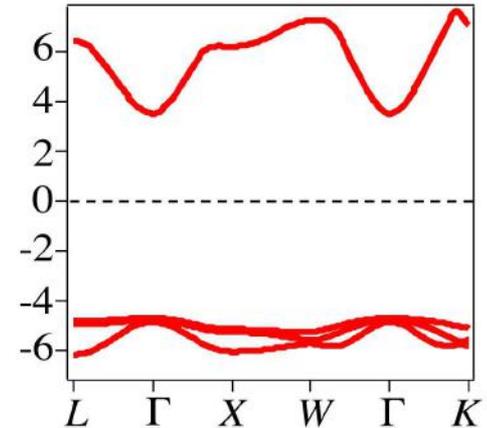


(c) Schematic Band
($a = \text{exp.}$)

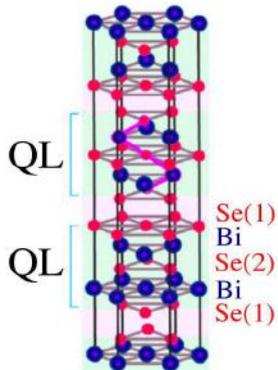


Bloch momentum (k)

(d) First-principles band cal.

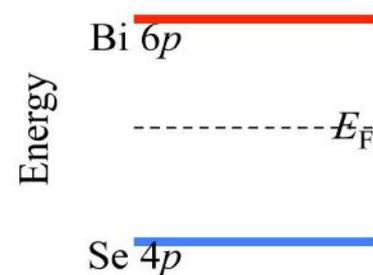


(e) Crystal Structure
Lattice constant = a

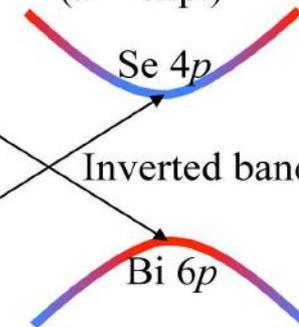


Topological Band Insulator - Bismuth selenide Bi_2Se_3

(f) Atomic limit
($a \rightarrow \infty$)

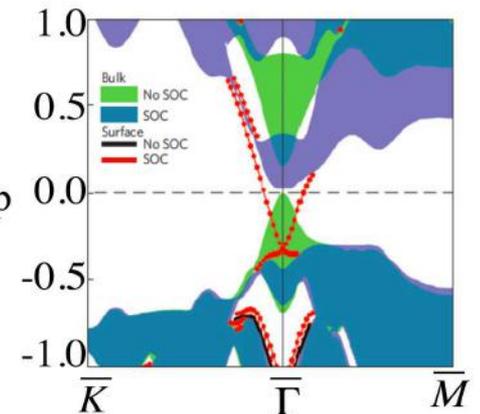


(g) Schematic Band
($a = \text{exp.}$)



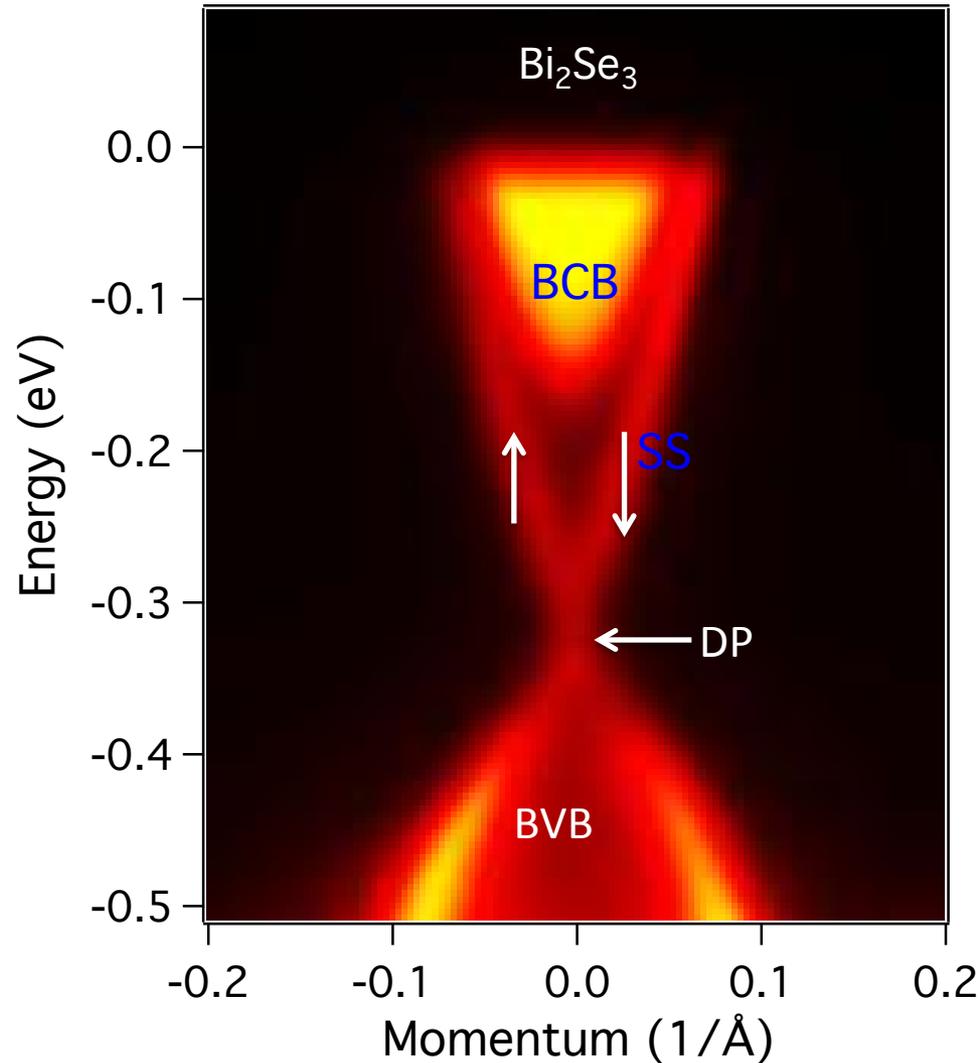
Bloch momentum (k)

(h) First-principles band cal.



Topological Insulator

- **DP:** The two branches (left-moving and right moving) of the surface states cross, forming a surface Dirac point
- **In bulk gap:** The Dirac surface states span across the bulk energy gap, and connect the bulk conduction and the bulk valence bands each other, forming a surface Dirac point
- **Enclosing Kramers points:** The surface state Fermi surfaces enclose the Kramers points of the surface BZ
- **Spin-momentum locking:** The surface state spin is locked with its momentum
- **Odd number:** There are an odd number of **robust** such spin-momentum locked surface state Fermi surfaces

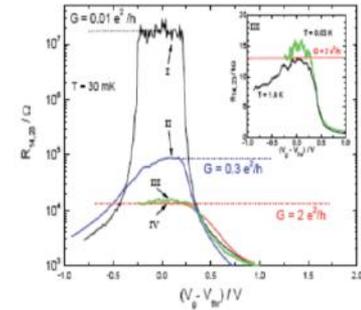
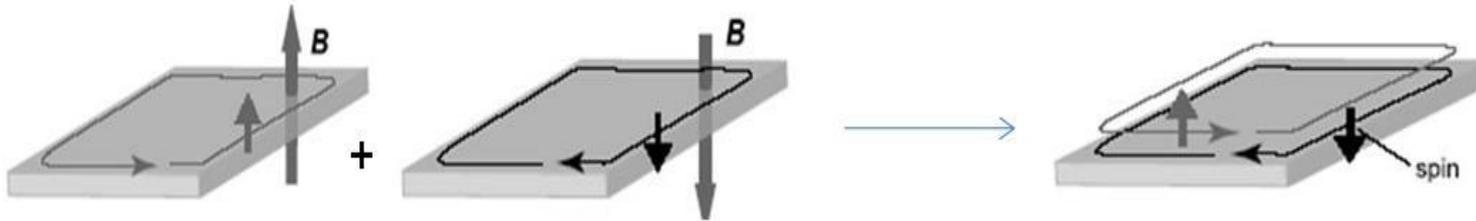


Experimental checklist

Experimental realization of TI

2D TI

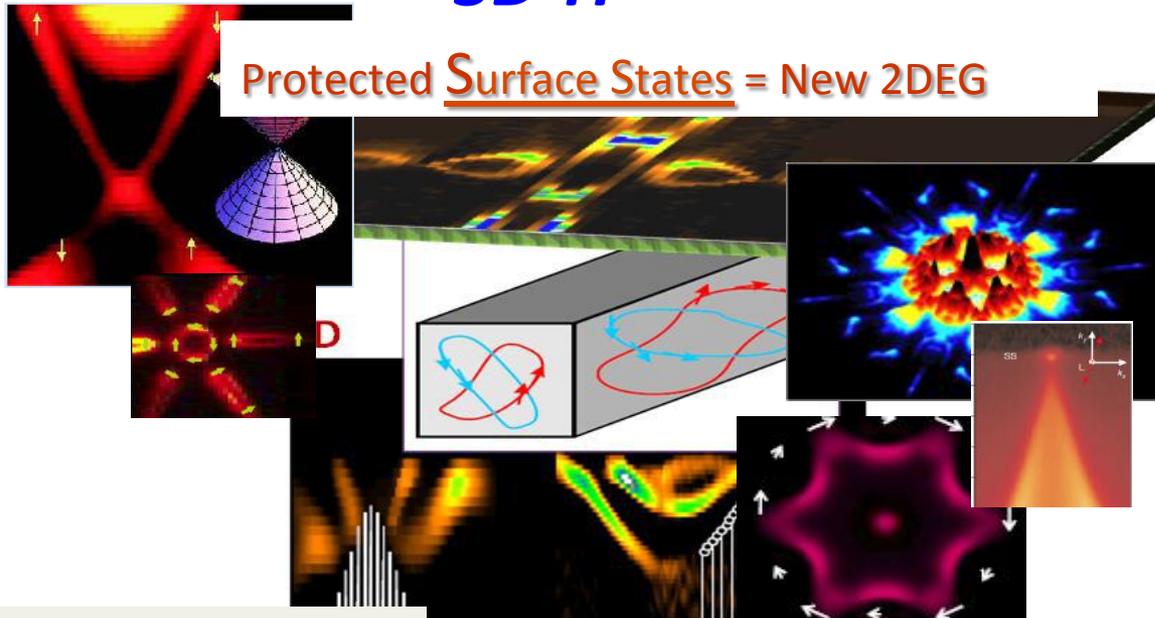
Science 07 (subm. 2007)



Edge States (1D) by TRS

3D TI

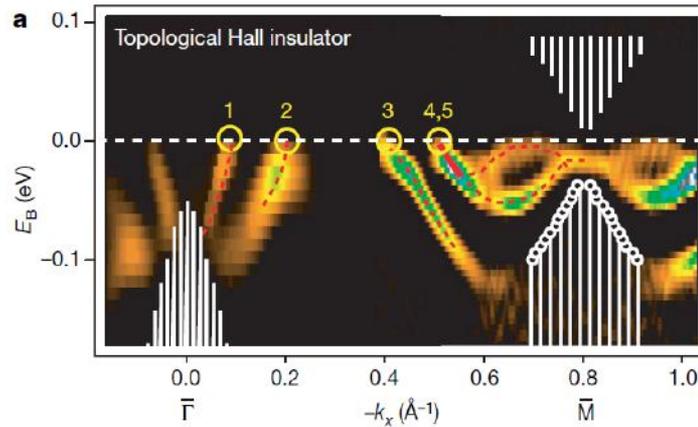
Protected Surface States = New 2DEG



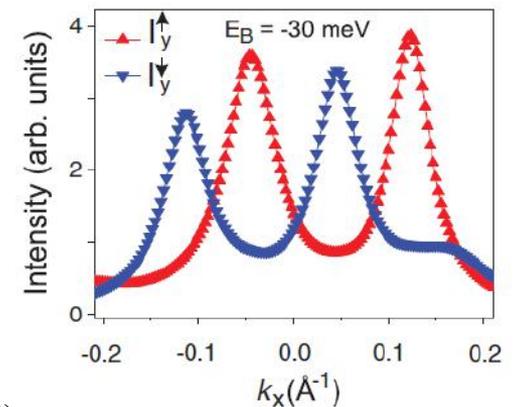
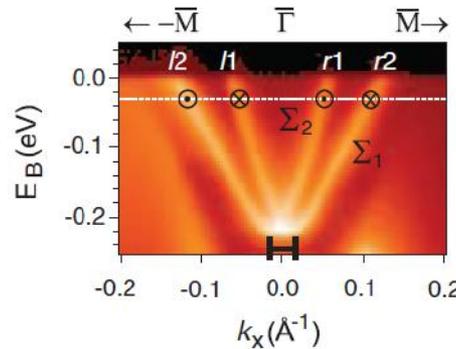
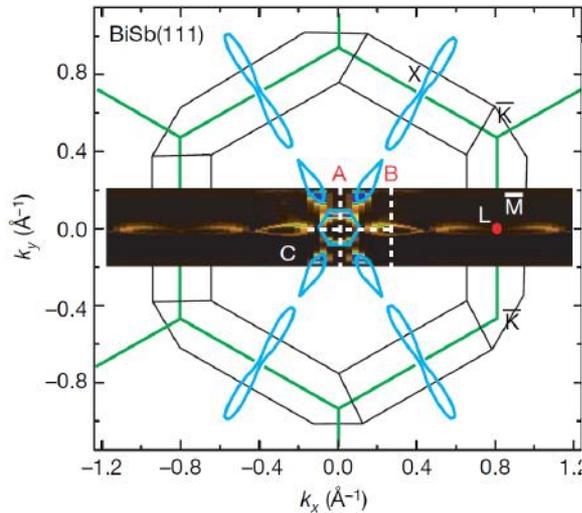
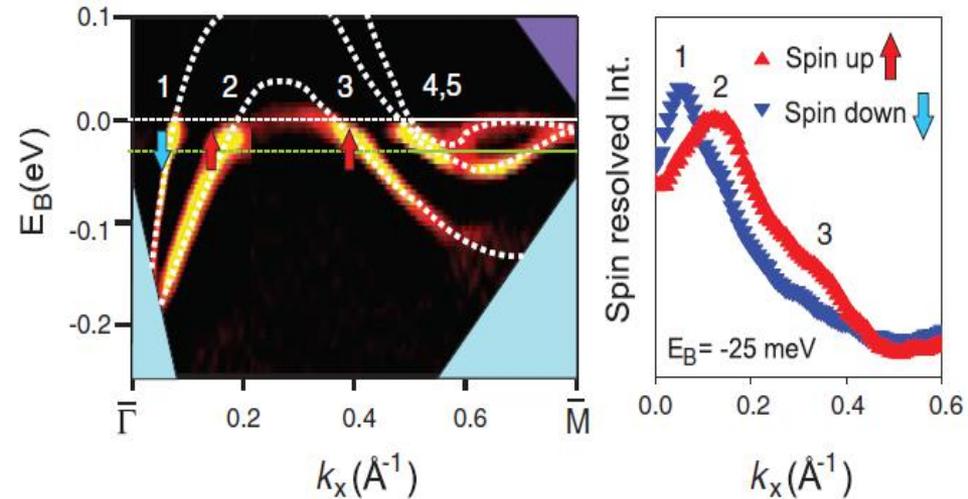
Nature 08 (subm. 2007)

Bi_{1-x}Sb_x: the first discovered 3D TI

Odd number of Dirac cones



spin helical structure



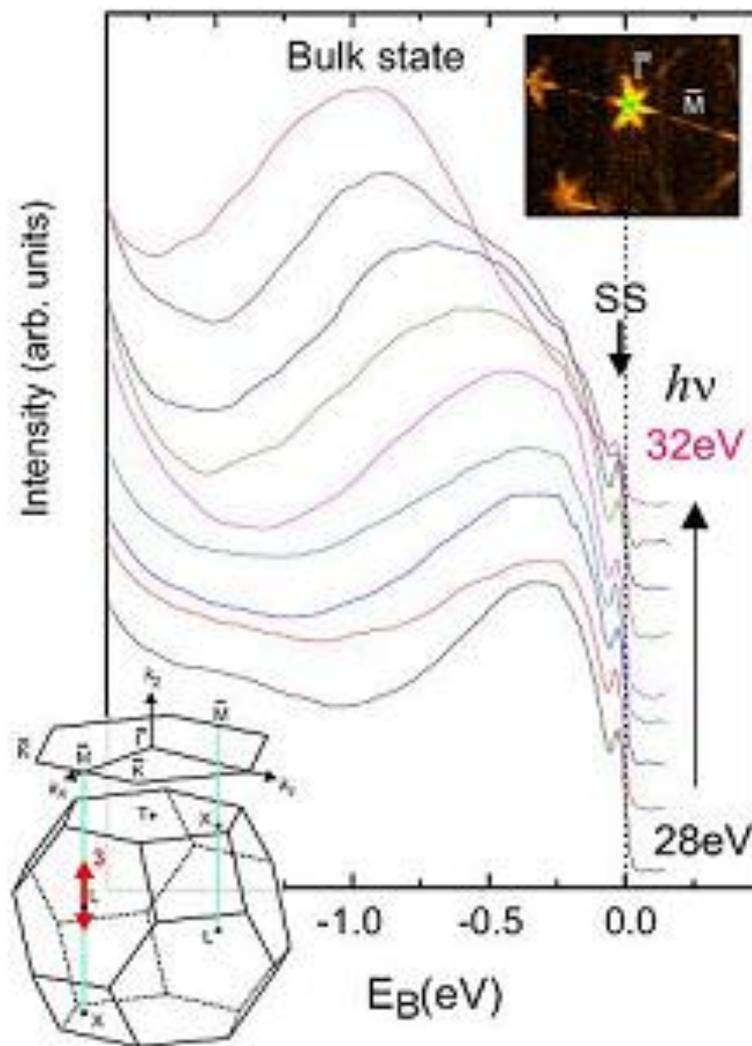
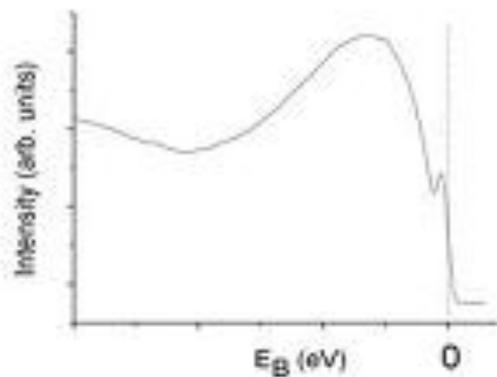
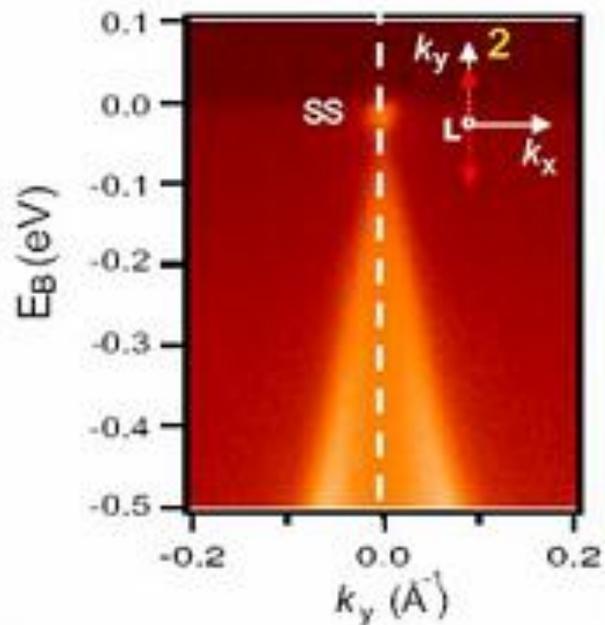
D. Hsieh *et al.* *Nature* **452**, 970 (2008);

D. Hsieh *et al.* *Science* **323**, 919 (2009)

Surface vs bulk

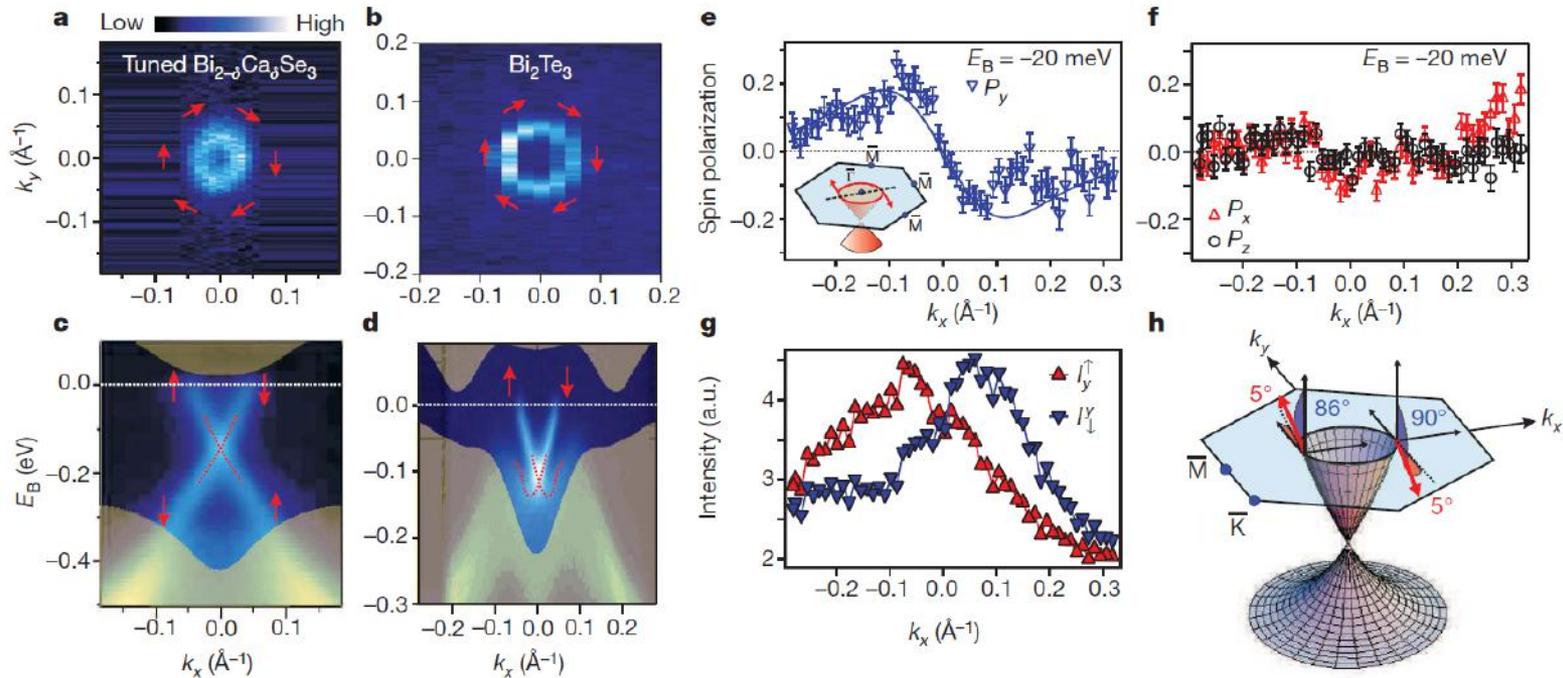
Band-structure of BiSb semiconductors : ARPES view

Fu-Kane PRB'07 Bi-Sb

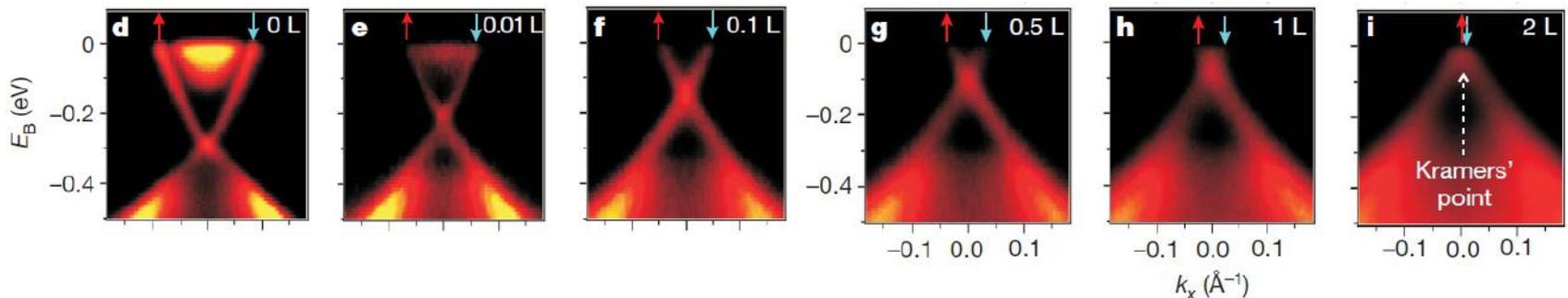


Bi₂Se₃- single Dirac cone TI

Bi₂(Se/Te)₃; Single Dirac cone and spin helical texture; stable at room T



Fermi level tunable by surface carrier deposition (NO₂ on Bi_{2-x}Ca_xSe₃)



Ternary Topological Insulators

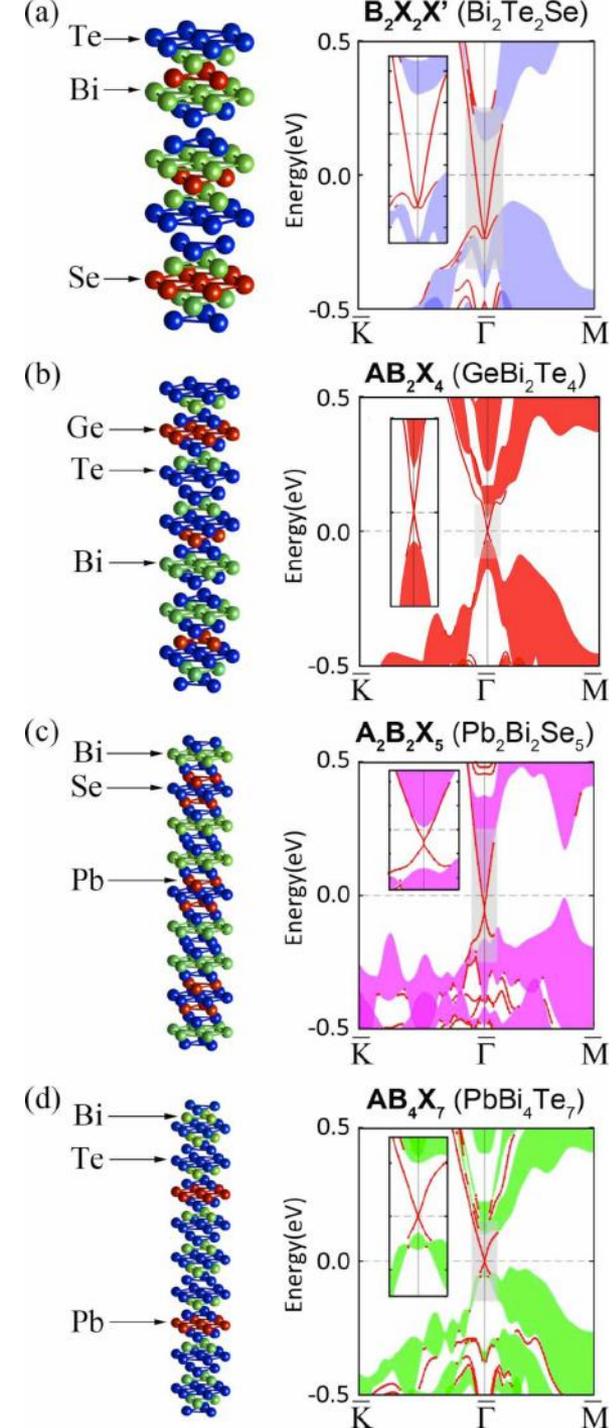
Ternary Topological Insulators

Many Ternary TIs

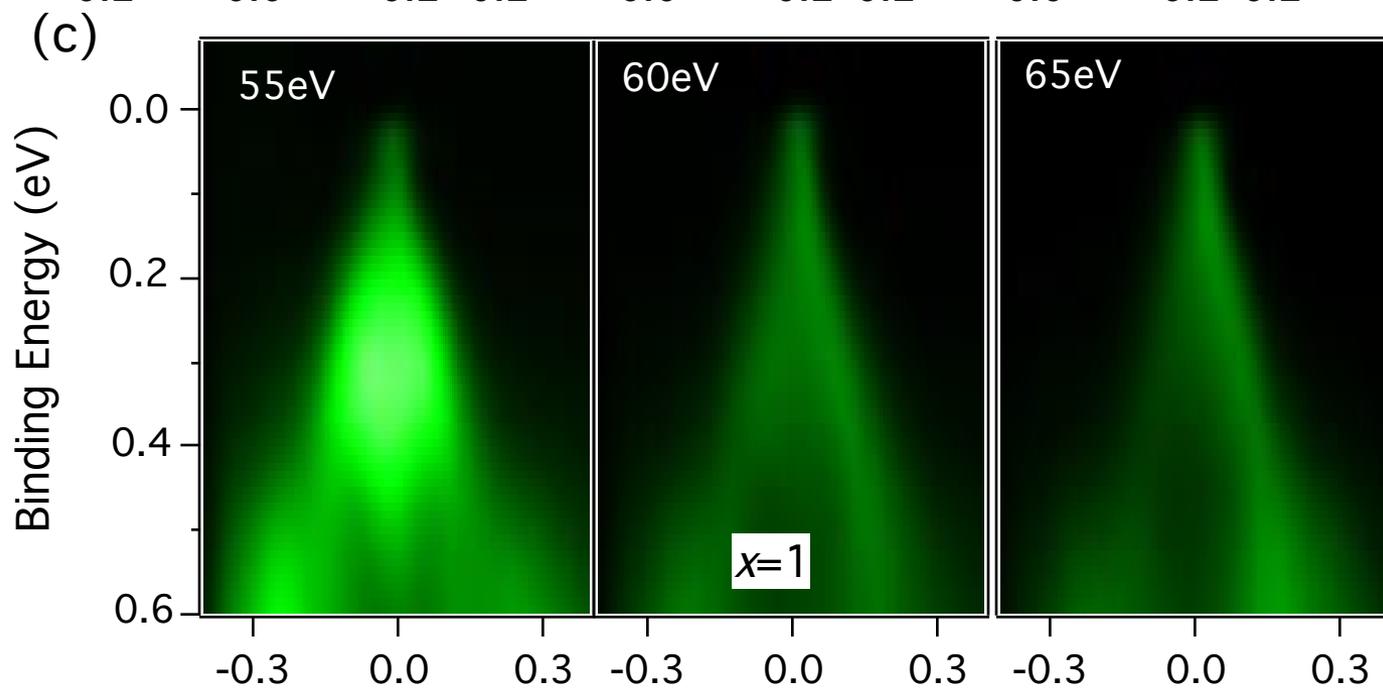
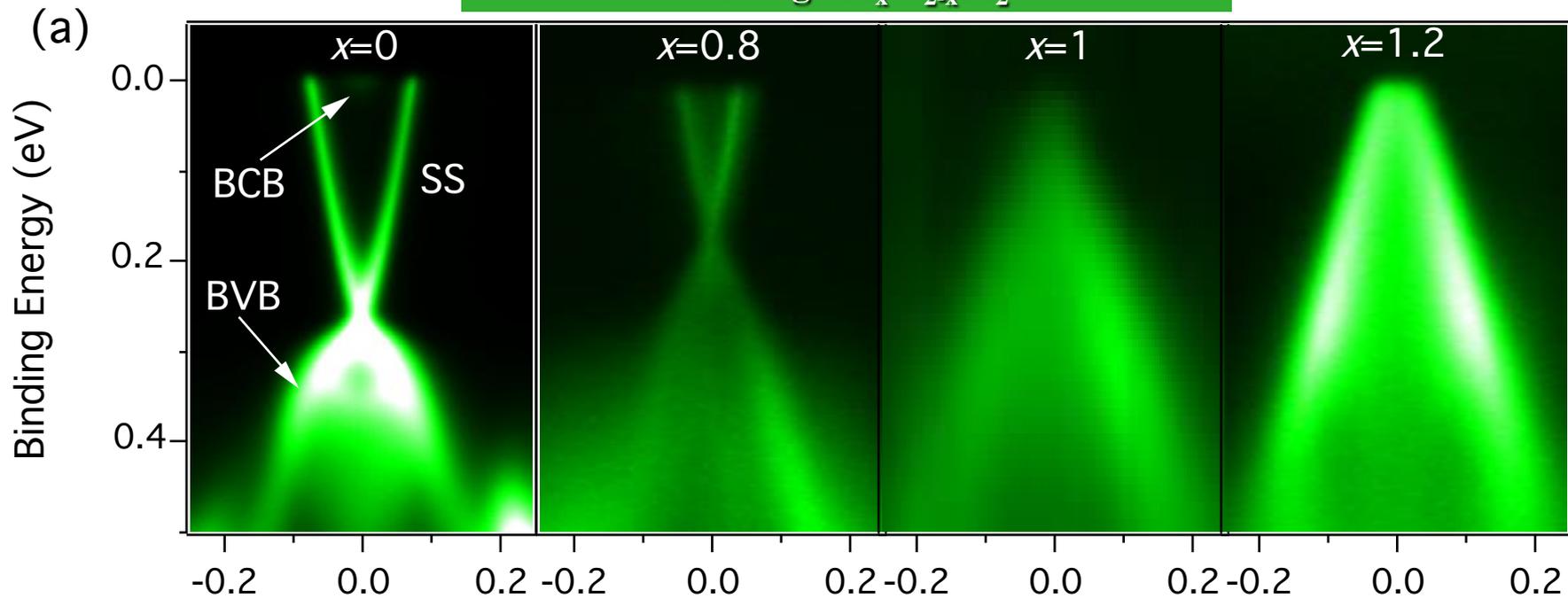
- Several new topological insulator classes
- Gaps up to ~ 0.35 eV
- New platforms to search for topological-superconductivity
- Single Dirac cone
- Bulk insulating nature

M. Neupane *et al.*, *Phys. Rev. B* **85**, 235406 (2012)

Also see Z. Ren *et al.*, *Phys. Rev. B (R)* **82**, 241306 (R) (2010)



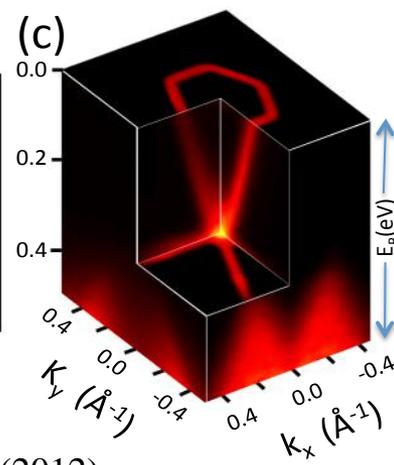
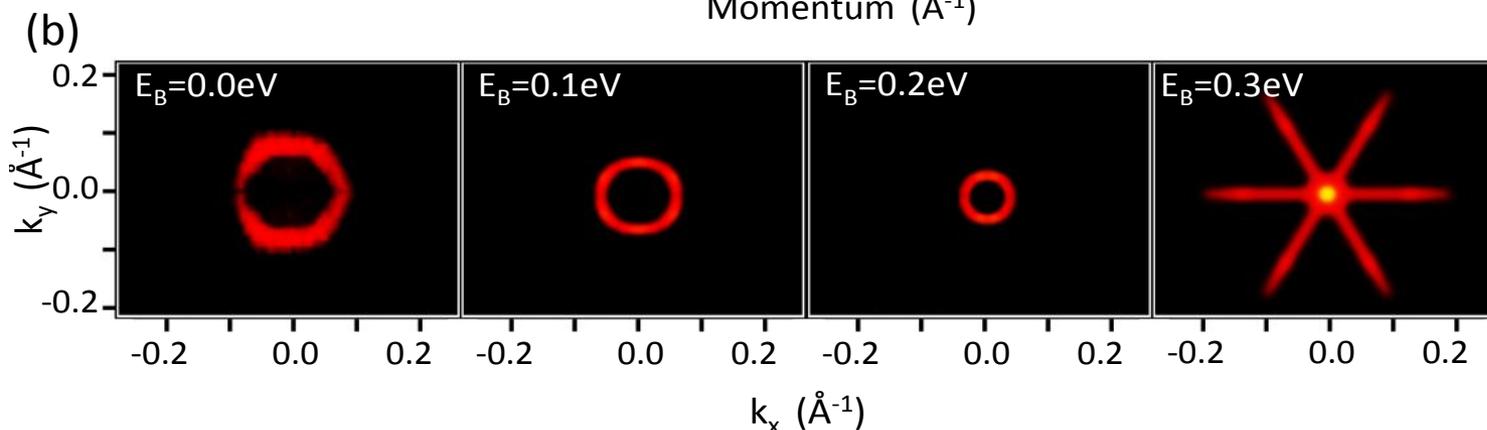
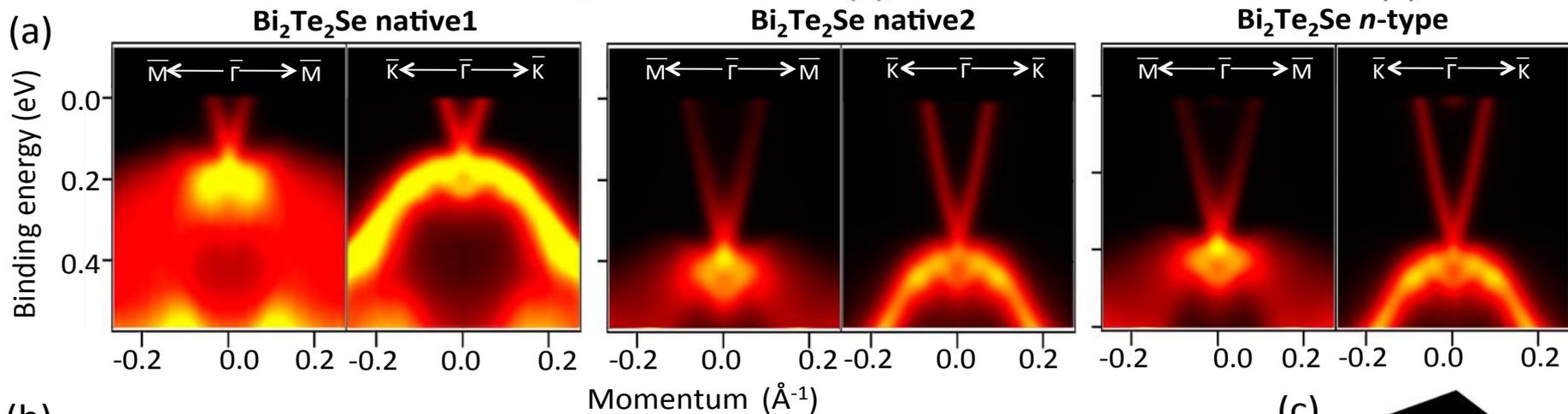
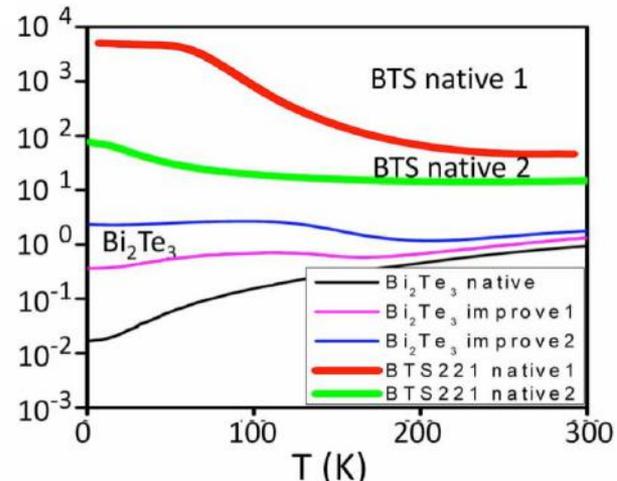
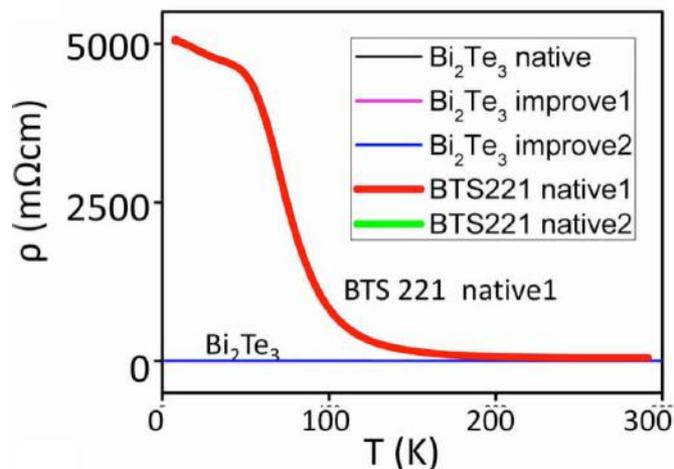
DP tuning: $\text{Sb}_x\text{Bi}_{2-x}\text{Se}_2\text{Te}$



M. Neupane *et al.*
Phys. Rev. B **85**,
 235406 (2012)

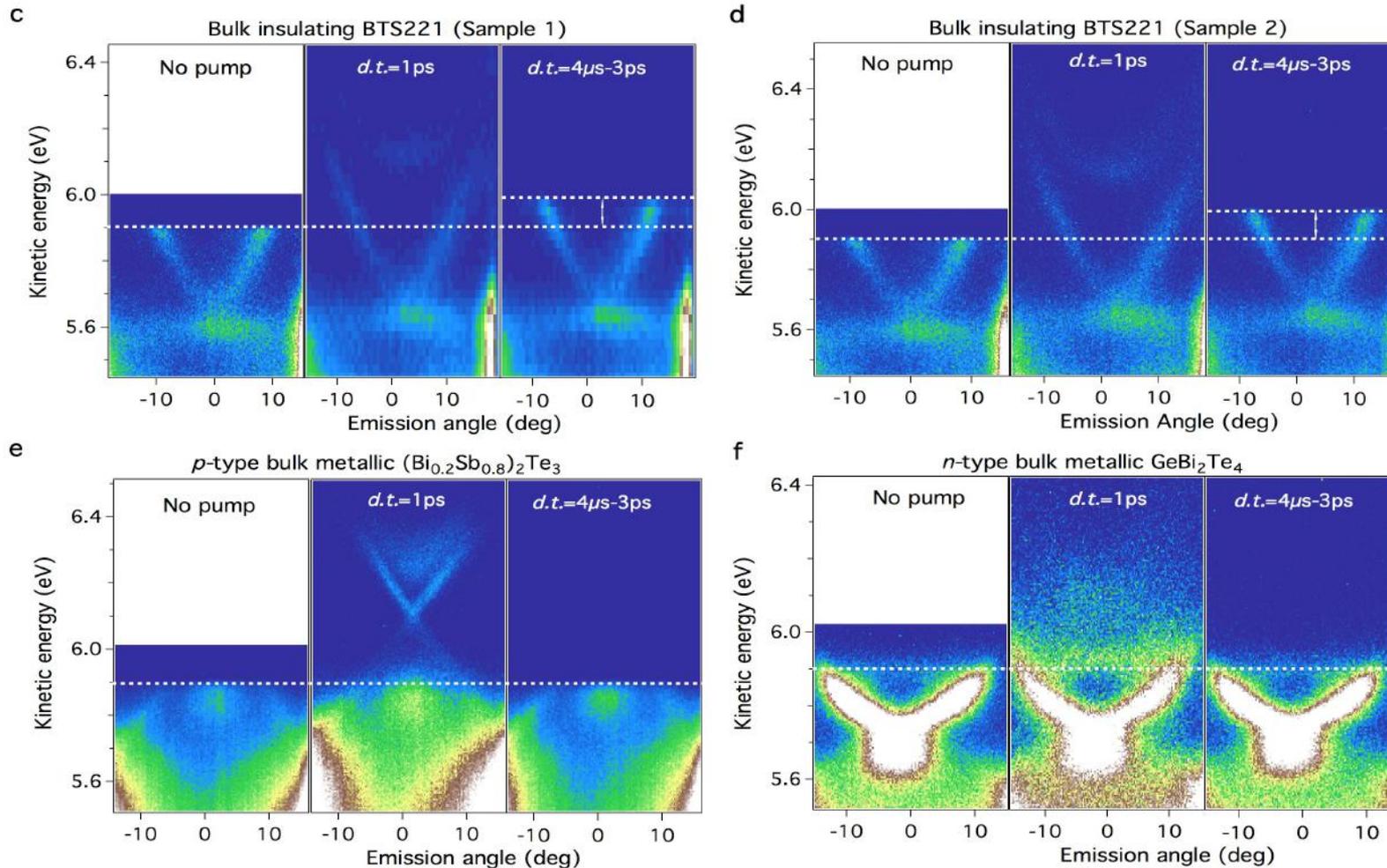
Highly bulk insulating TI

$\text{Bi}_2\text{Te}_2\text{Se}$



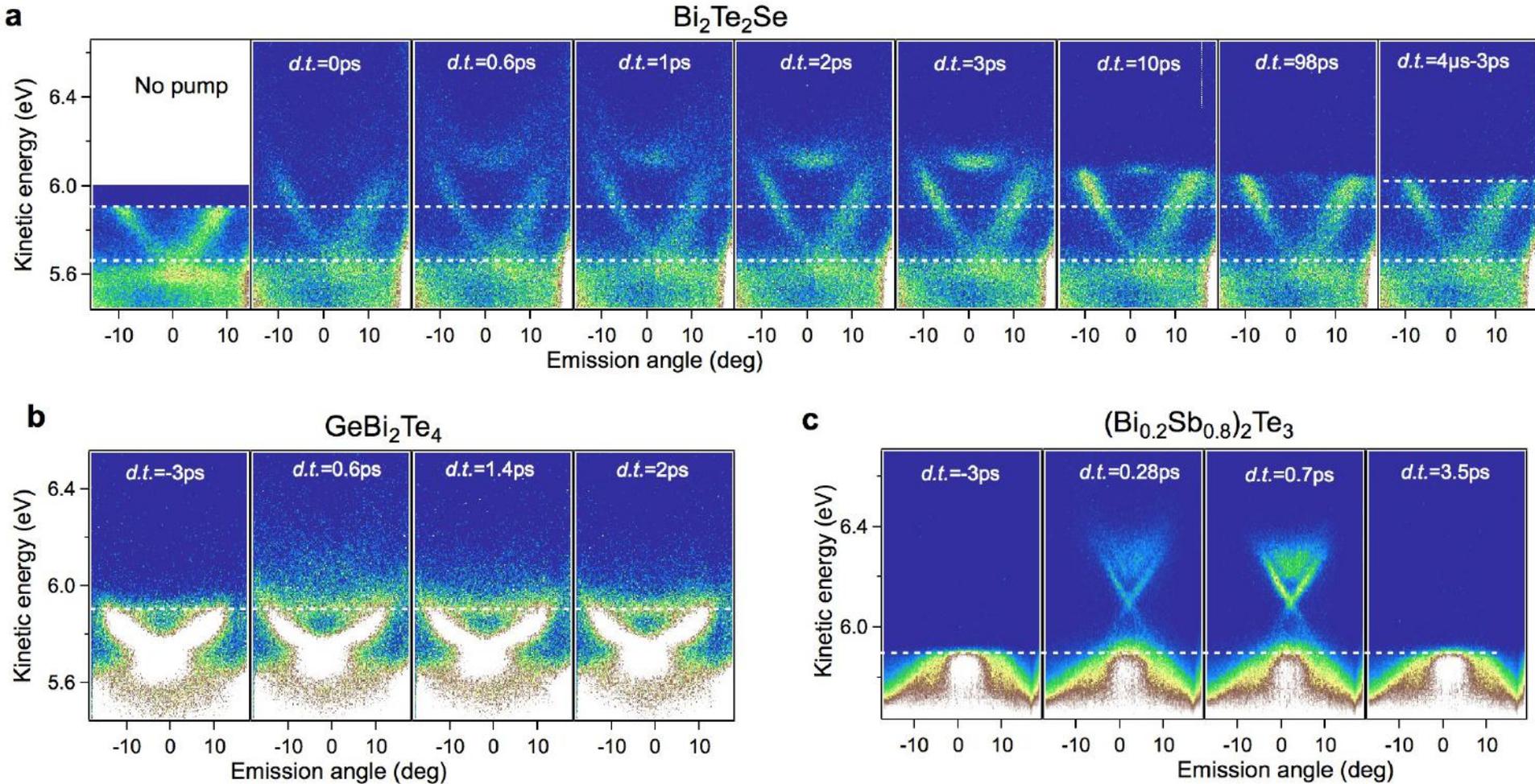
TrARPES on highly bulk insulating TI: $\text{Bi}_2\text{Te}_2\text{Se}$

Gigantic surface life-time of an intrinsic topological insulator



For binary TIs
ZX Shen group
Gedik group
Parmigiani group
Marsi group
Shin group

Time-resolved spectra: Bulk insulating vs bulk metallic



Time-resolved spectra: time evolution

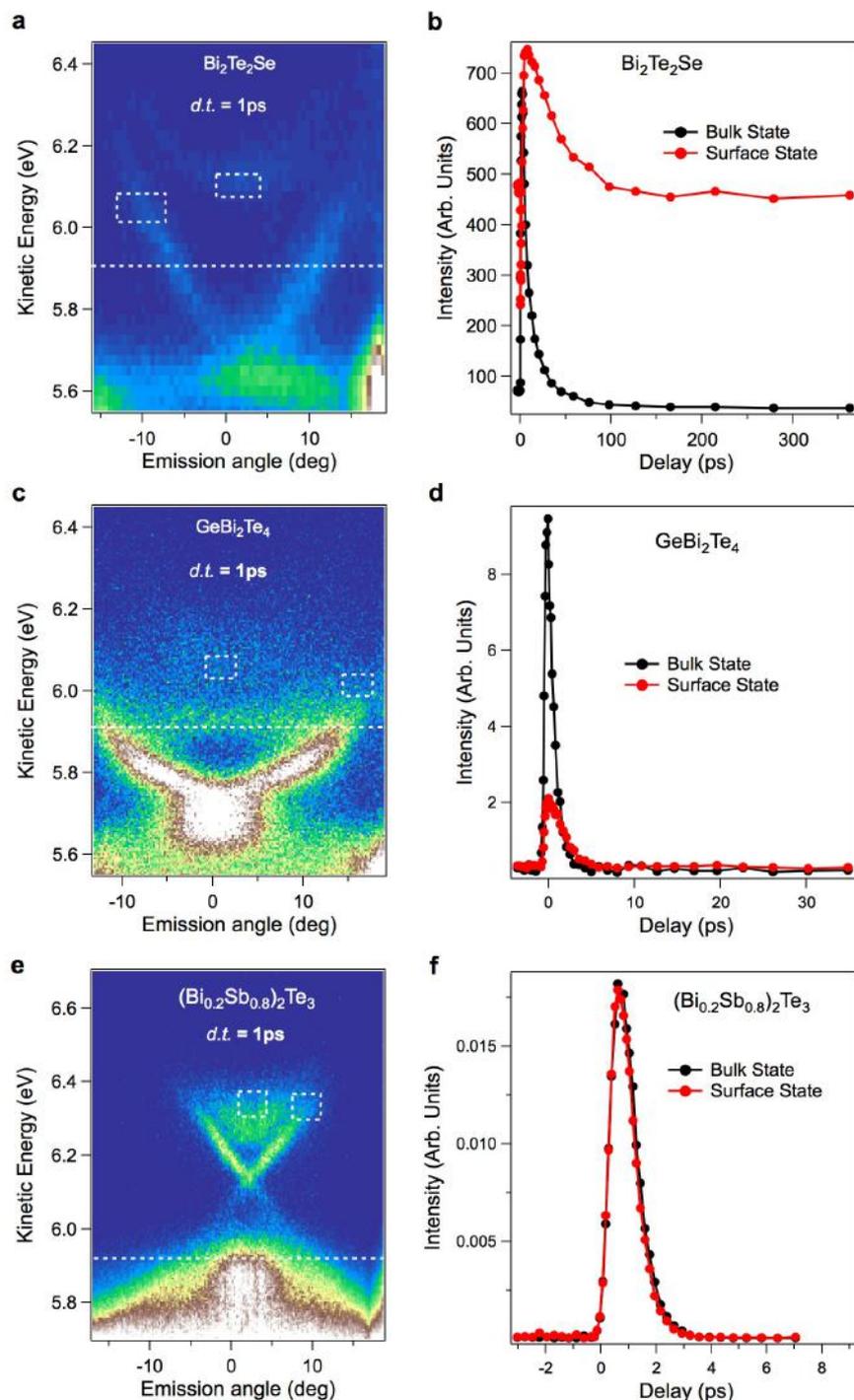
$\text{Bi}_2\text{Se}_3/\text{Bi}_2\text{Te}_3$ vs $\text{Bi}_2\text{Te}_2\text{Se}$

Bulk-metallic vs bulk-insulating TI

Pico-second vs Micro-second

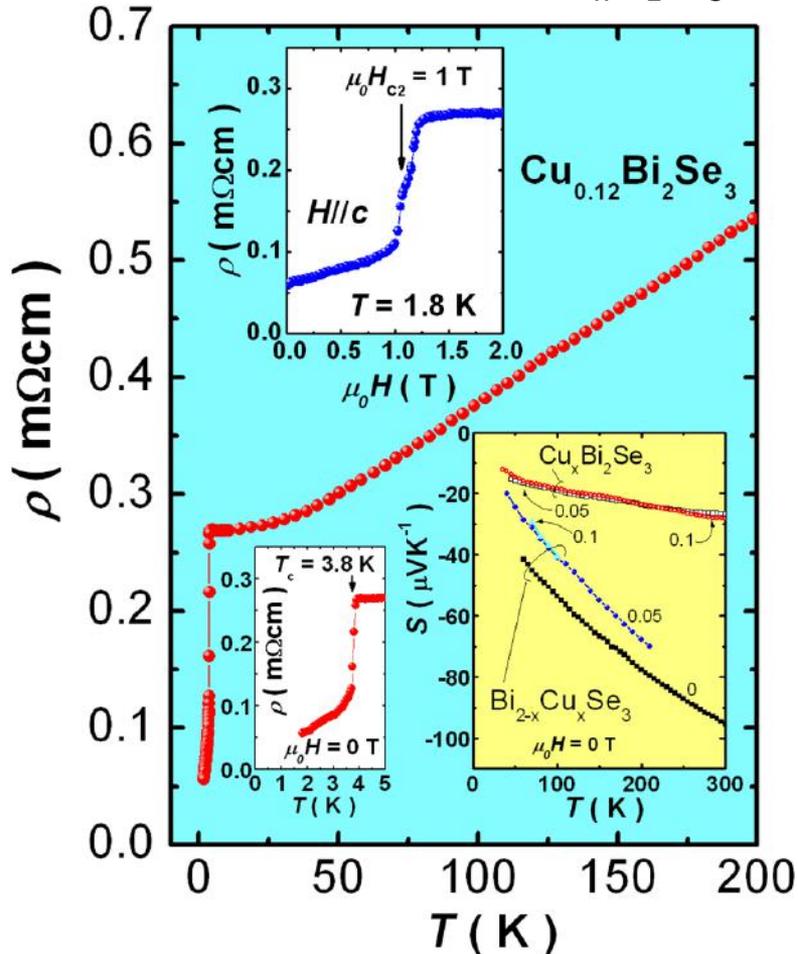
Absence (SPV) vs presence (SPV)

*Charge relaxation:
Exponential vs power law*

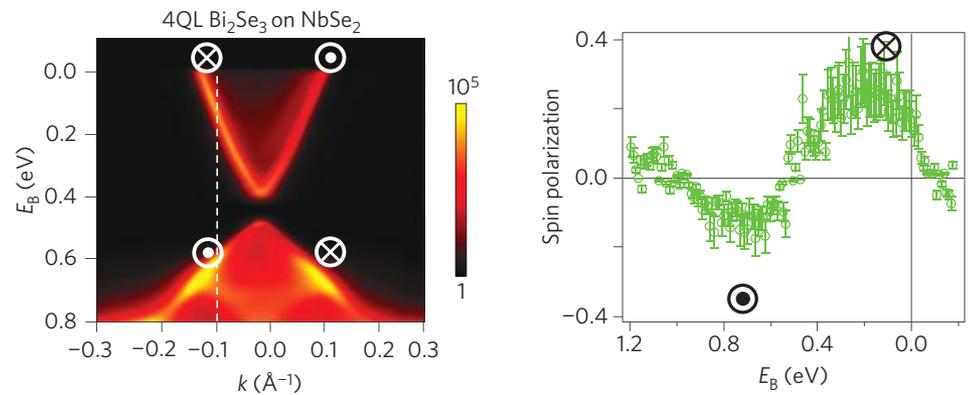
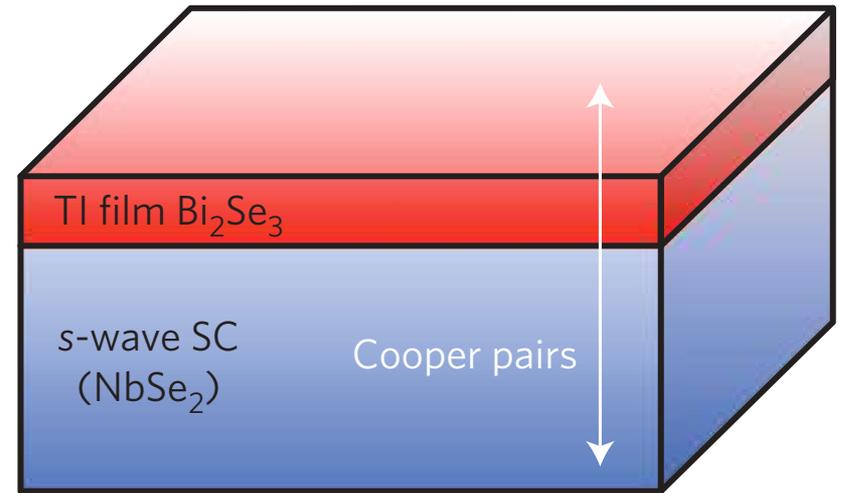


Relaxation dynamics in a superconducting topological insulator

Superconductivity in $\text{Cu}_x\text{Bi}_2\text{Se}_3$



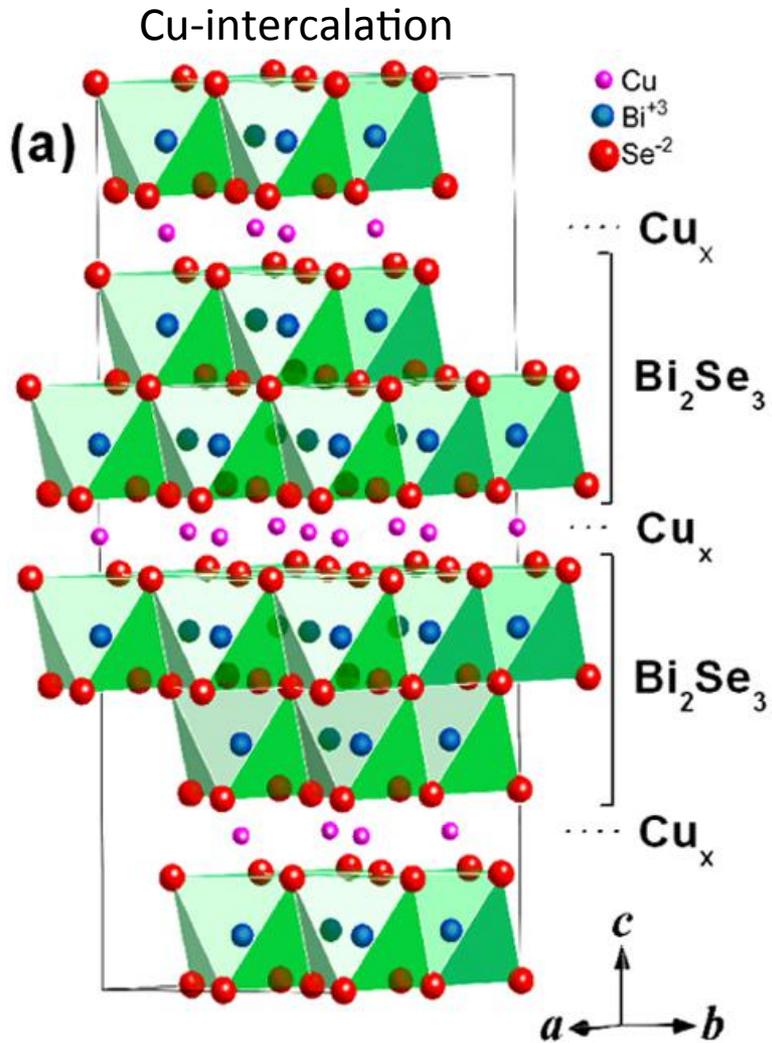
Proximity induced superconductivity



SY Xu *et al.*, *Nat. Phys.* **10**, 943 (2014)

Motivation:

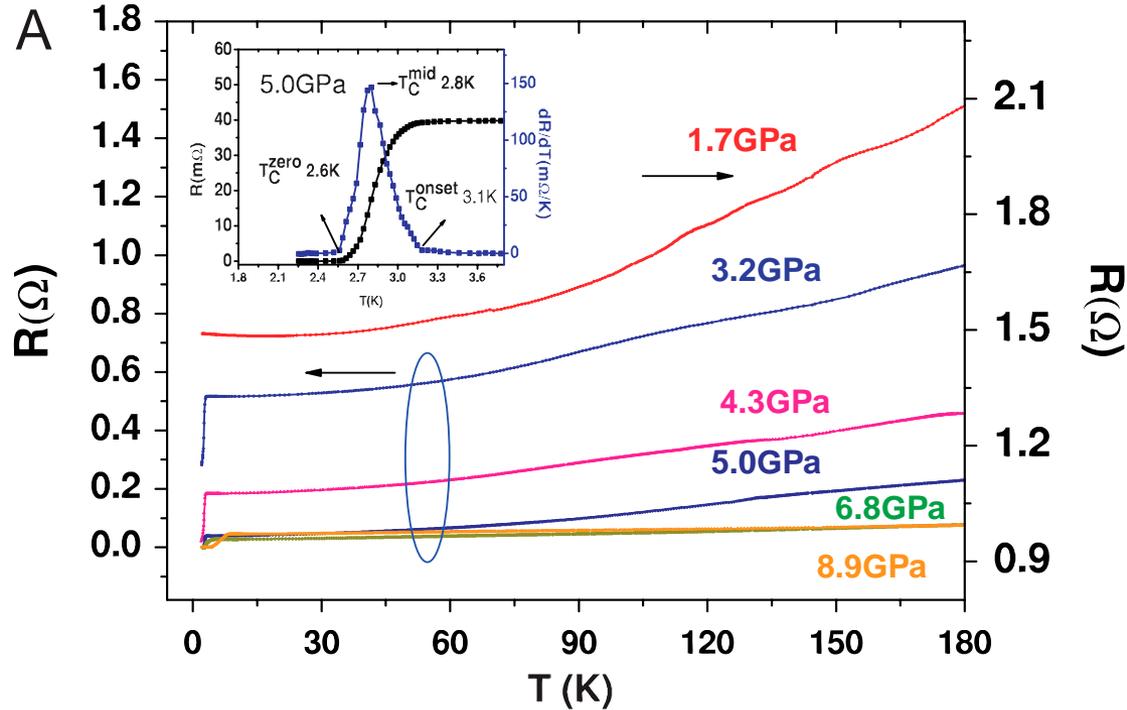
- Search for a bulk topological superconductor



Y.S. Hor *et al.*, *Phys. Rev. Lett.* 104, 05701 (2010).

Intercalation versus substitution

Pressured induced SC on Bi₂Te₃

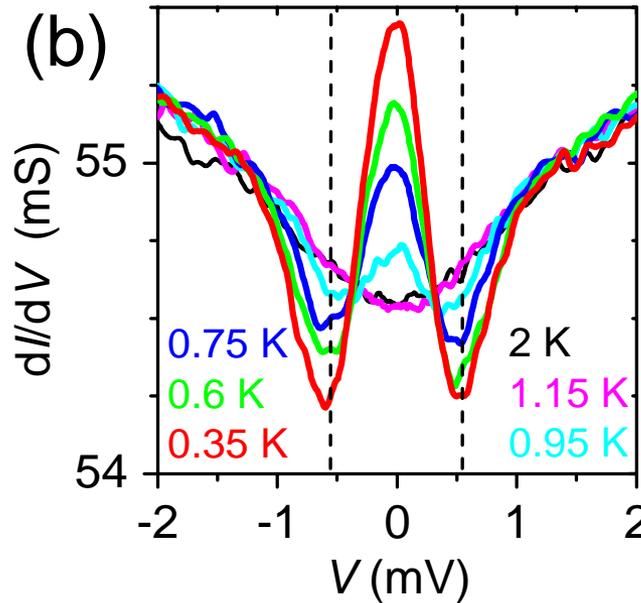
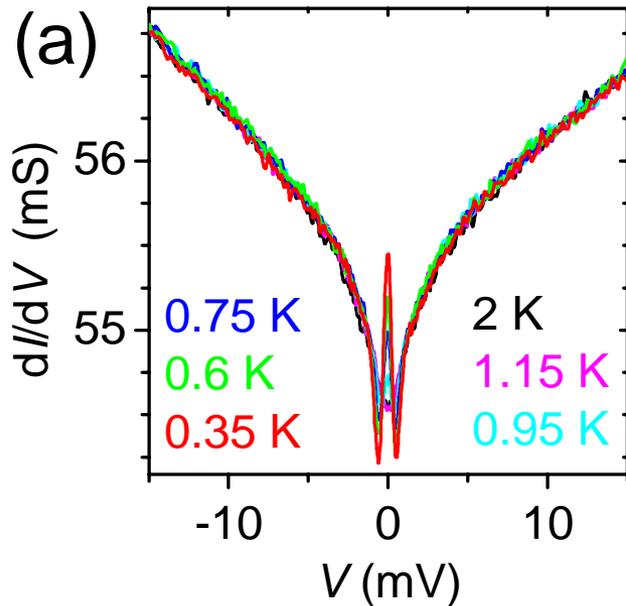


J. L. Zhang *et al.*, *Proc. Natl. Acad. Sci.* **108**, 24 (2011).

- No crystal structure phase transition
- $T_c \sim 3K$ between 3-6 GPa

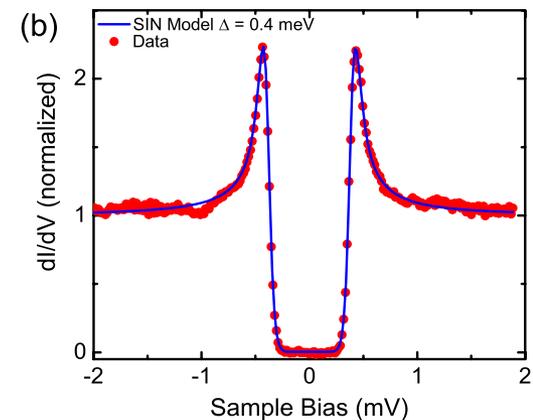
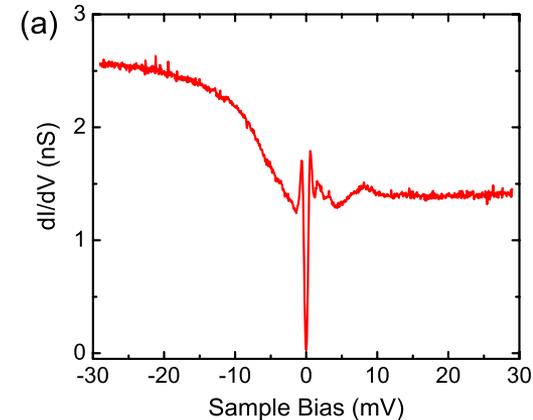
ZBP vs gap in $\text{Cu}_x\text{Bi}_2\text{Se}_3$

Zero-biased conductance peak $\text{Cu}_x\text{Bi}_2\text{Se}_3$ ($x=0.3$)



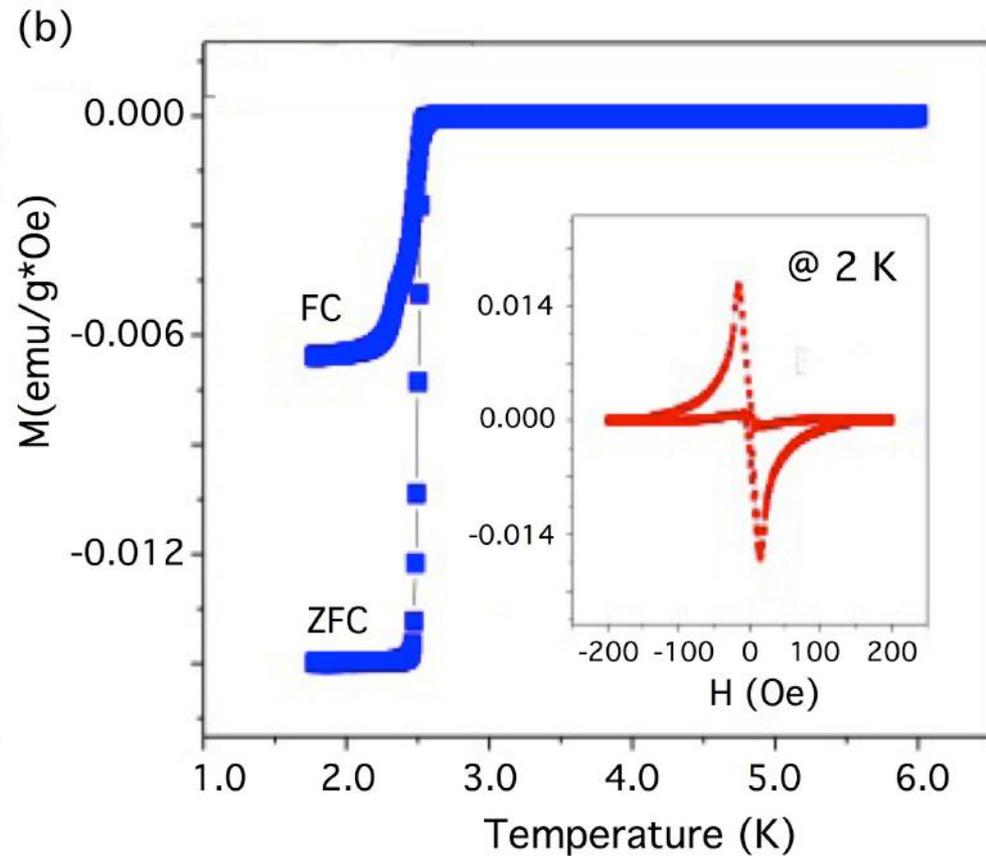
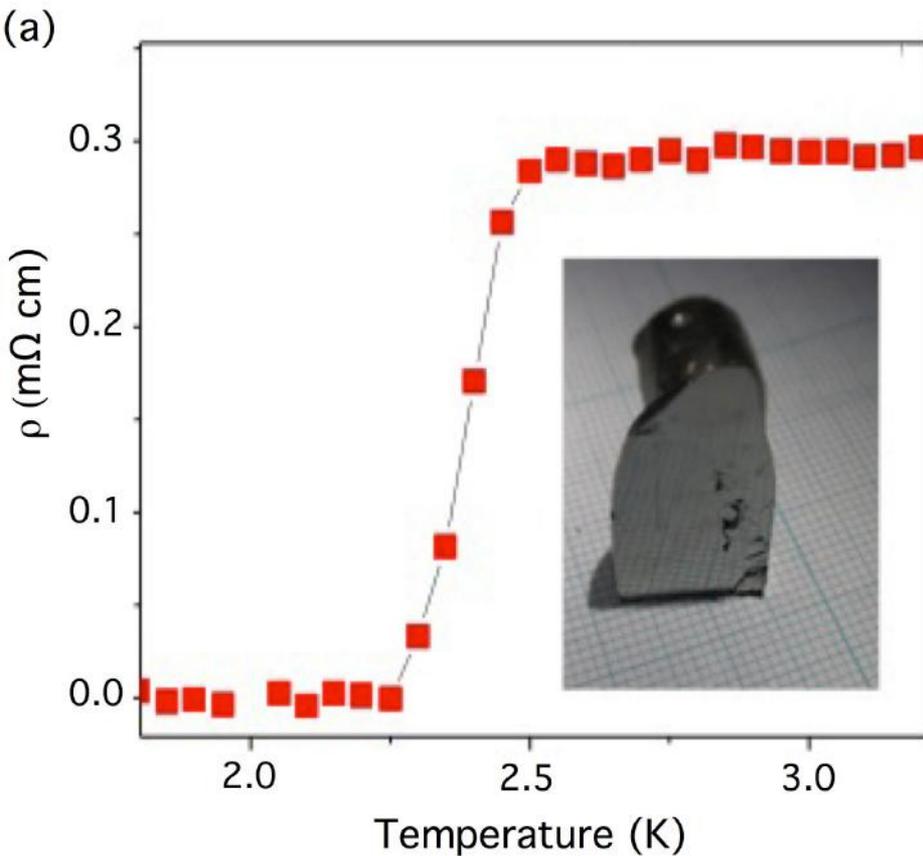
S. Sasaki et al., *Phys. Rev. Lett.* **107**, 217001 (2011).

s-wave pairing gap



N. Levy et al., *Phys. Rev. Lett.* **110**, 117001 (2013).

Search for better candidates for TSC continue?



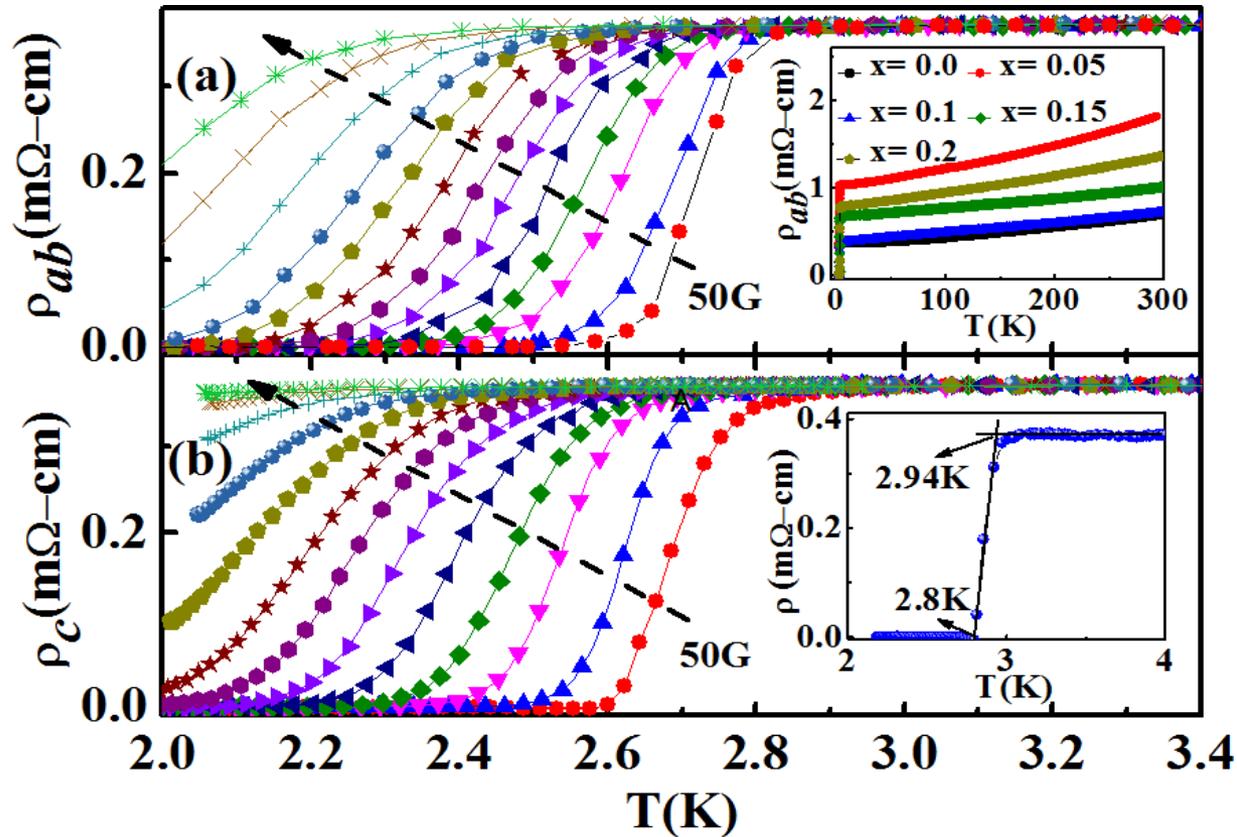
M. Neupane *et al.*, *Sci. Rep.* **6**, 22557 (2016)

- $T_c \sim 2.5$ K
- The shielding volume fraction at 0.5 K is about 90%.

Z. Liu *et al.*, *Jour. Ame., Che. Soc.* **137**, 10512 (2015)

Shruti *et al.*, arXiv:1505.05394v1 (2015)

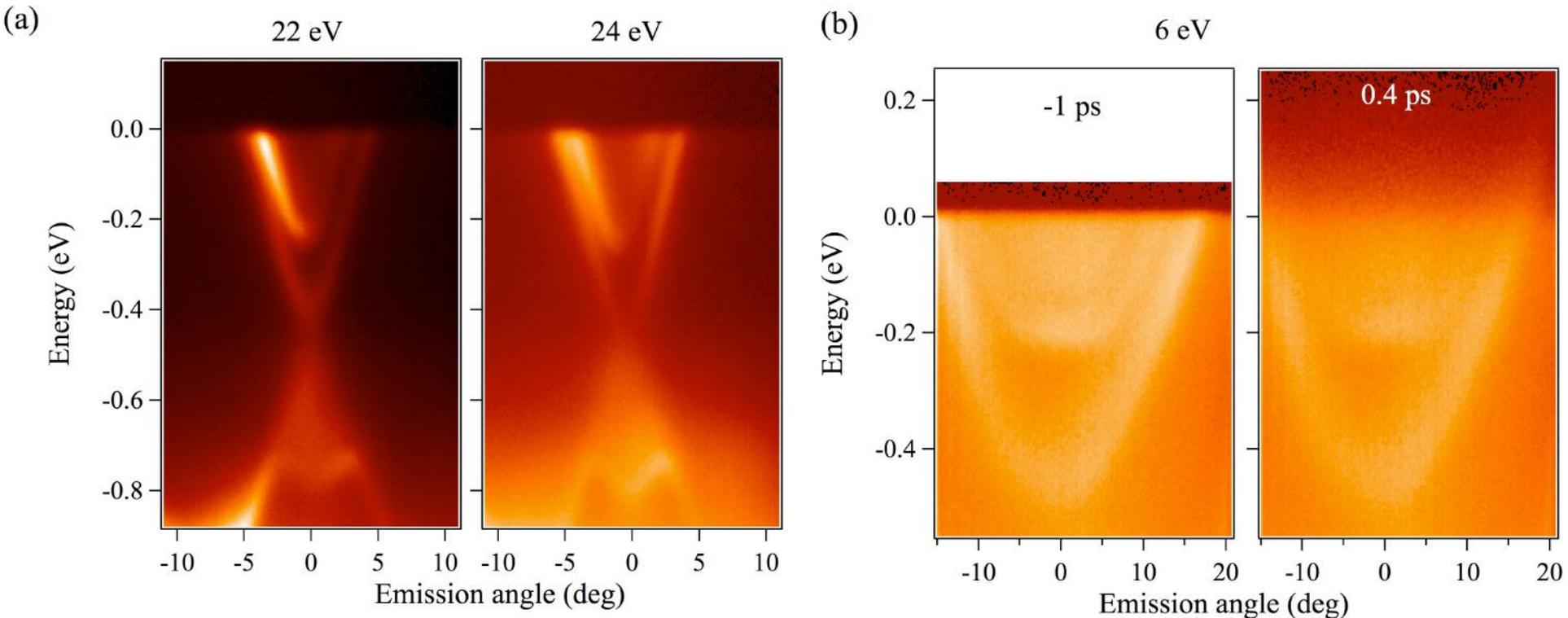
$T_c \sim 2.9$ K for $\text{Sr}_{0.1}\text{Bi}_2\text{Se}_3$



Shruti *et al.*, (2015)

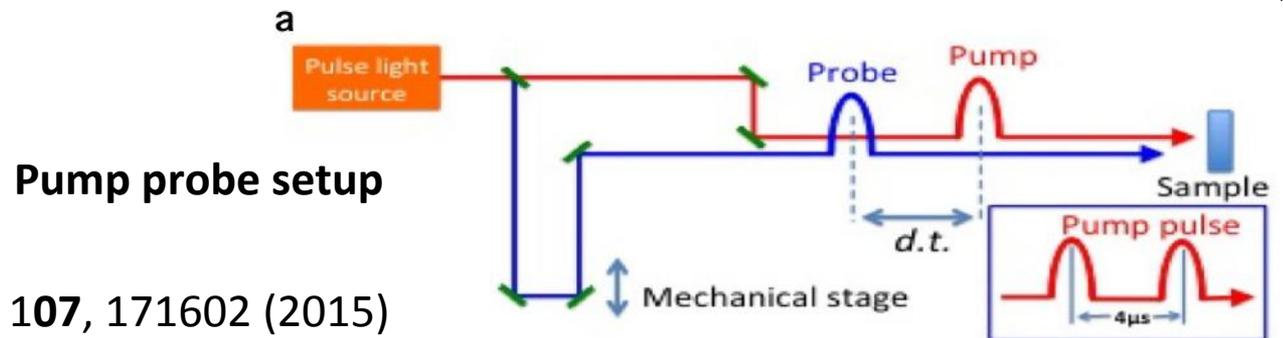
Figure 3. The resistivity as a function of magnetic field applied parallel to ab plane (a) and parallel to c -axis (b) is plotted for $\text{Sr}_{0.1}\text{Bi}_2\text{Se}_3$. External field $H = 0.005, 0.02, 0.05, 0.08, 0.11, 0.14, 0.17, 0.20, 0.24, 0.28, 0.34, 0.42$ and 0.50 T. ρ_c in (a) shows the resistivity behaviour from 2 K to 300 K. Inset in (a) shows the resistivity behaviour from 2 K to 300 K. Inset in (b) shows the expanded view of the superconducting transition.

ARPES dispersion maps of $\text{Sr}_{0.06}\text{Bi}_2\text{Se}_3$



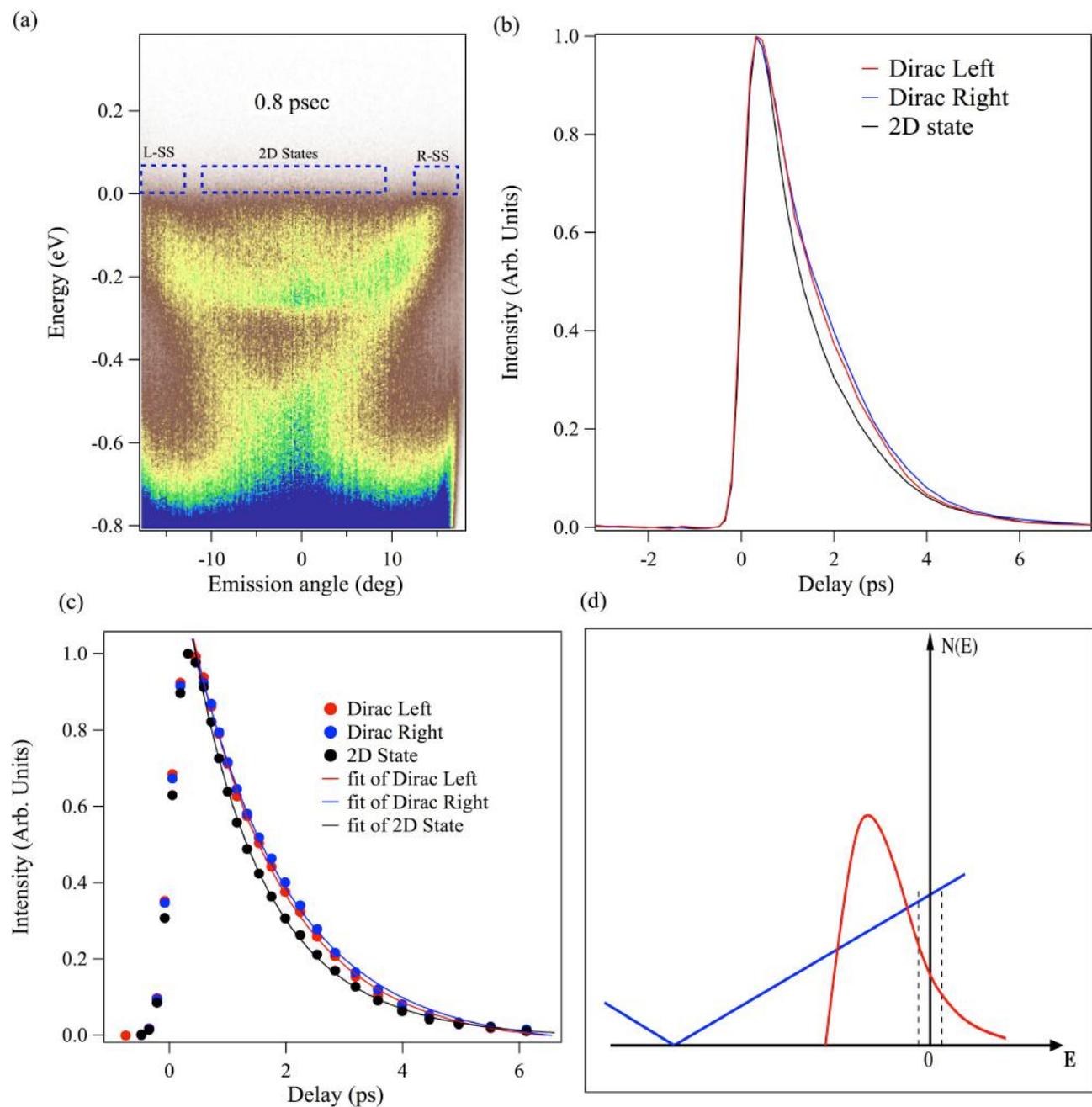
- Dirac point is located about 450 meV below the Fermi level.
- Coexistence of the topological surface states and a 2D states.
- 2D quantum well state is a generic property of the Sr intercalated topological insulator Bi_2Se_3 .

M. Neupane *et al.* (2016)



For normal ARPES, also see
C.Q. Han *et al.*, *Appl. Rev. Lett.* **107**, 171602 (2015)

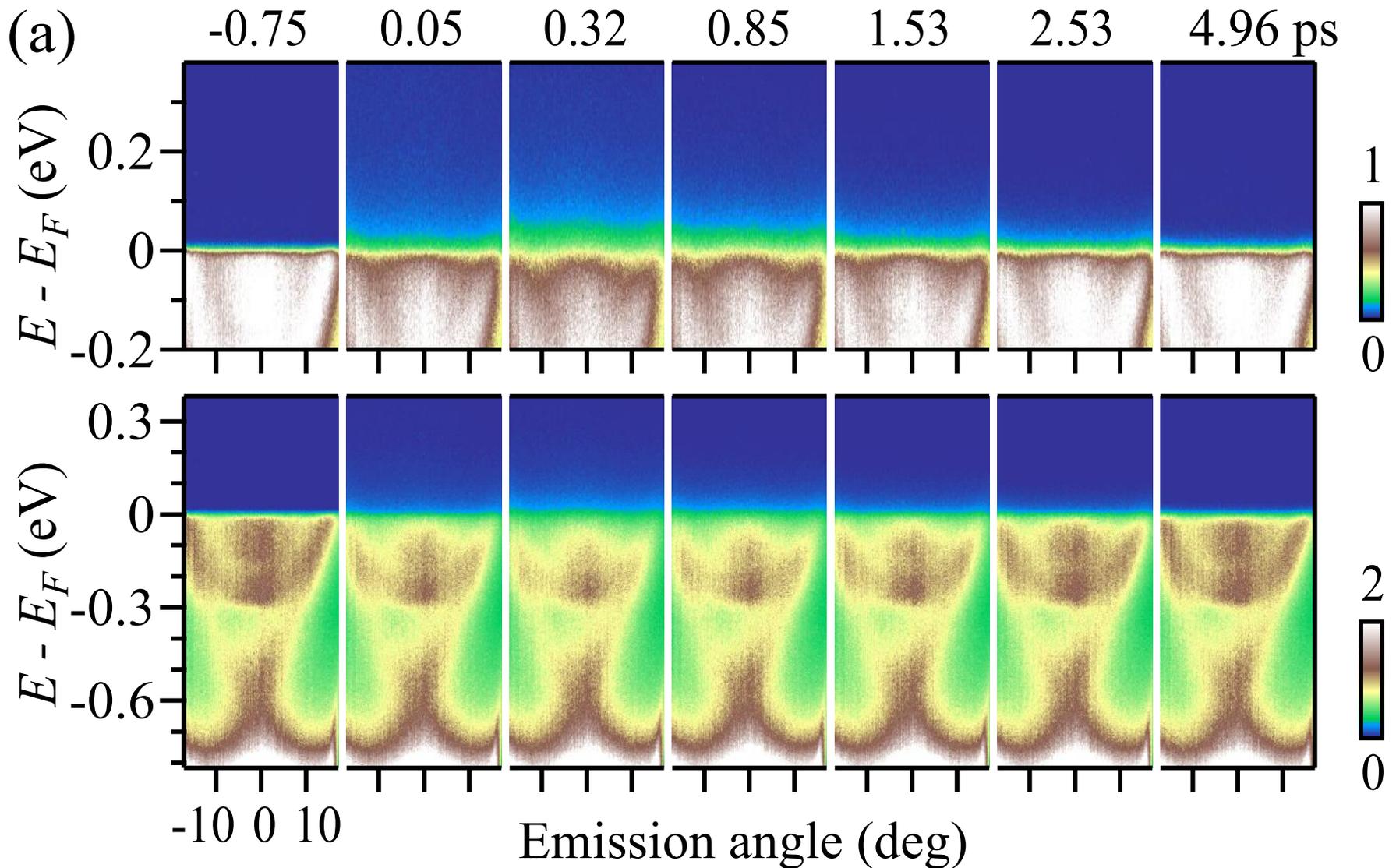
TR-ARPES result



- Both relax within 5 ps
- Different decay dynamics
- Short lifetime

Spread of the intensity into the unoccupied side is less pronounced

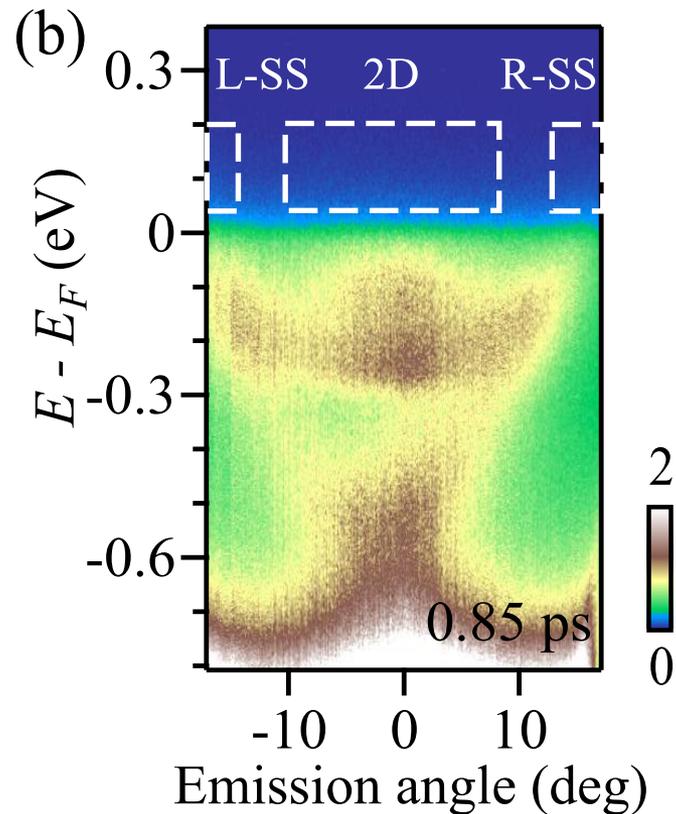
Carrier evolution



- Both (2D and TI SSs) relax within 5 ps
- Short lifetime
- Spread of the intensity into the unoccupied side is less pronounced (metallic)

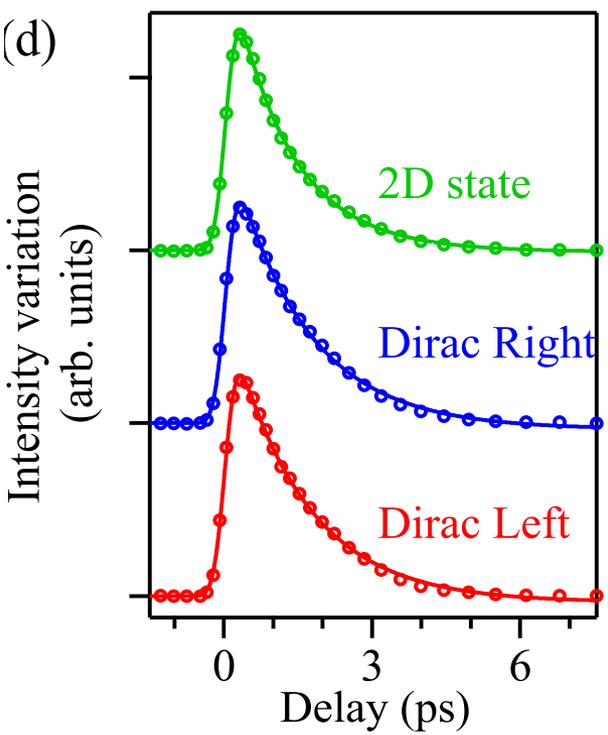
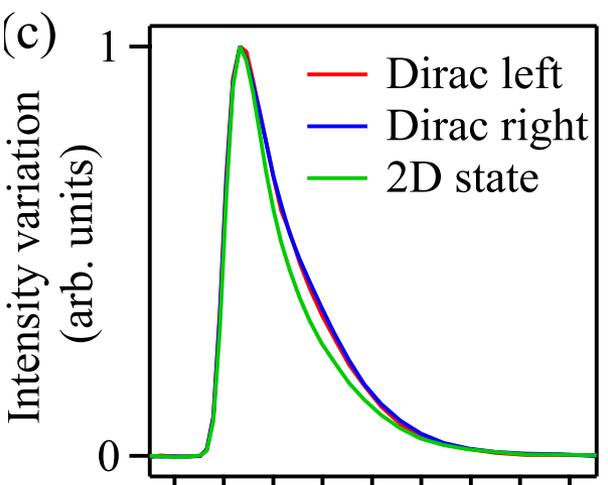
M. Neupane *et al.*, *Sci. Rep.* **6**, 22557 (2016)

Decay channels



Band	Decay constants (ps)	r^2	Amplitude (A)
L-SS	$\tau_1 = \tau_2 = 1.58$	0.99	A=1.382
R-SS	$\tau_1 = \tau_2 = 1.69$	0.99	A=1.347
2D state	$\tau_1 = 0.70$ and $\tau_2 = 1.46$	0.99	A1=0.33, A2=1.14

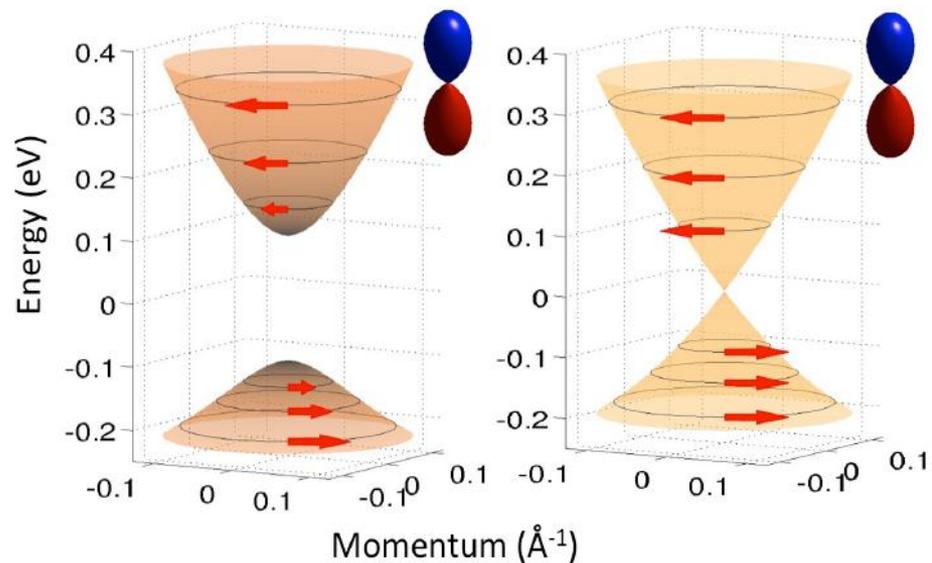
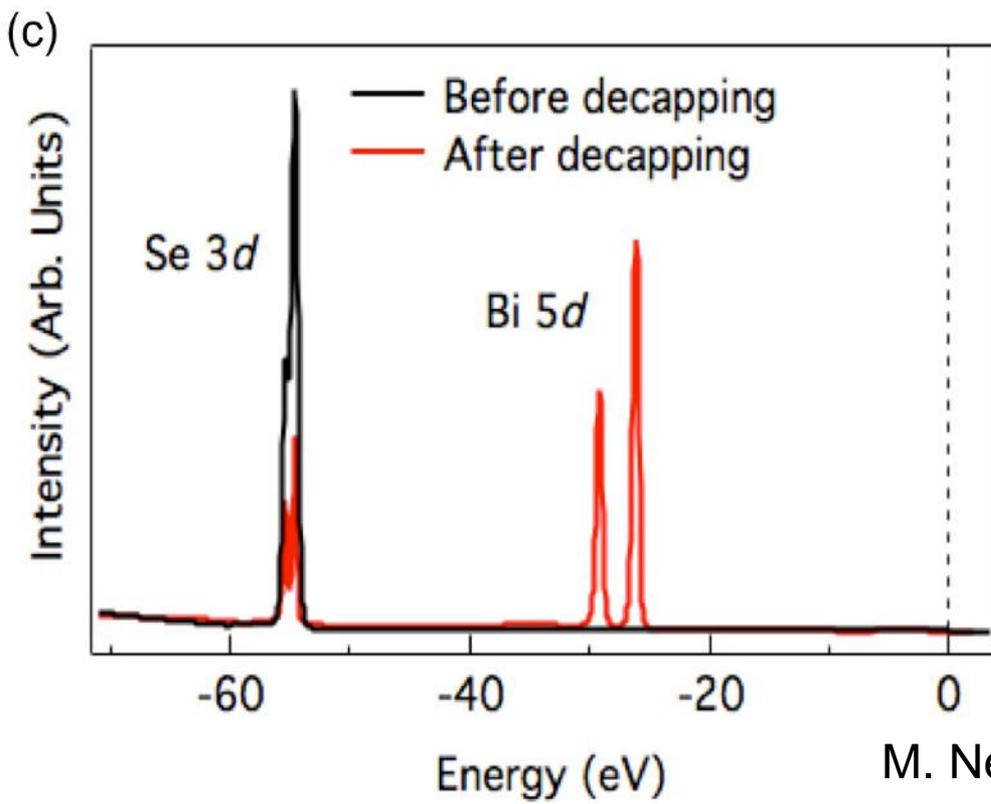
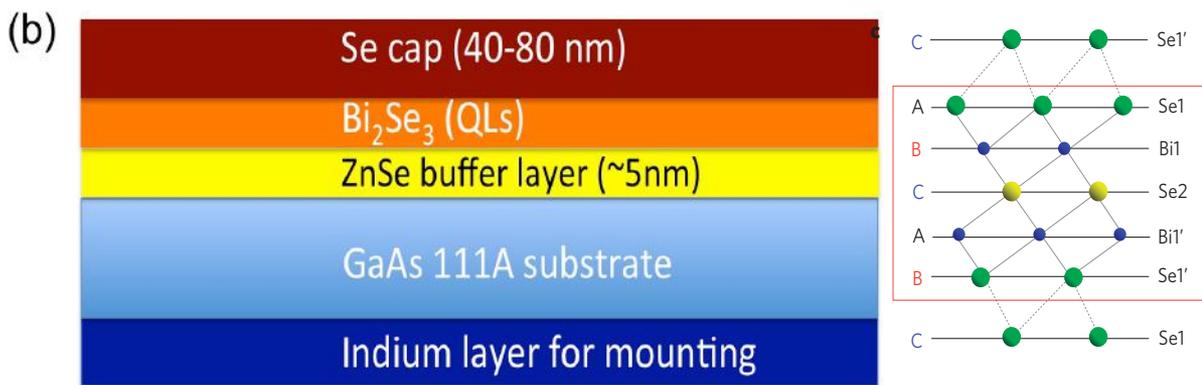
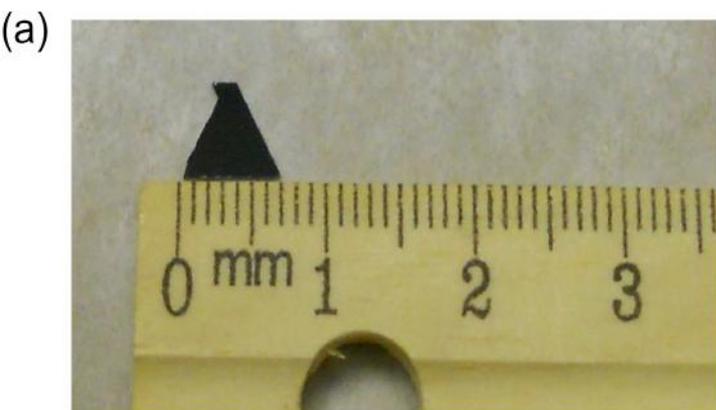
M. Neupane *et al.*, *Sci. Rep.* **6**, 22557 (2016)



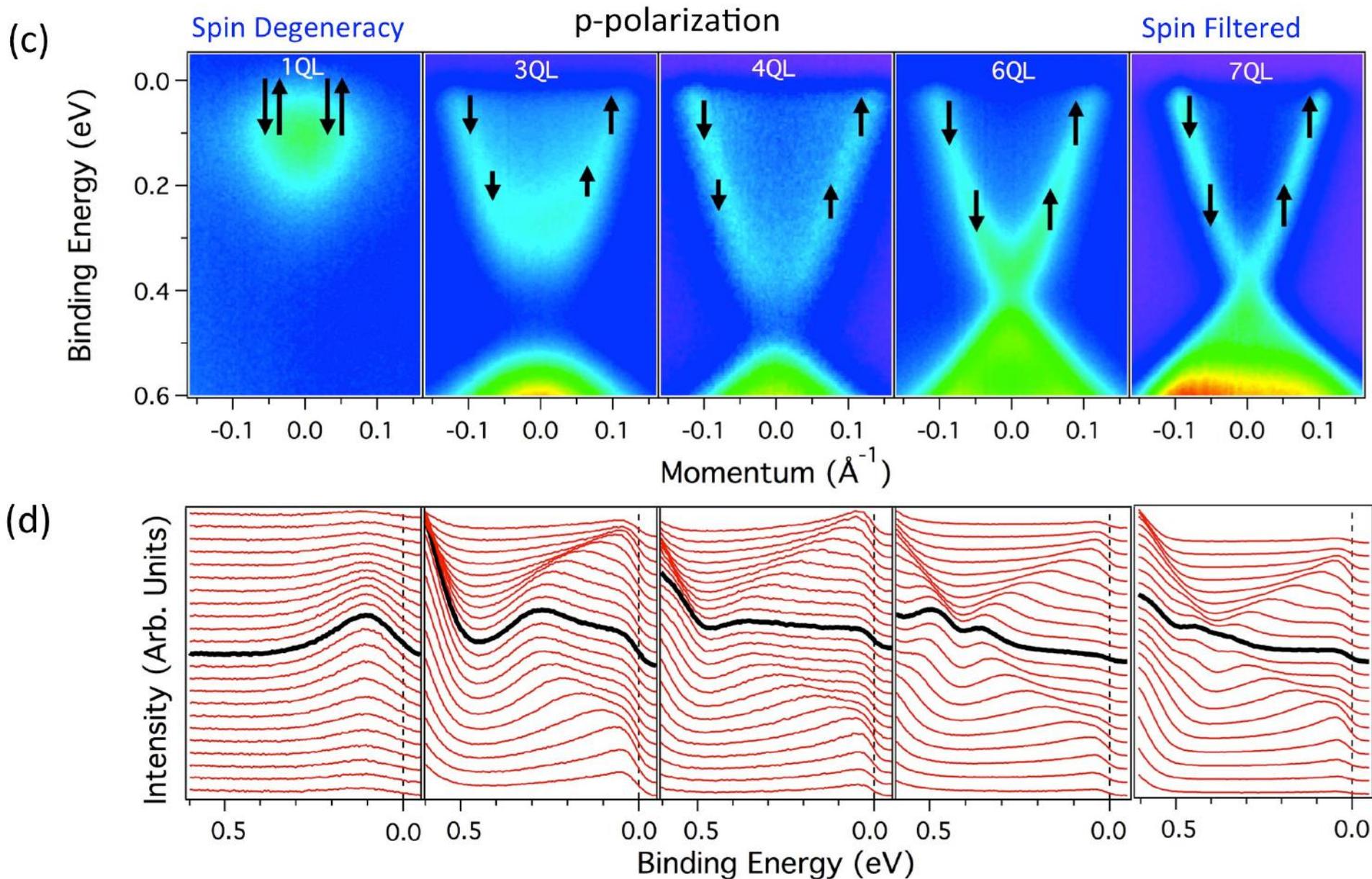
- Single and double exponential decay fitting functions
- TSS: single decay function; 2D states: double decay function

Thin films based TIs:

Ultrathin Bi_2Se_3 TI films



Quantum tunneling modulated spectra: ultrathin Bi_2Se_3 TI films



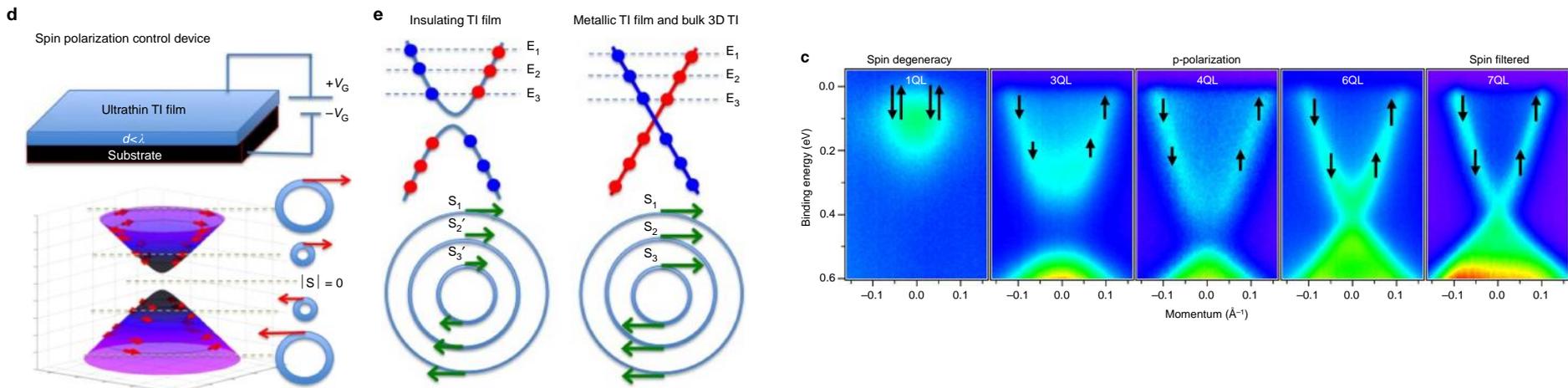
ARTICLE

Received 10 Nov 2013 | Accepted 9 Apr 2014 | Published 12 May 2014

DOI: 10.1038/ncomms4841

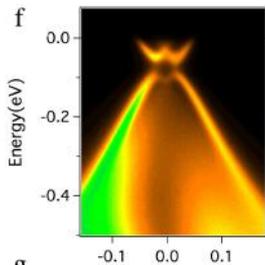
Observation of quantum-tunnelling-modulated spin texture in ultrathin topological insulator Bi_2Se_3 films

Madhab Neupane¹, Anthony Richardella², Jaime Sánchez-Barriga³, SuYang Xu¹, Nasser Alidoust¹, Ilya Belopolski¹, Chang Liu¹, Guang Bian¹, Duming Zhang², Dmitry Marchenko^{3,4}, Andrei Varykhalov³, Oliver Rader³, Mats Leandersson⁵, Thiagarajan Balasubramanian⁵, Tay-Rong Chang⁶, Horng-Tay Jeng^{6,7}, Susmita Basak⁸, Hsin Lin⁹, Arun Bansil⁸, Nitin Samarth² & M. Zahid Hasan^{1,10}



New topological phases beyond TIs

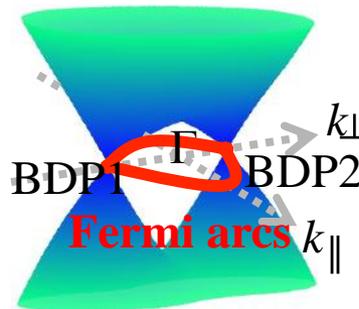
Topo. Crystalline Ins. (TCI)



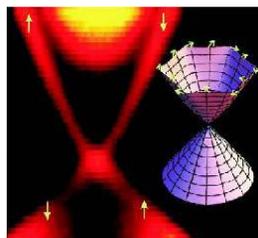
Protected by symmetries beyond TR-symm.?

Topo. Dirac & Weyl Semimetal

SOC does not open full bulk gap?
Topological semimetals?



TI

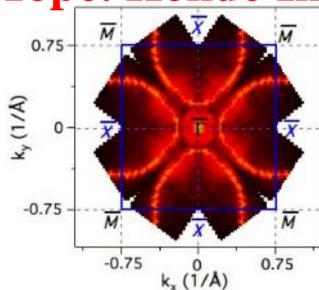


Bi₂Se₃

Superconductivity
Magnetism

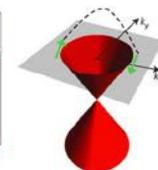
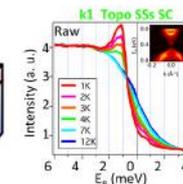
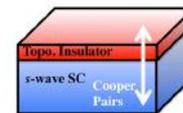
Interaction?

Topo. Kondo Ins. (TKI)



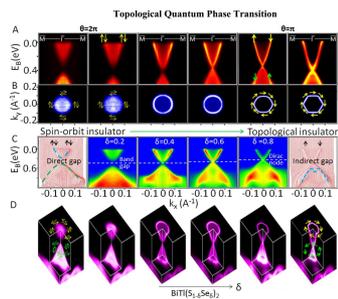
Topo. Superconductor (TSC) Mag. TI (MTI)

A Topological Superconductor



Trivial to TI
Band inversion

Topo. Phase Transition (TPT)



New topological phases beyond TIs

Topo. Kondo Ins.

Neupane, *et al.*, *Nature Commun.* **4**, 2991 (2013).

Neupane *et al.*, *PRL* (2015).

Correlated TI:

Neupane *et al.*, *PRL* (2015).

Neupane *et al.*, arXiv:1411.0302 (2014), in review

Topo. Dirac, Weyl & nodal Semimetal

Neupane *et al.*, *Nature Commun.* **5**, 4786 (2014).

Neupane *et al.*, *PRB (R)* (2015)

Topo. Phase Transition

Xu, Neupane *et al.*, *Nature Commun.* (2015).

Xu *et al.*, *Science* **332**, 560-564 (2011).

Topo. Crystalline Ins.

Neupane, *et al.*, *PRB* (2015); arXiv:1403.1560 (2014).

Xu, Liu, Neupane *et al.*, *Nature Commun.* **3**, 1192 (2012).

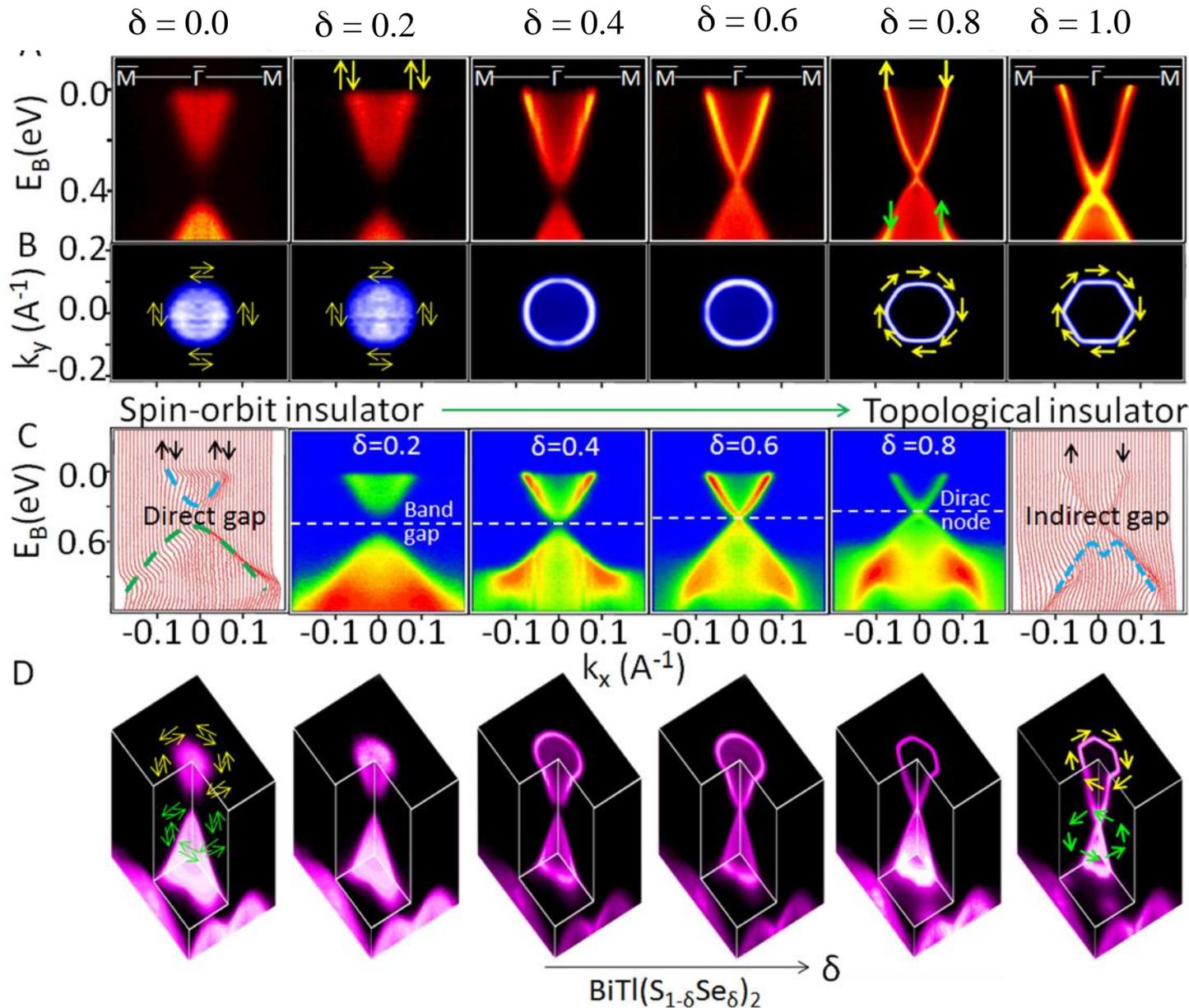
TSC and MTI

Xu...Neupane *et al.*, *Nature Phys.* doi:10.1038/nphys3139 (2014).

Xu, Neupane *et al.*, *Nature Phys.* **8**, 616-622 (2012).

Topological Dirac semimetals

Band inversion and topological phase transition in $\text{BiTl}(\text{S}_{1-\delta}\text{Se}_\delta)_2$



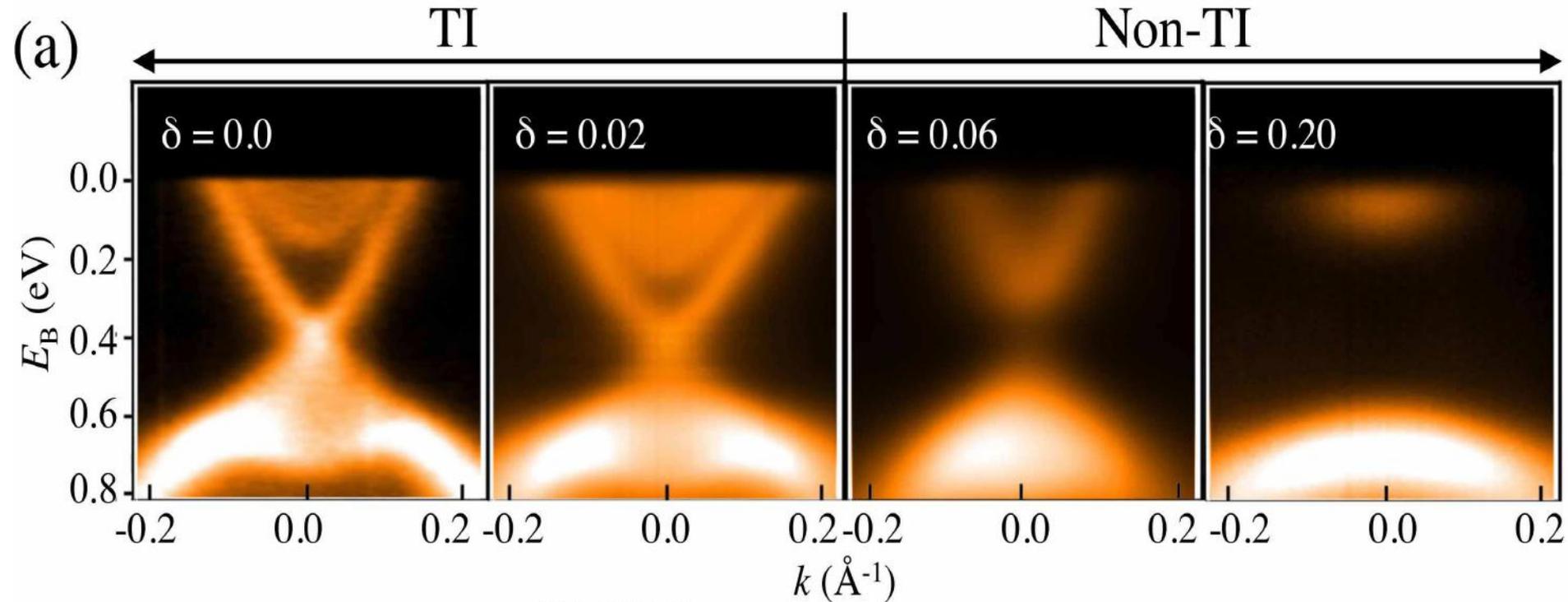
Band inversion happens at $\delta \sim 0.5$;

Fermi gas \rightarrow Dirac gas;

Spin degenerate \rightarrow spin-momentum locked

Topological phase transition in $(\text{Bi}_{1-\delta}\text{In}_\delta)_2\text{Se}_3$

$(\text{Bi}_{1-\delta}\text{In}_\delta)_2\text{Se}_3 - \delta_c \sim 0.04$



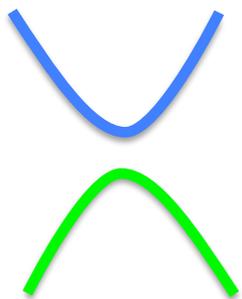
- Requires fine-tuning of the chemical doping
- Introduces chemical disorder into the system

The search for TBDS phase in stoichiometric materials continues ----

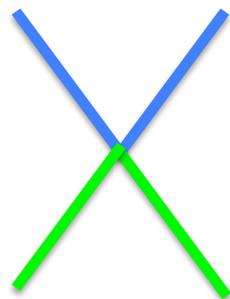
M. Brahlek, ... M. Neupane, M. Z. Hasan, *Phys. Rev. Lett.* 109, 186403 (2012)

Topological Dirac semimetals

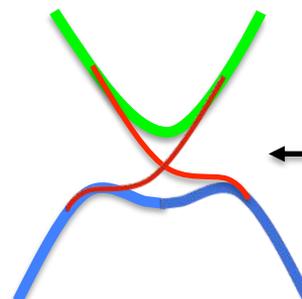
Band inversion in $\text{BiTl}(\text{S}_{1-\delta}\text{Se}_\delta)_2$



Trivial
insulator

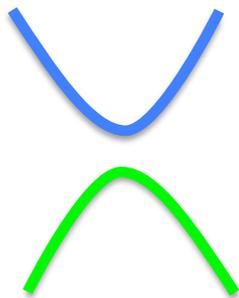


3D Dirac at the band
inversion critical xc

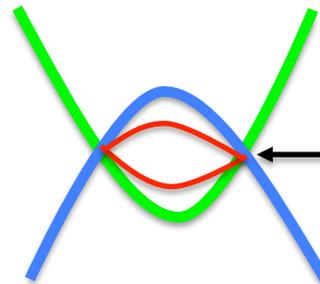
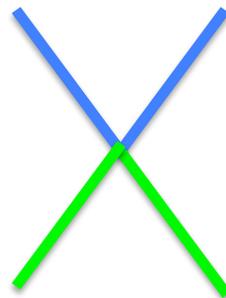


Topological
insulator

Topo. Dirac Semimetal



Trivial
insulator

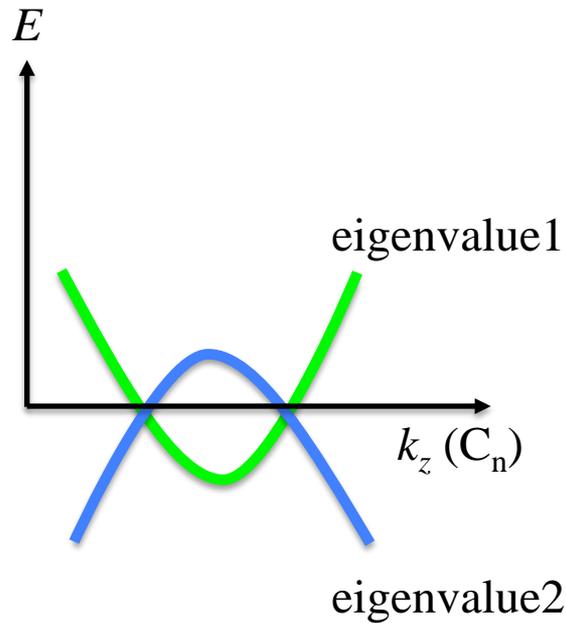
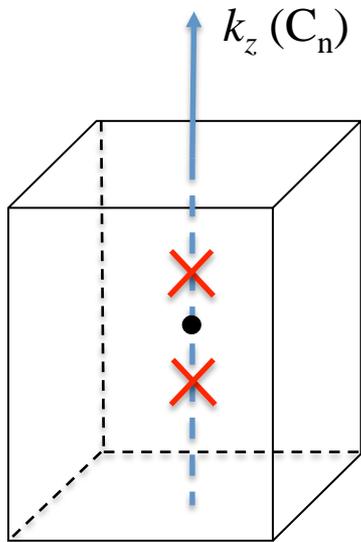


3D Dirac nodes
protected by C_n

SOC

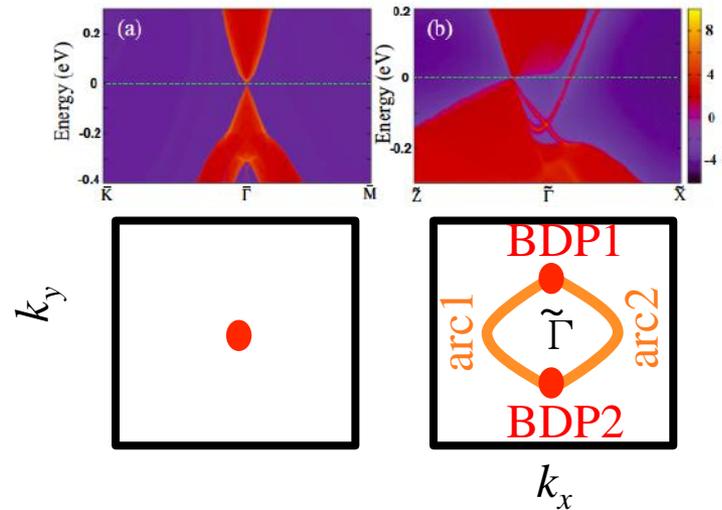
TDSM states protected by uniaxial rotational symmetries

Cd_3As_2



Top surface

Side surface

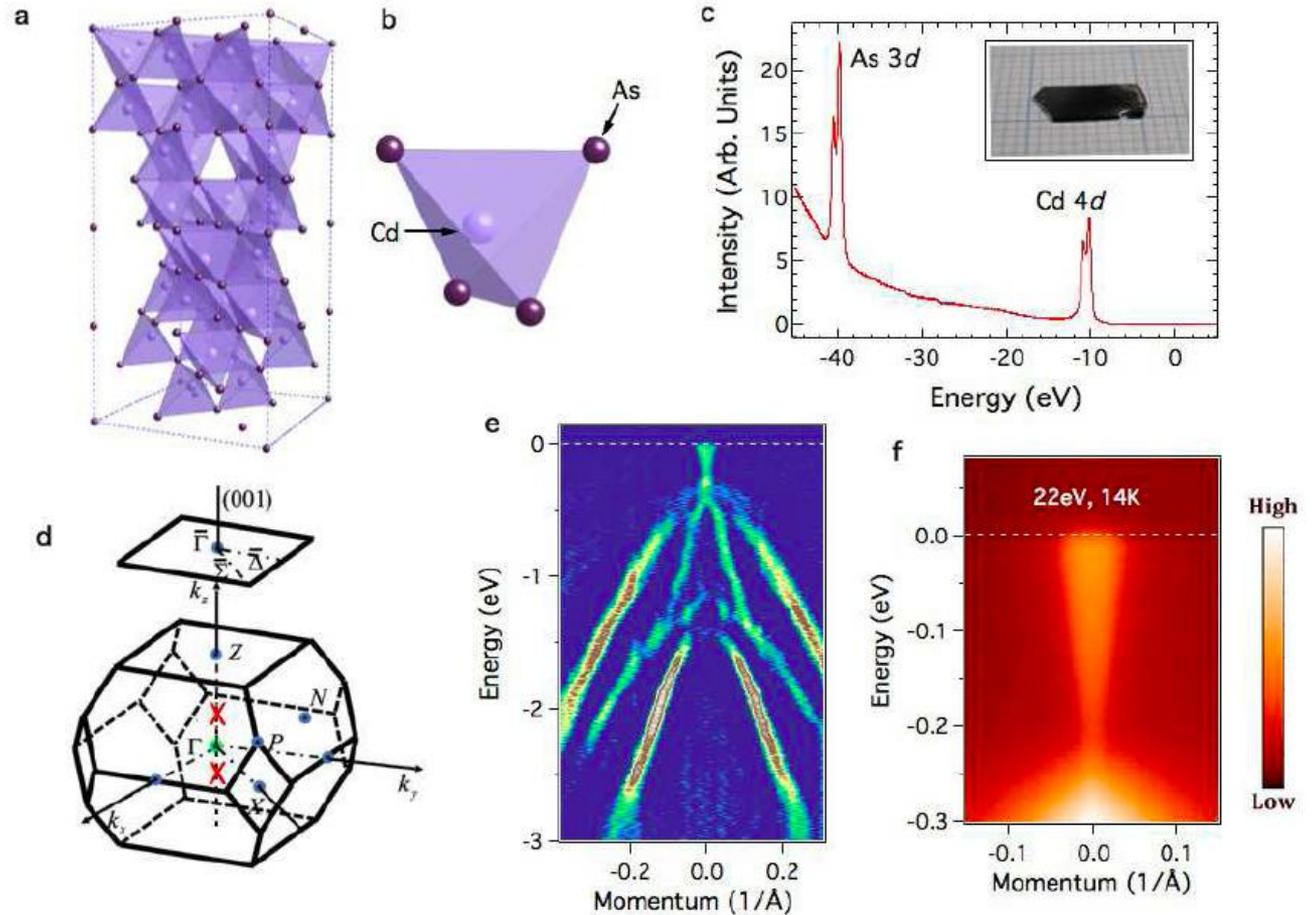
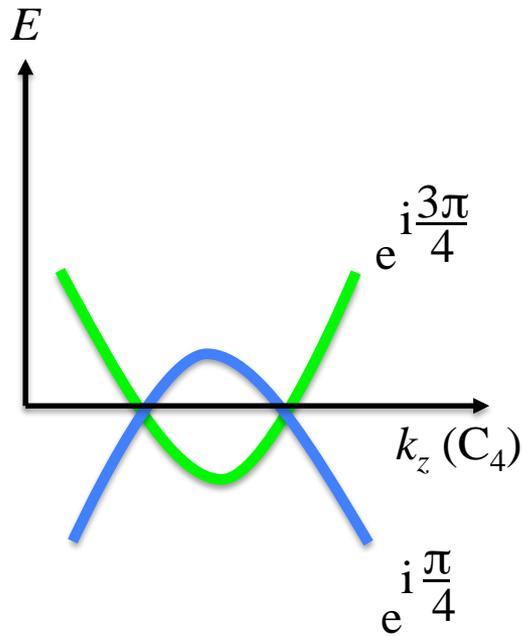


Wang *et al.*, *Phys. Rev. B* **85**, 195320 (2010)

For Na_3Bi , Z. Wang *et al.*, *Phys. Rev. B* **95**, 195320 (2011)

TDSM state in high mobility Cd_3As_2

3D analog of graphene



For Na_3Bi :

Z. Wang *et al.*, *Phys. Rev. B* **95**, 195320 (2011)

Z.K. Liu *et al.*, *Science* **343**, 864 (2014)

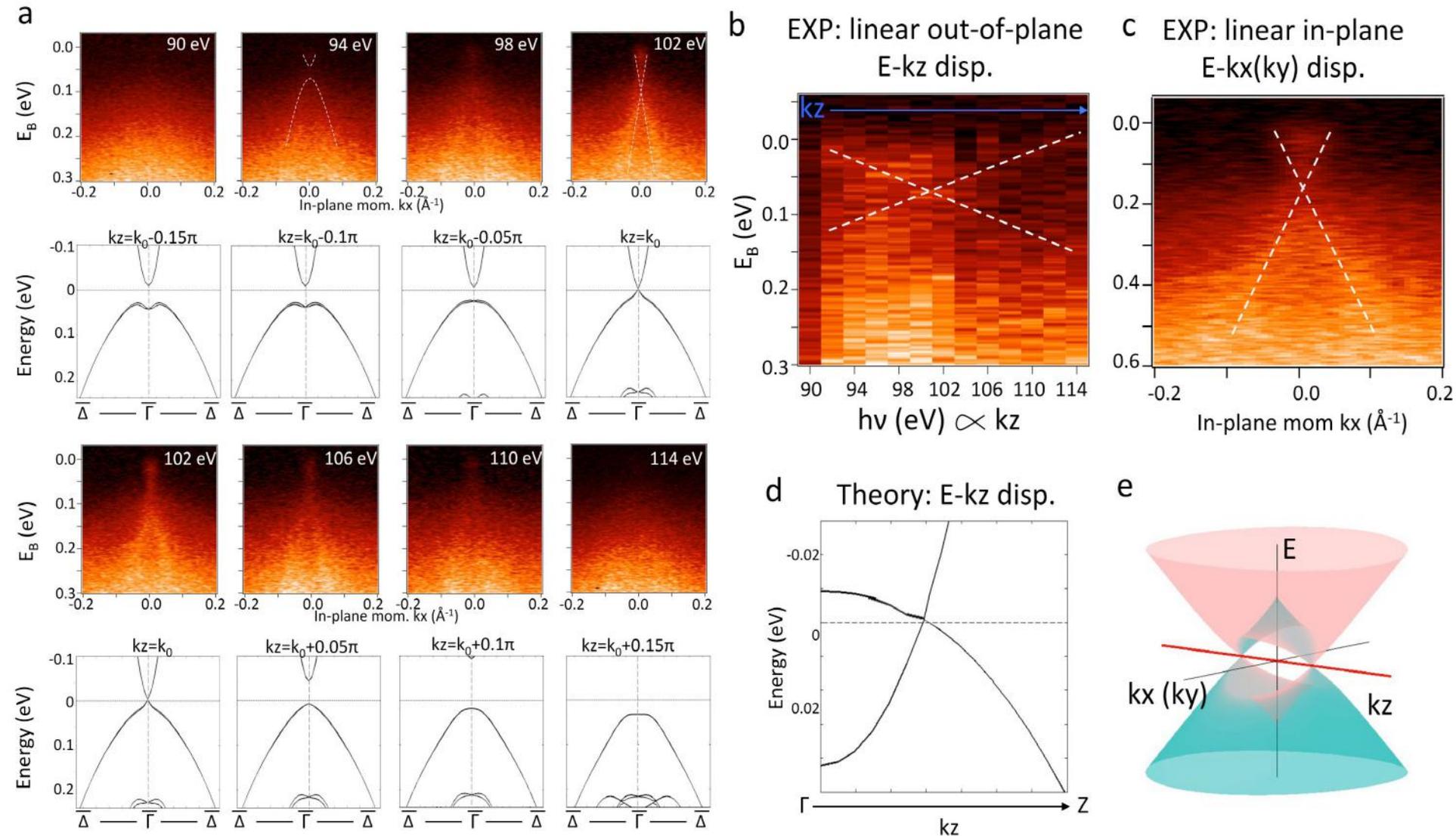
S.Y. Xu *et al.*, *Science* **347**, 294 (2015)

M. Neupane *et al.*, *Nature Commun.* **5**, 4786 (2014).

S. Borisenko *et al.*, *Phys. Rev. Lett.* **113**, 027603 (2014)

Z.K. Liu *et al.*, *Nat. Mat.* **13**, 677 (2014)

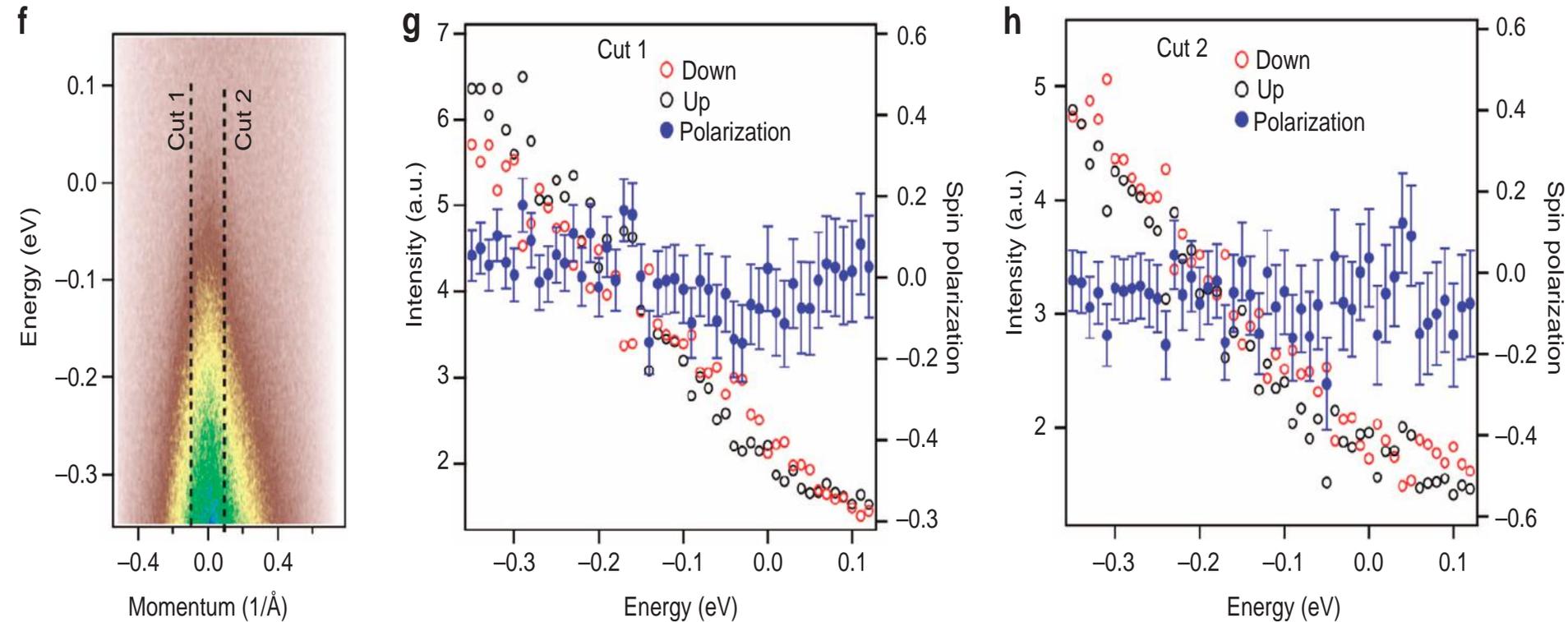
3D band dispersion: Cd_3As_2



M. Neupane *et al.*, *Nature Commun.* **5**, 4786 (2014).

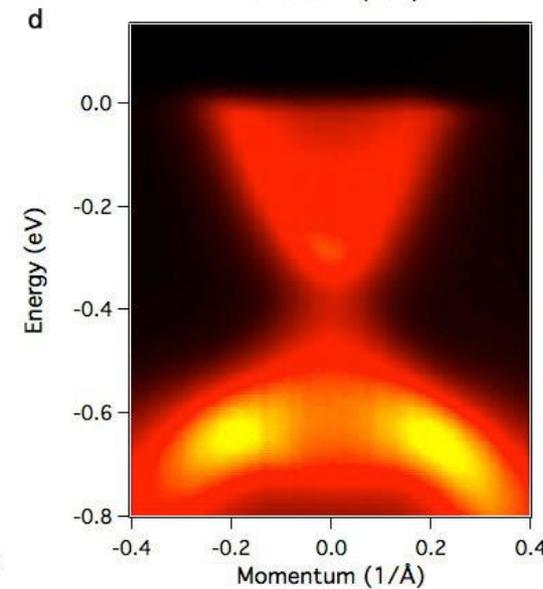
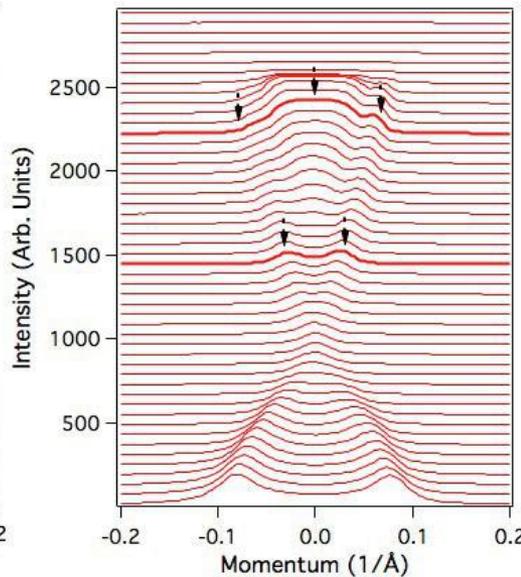
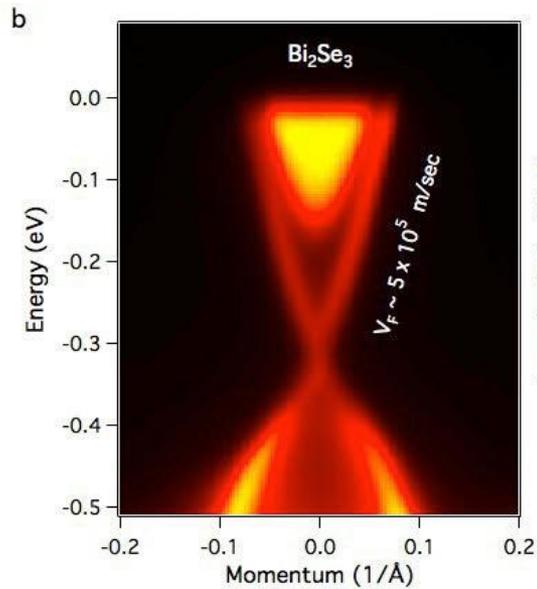
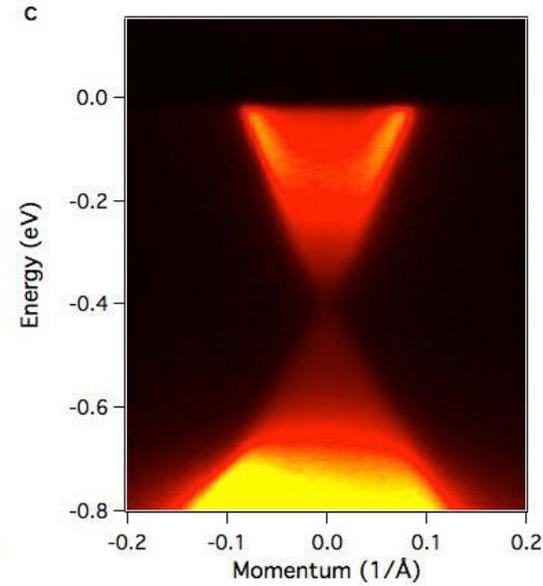
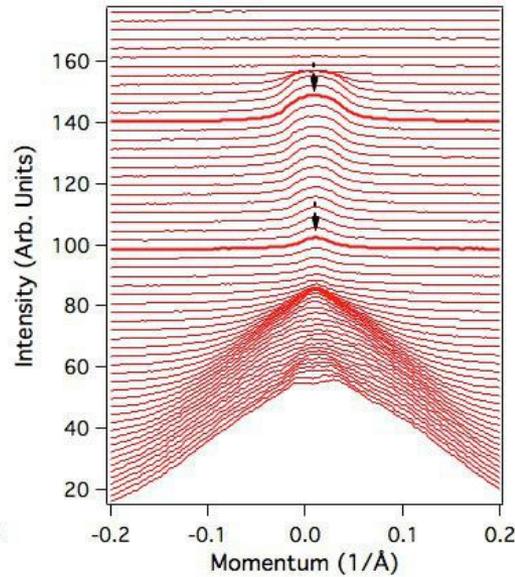
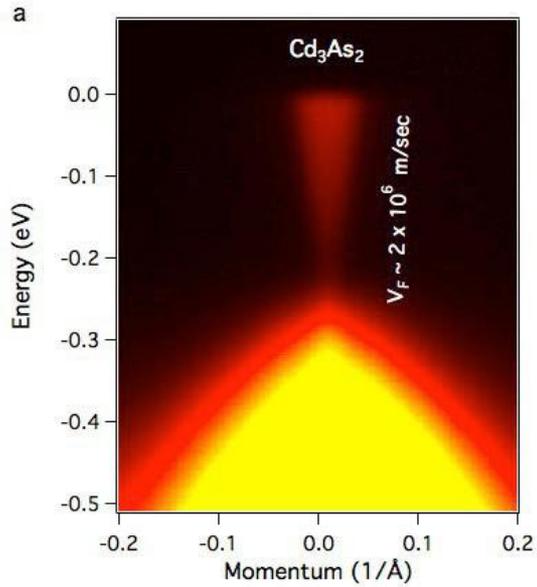
3D band dispersion: Cd_3As_2

Spin-degenerate property: bulk Dirac cone

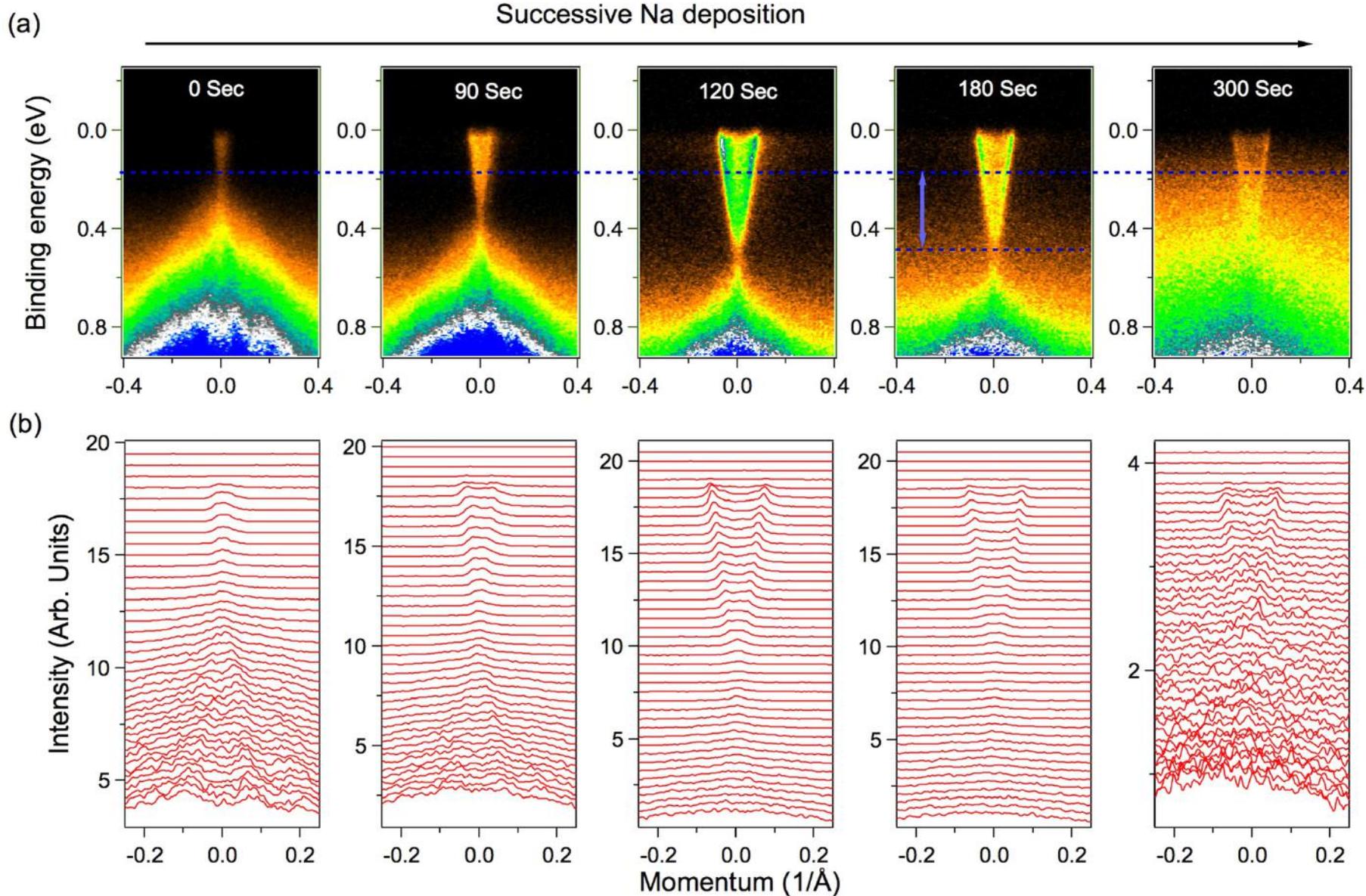


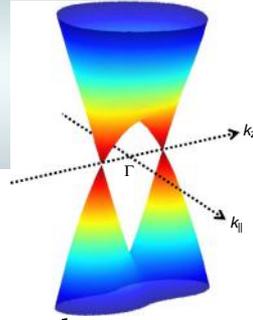
M. Neupane *et al.*, *Nature Commun.* **5**, 4786 (2014).

2D vs 3D Dirac semimetals



Surface deposition





ARTICLE

Received 2 Dec 2013 | Accepted 2 Apr 2014 | Published 7 May 2014

DOI: 10.1038/ncomms4786

Observation of a three-dimensional topological Dirac semimetal phase in high-mobility Cd_3As_2

Madhab Neupane^{1,*}, Su-Yang Xu^{1,*}, Raman Sankar^{2,*}, Nasser Alidoust¹, Guang Bian¹, Chang Liu¹, Ilya Belopolski¹, Tay-Rong Chang³, Horng-Tay Jeng^{3,4}, Hsin Lin⁵, Arun Bansil⁶, Fangcheng Chou² & M. Zahid Hasan^{1,7}

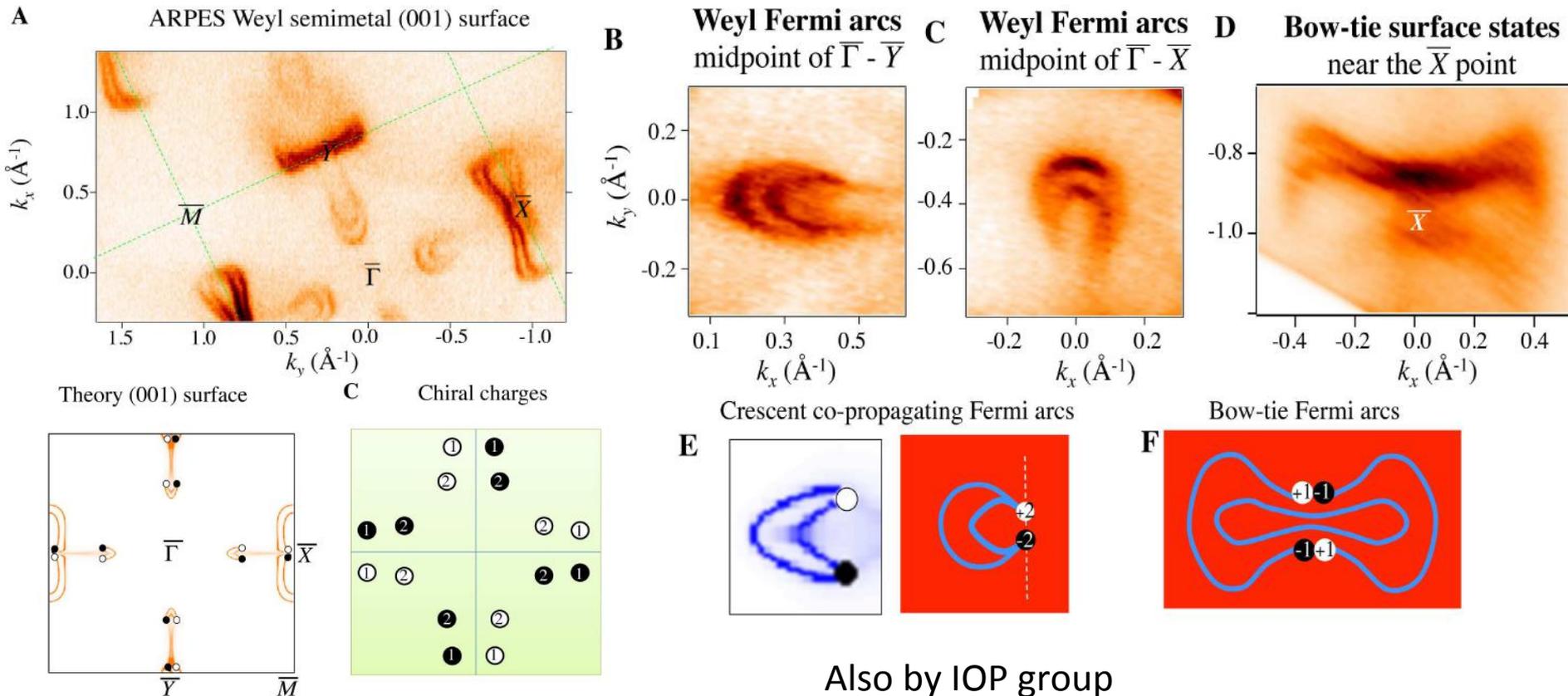
Conclusions:

- Experimental observation of the bulk Dirac semimetal phase in Cd_3As_2
- High Fermi velocity
- 3D BDS phase in stoichiometric compound
- ***Basis for Weyl semimetal phase: break symmetry (TR and IS)***

Discovery of a Weyl Fermion semimetal and topological Fermi arcs

Su-Yang Xu,^{1,2*} Ilya Belopolski,^{1*} Nasser Alidoust,^{1,2*} Madhab Neupane,^{1,3*} Guang Bian,¹ Chenglong Zhang,⁴ Raman Sankar,⁵ Guoqing Chang,^{6,7} Zhujun Yuan,⁴ Chi-Cheng Lee,^{6,7} Shin-Ming Huang,^{6,7} Hao Zheng,¹ Jie Ma,⁸ Daniel S. Sanchez,¹ BaoKai Wang,^{6,7,9} Arun Bansil,⁹ Fangcheng Chou,⁵ Pavel P. Shibayev,^{1,10} Hsin Lin,^{6,7} Shuang Jia,^{4,11} M. Zahid Hasan^{1,2†}

correspondence in a topological phase. In contrast to topological insulators where only the surface states are interesting (21, 22), a Weyl semimetal features unusual band structure in the bulk and on the surface. The Weyl fermions in the bulk are predicted to provide a condensed matter realization of the chiral anomaly, giving rise to a negative magnetoresistance under parallel electric and



PHYSICAL REVIEW B **93**, 201104(R) (2016)

Observation of topological nodal fermion semimetal phase in ZrSiS

Madhab Neupane,^{1,*} Ilya Belopolski,² M. Mofazzel Hosen,¹ Daniel S. Sanchez,² Raman Sankar,³ Maria Szlawska,⁴ Su-Yang Xu,² Klauss Dimitri,¹ Nagendra Dhakal,¹ Pablo Maldonado,⁵ Peter M. Oppeneer,⁵ Dariusz Kaczorowski,⁴ Fangcheng Chou,³ M. Zahid Hasan,² and Tomasz Durakiewicz⁶

¹*Department of Physics, University of Central Florida, Orlando, Florida 32816, USA*

²*Joseph Henry Laboratory and Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*

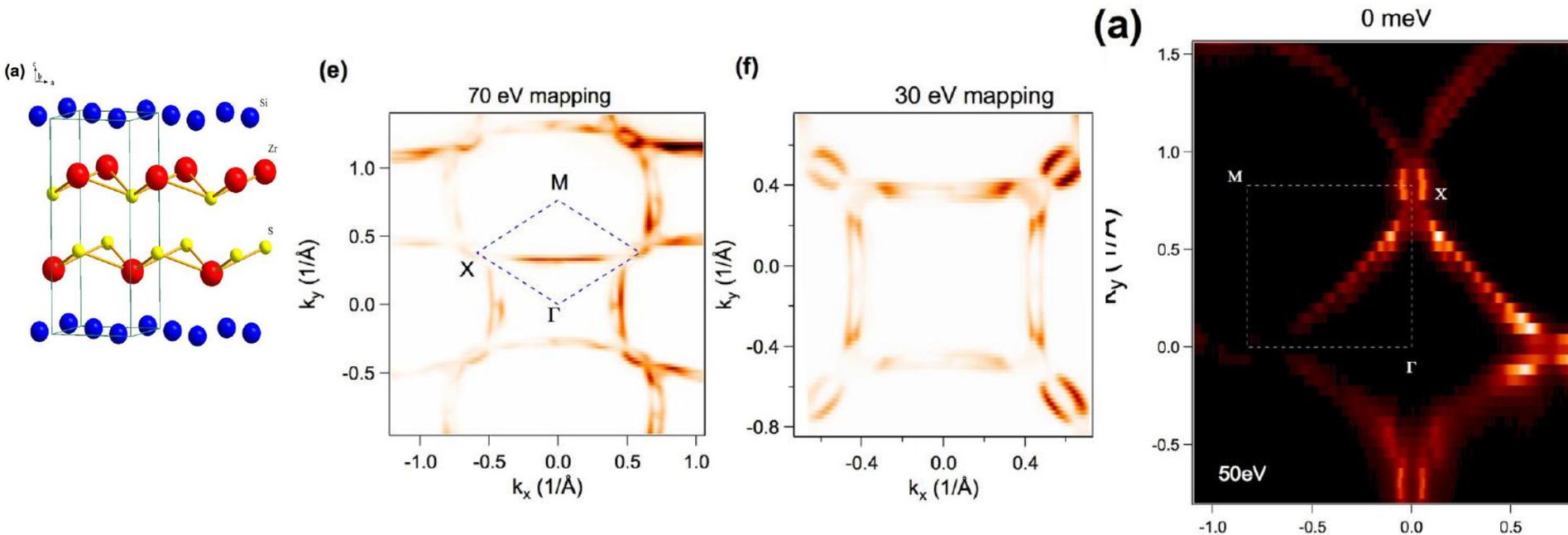
³*Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan*

⁴*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, 50-950 Wroclaw, Poland*

⁵*Department of Physics and Astronomy, Uppsala University, P.O. Box 516, S-75120 Uppsala, Sweden*

⁶*Condensed Matter and Magnet Science Group, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

(Received 4 March 2016; published 11 May 2016)



Letter

Observation of Dirac-like semi-metallic phase in NdSb

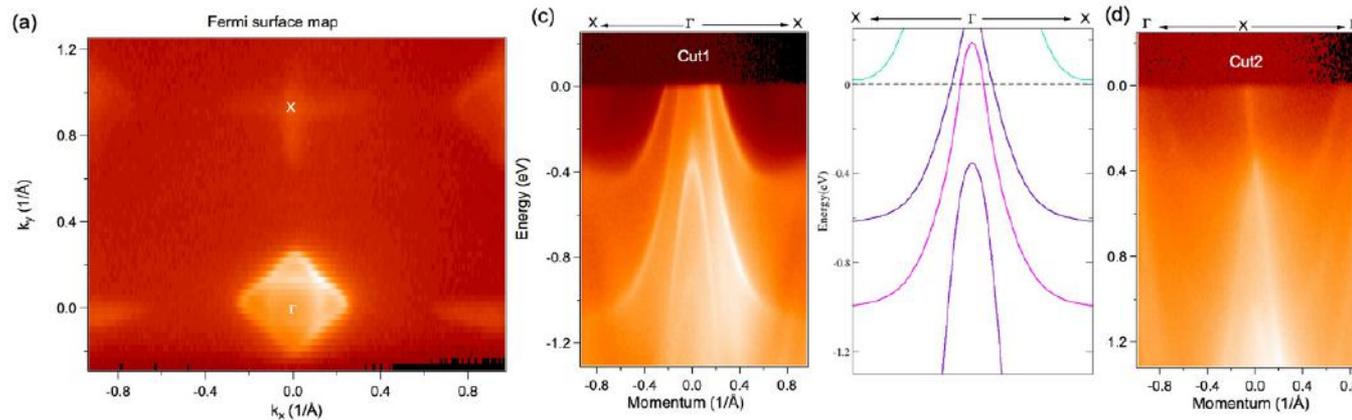
Madhab Neupane^{1,5}, M Mofazzel Hosen¹, Ilya Belopolski²,
Nicholas Wakeham³, Klauss Dimitri¹, Nagendra Dhakal¹, Jian-Xin Zhu⁴,
M Zahid Hasan², Eric D Bauer³ and Filip Ronning³

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⁴ Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA



Thank you!