Photoemission Study on Topological Semimetals

SPICE Workshop

New Paradigms in Dirac-Weyl Nanoelectronics

June 15th, 2016

Zhongkai Liu

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Outline

- Probing the electronic structure of TI with ARPES
- ARPES study on Dirac/Weyl Semimetal
- Multi Dimensional ARPES techniques

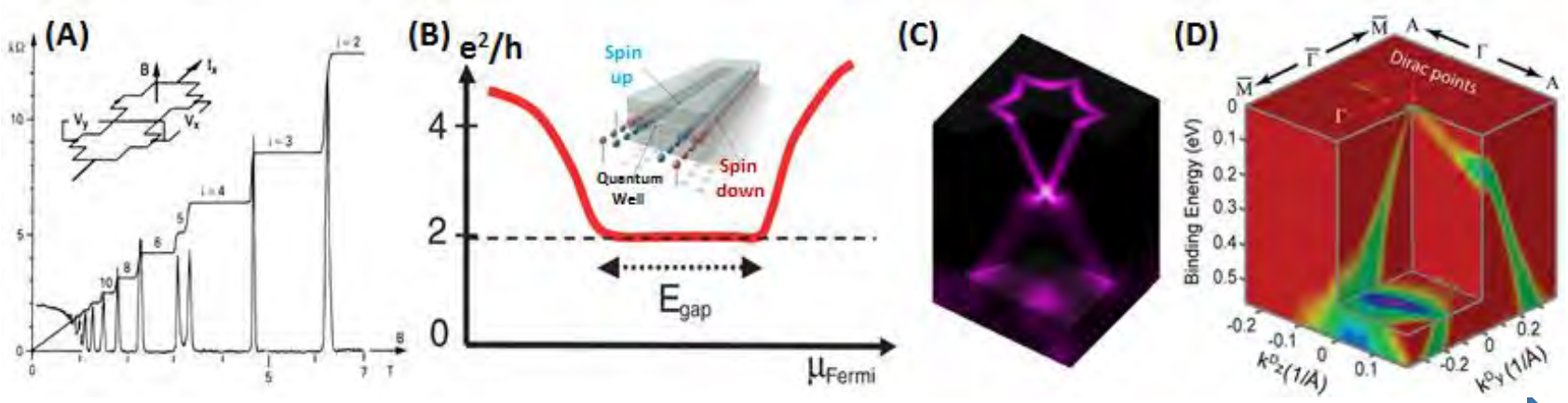
Topological Quantum Materials

QH Insulator

QSH Insulator

Topological Insulator

Topological Semimetal



1980 — 2006-2013 — 2014

Topological invariant:
"**first Chern number**"

Topological invariant:
"**Z_2 invariant**"

Topological invariant:
"**Chern number** (of some sort?)"

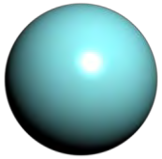
Why “topological”

Topologically distinct objects

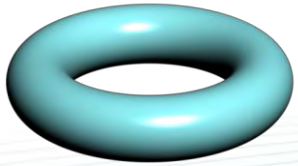
Regular insulator

Topological insulator

Sphere

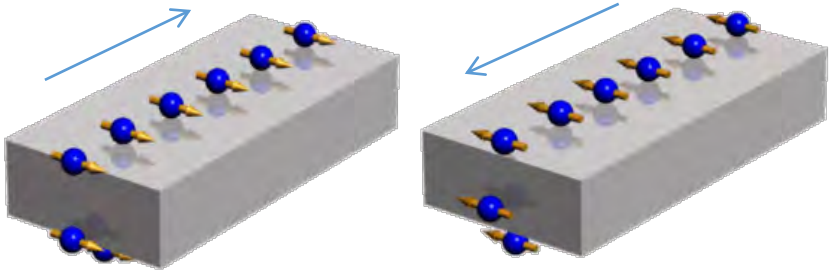


Torus

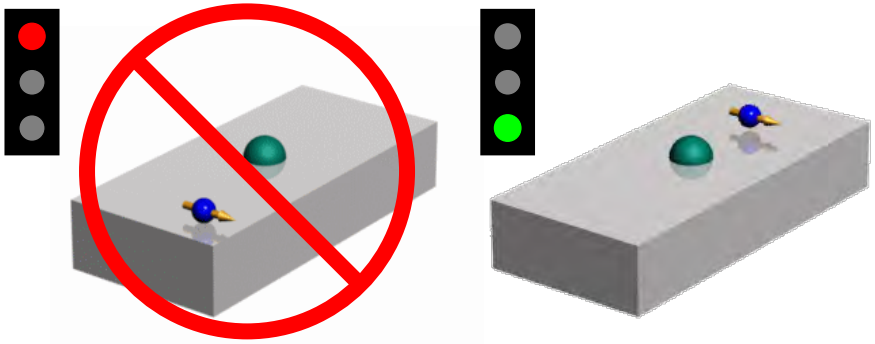


Unique surface state properties of TIs

"Locking" between current & spin

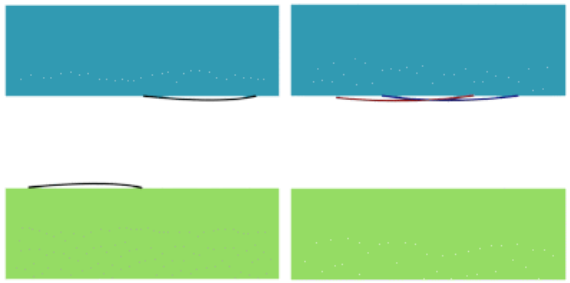


No back-scattering rule
(by non-magnetic impurities)

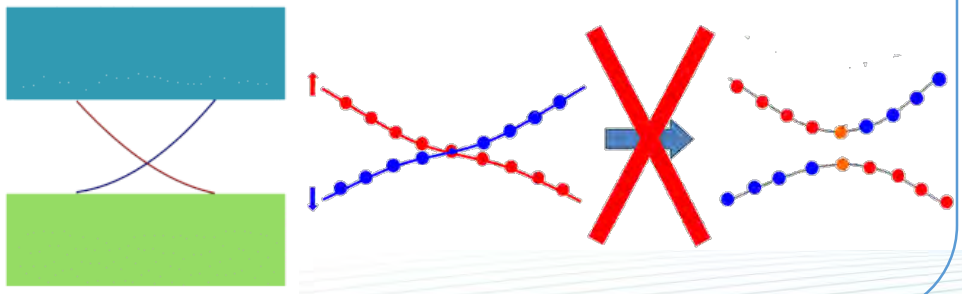


Robustness of the topological surface state

Surface state in regular insulator
vulnerable



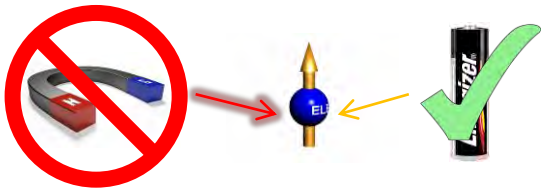
Surface state in topological insulator
robust



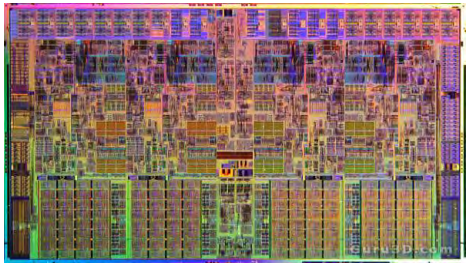
Application potentials

Electronics more efficient
(Longer functional time)

Spintronics without magnet
(Faster & less consumption)

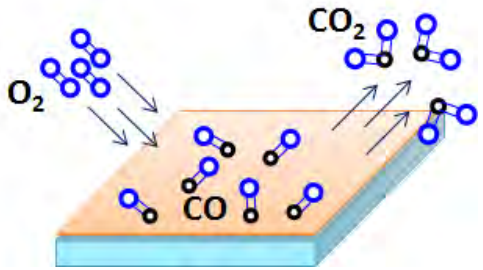


Higher density integrated circuit

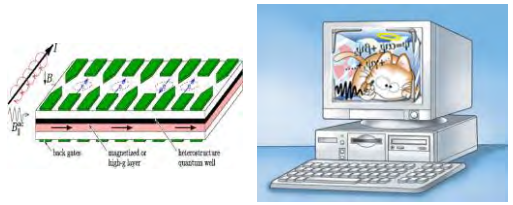


Thermoelectric generators

New catalysts



Quantum computation



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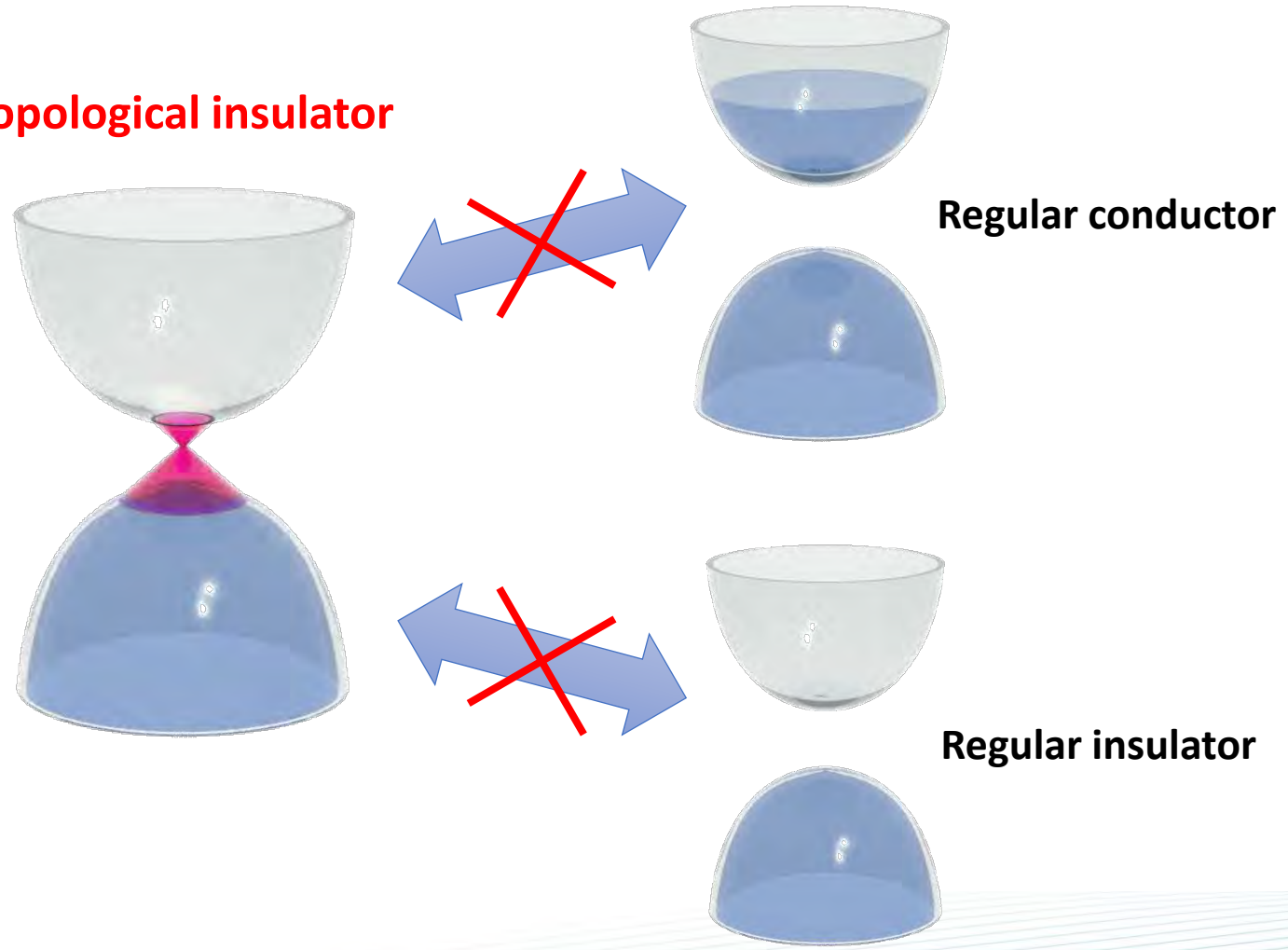
How to find TIs

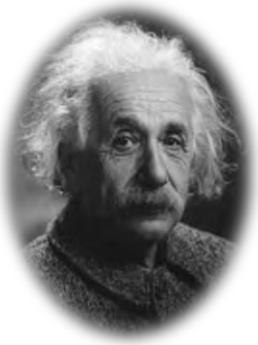
Search for the unique band structure



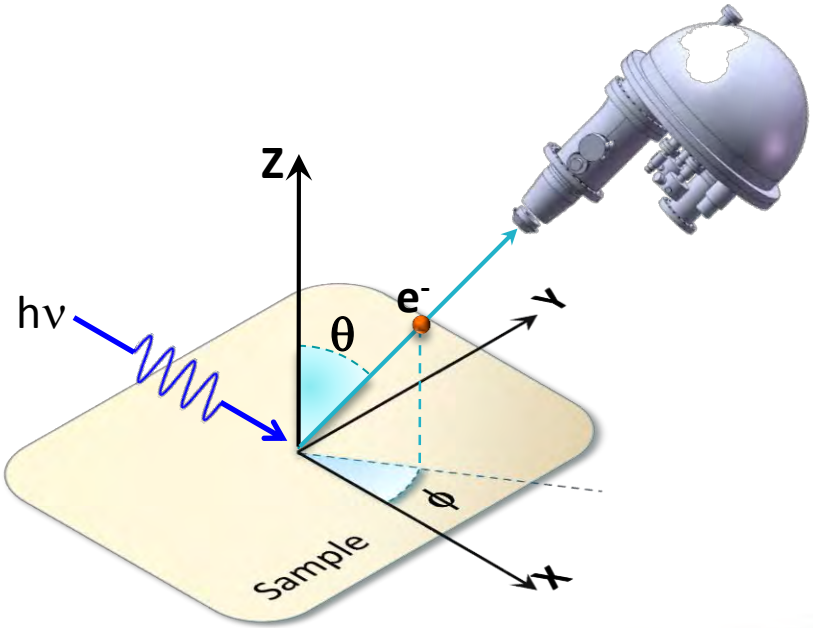
How to “see” band structures

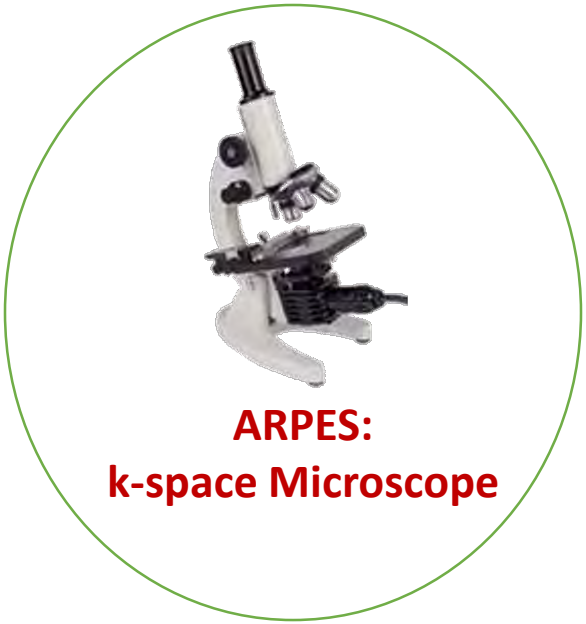
Angle Resolved Photoemission Spectroscopy (ARPES)

Heinrich Hertz



Albert Einstein





Energy Conservation

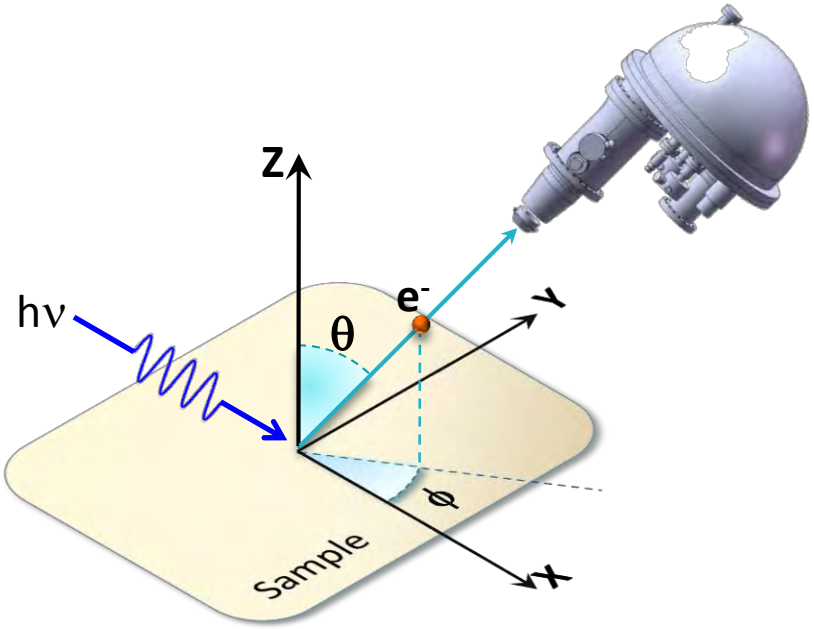
$$E_B = h\nu - E_{kin} - \Phi$$

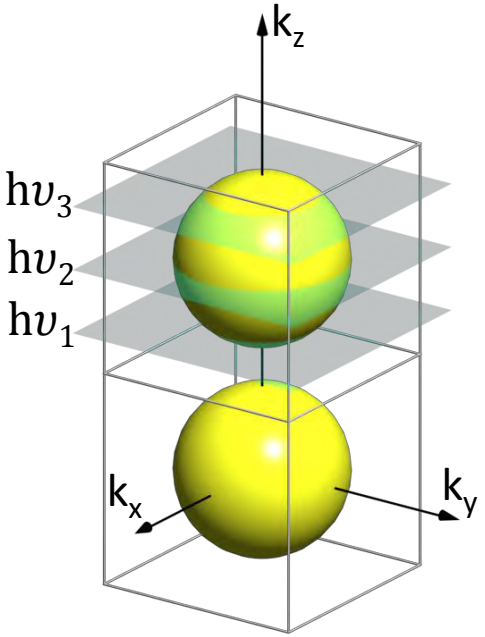
Momentum Conservation

$$K_{\parallel} = k_{\parallel} + G_{\parallel}$$

How to determine *kz*?

Photon energy dependent ARPES measurement





$$E_k = h\upsilon - w - E_B$$

In vacuum:

$$k^V{}_x = \frac{\sqrt{2m_e E_k}}{\hbar}\sin(\theta)\cos(\Phi)$$

$$k^V{}_y = \frac{\sqrt{2m_e E_k}}{\hbar}\sin(\theta)\sin(\Phi)$$

$$k^V{}_z = \frac{\sqrt{2m_e E_k}}{\hbar}\cos(\theta)$$

In crystal:

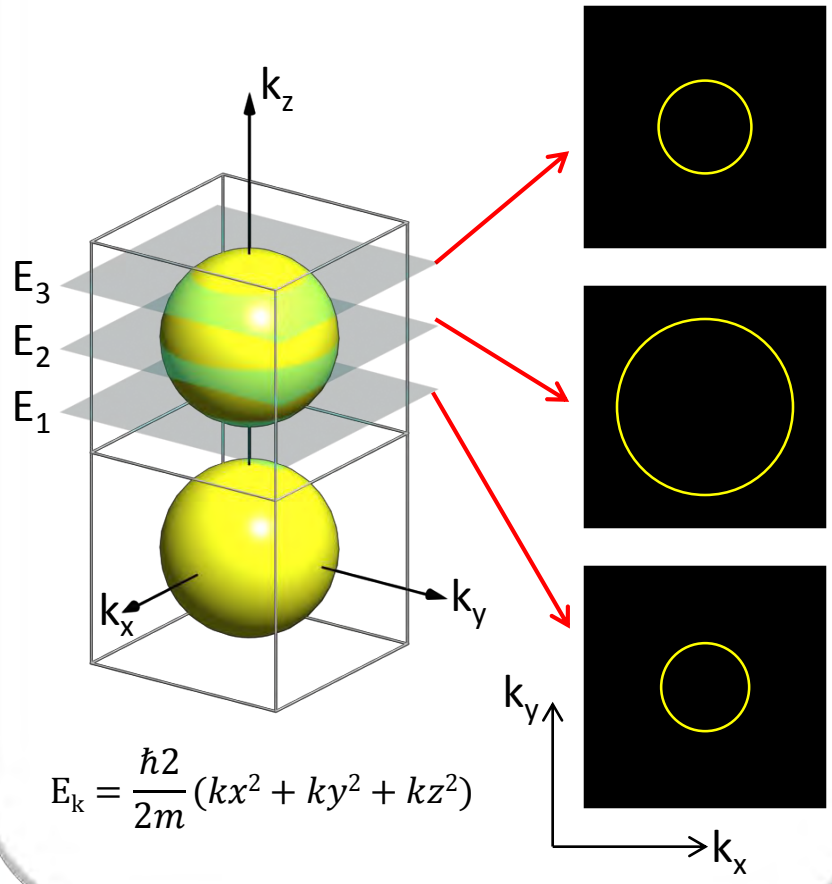
$$k_x = \frac{\sqrt{2m_e E_k}}{\hbar}\sin(\theta)\cos(\Phi) = k^V{}_x$$

$$k_y = \frac{\sqrt{2m_e E_k}}{\hbar}\sin(\theta)\,sin(\Phi) = k^V{}_y$$

$$k_z = \sqrt{\frac{2m_e{}^*}{\hbar^2}(E_k + V_0) - \frac{2m_e E_k}{\hbar^2}\sin^2\theta} \neq k^V z$$

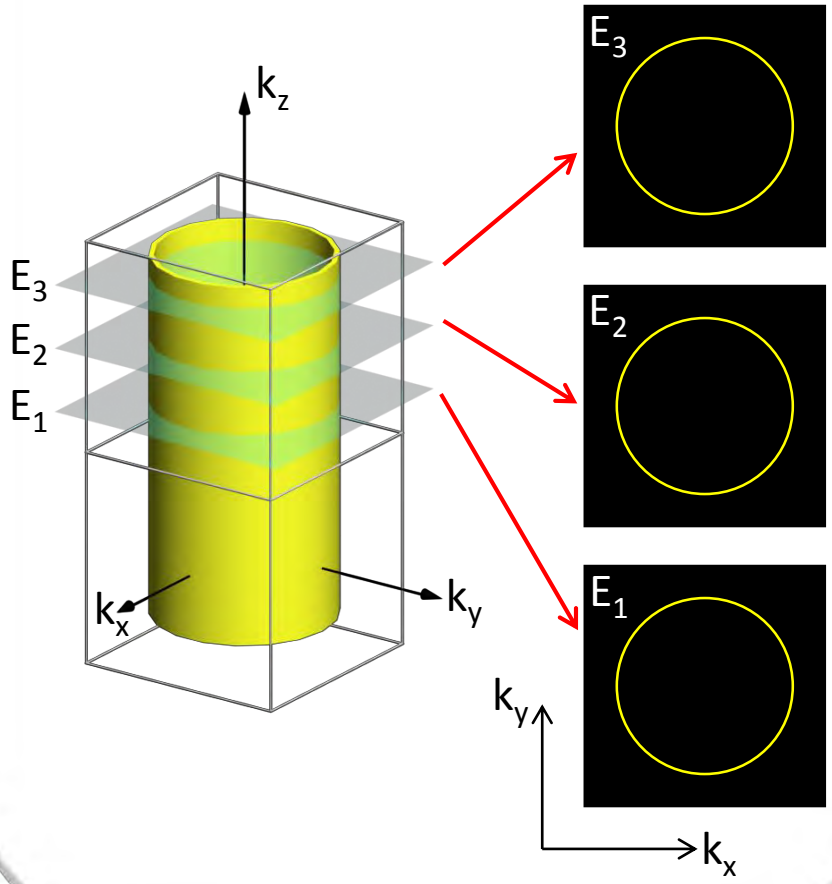
How to discriminate bulk & surface?

3D FS
(e.g. FS from bulk state)



$$E_k = \frac{\hbar 2}{2m}(kx^2 + ky^2 + kz^2)$$

2D FS
(e.g. FS from surface state)

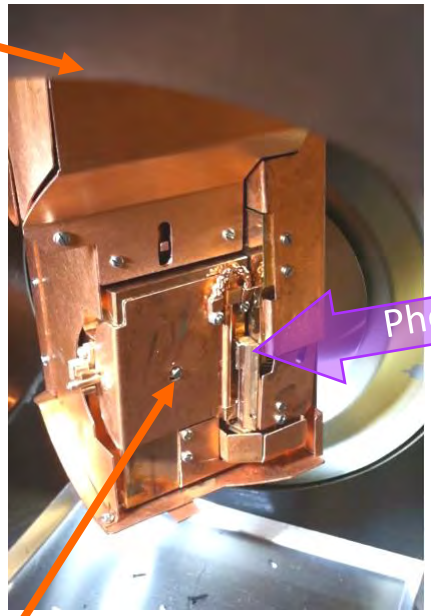


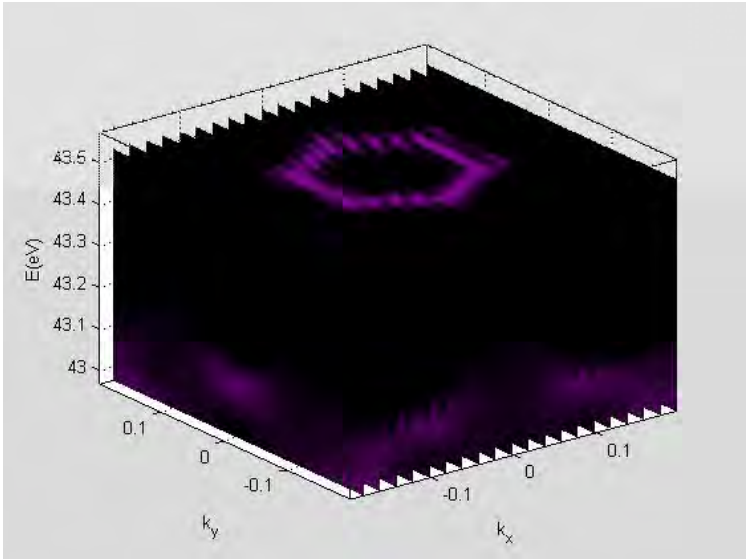
Modern ARPES

Experimental setup

Data acquired

Experiment Chamber

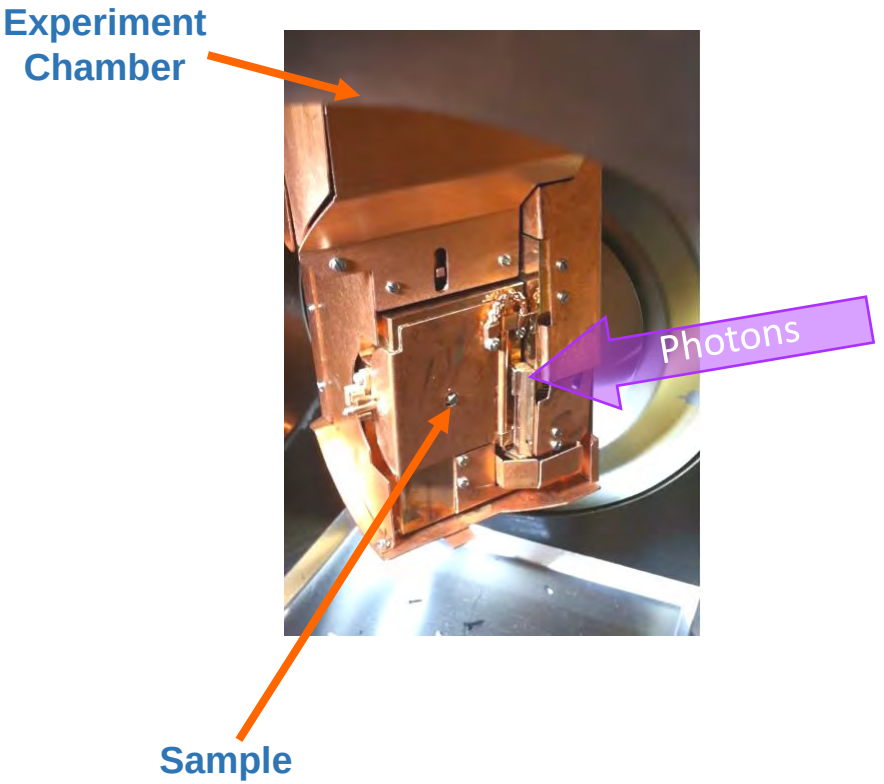


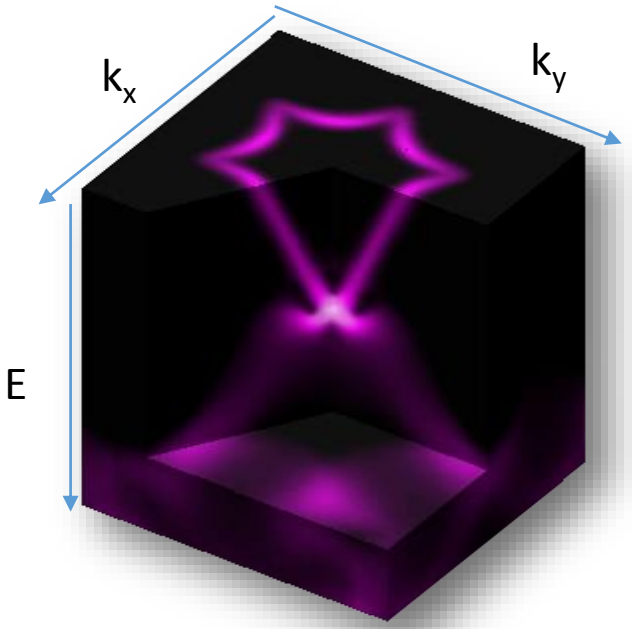


Modern ARPES

Experimental setup

Data acquired

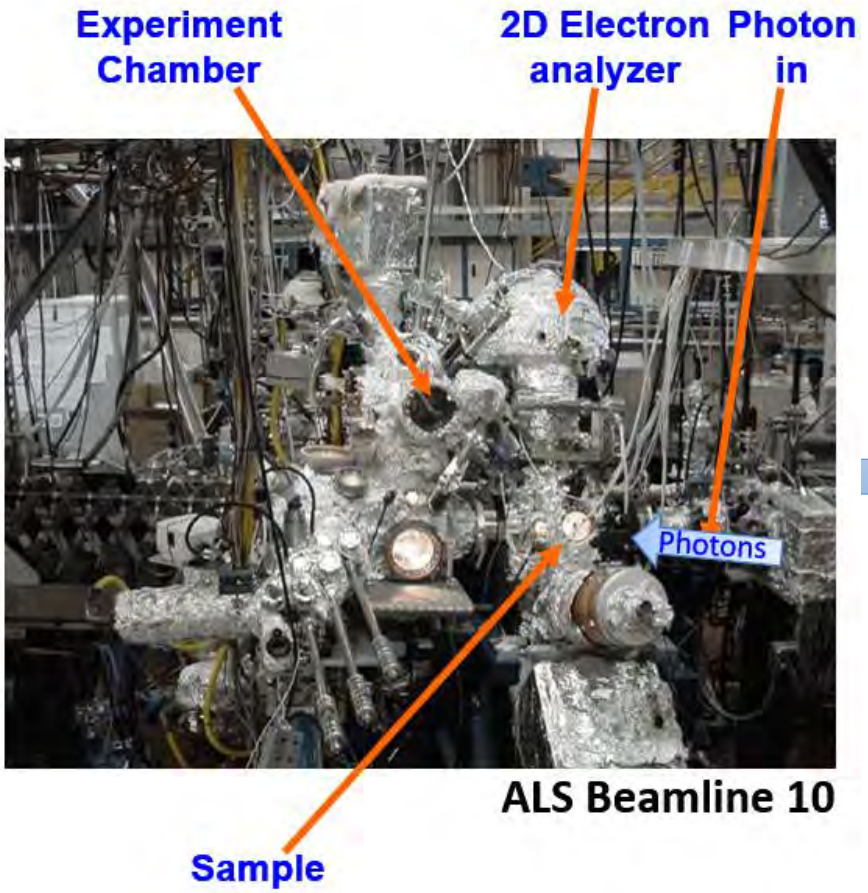


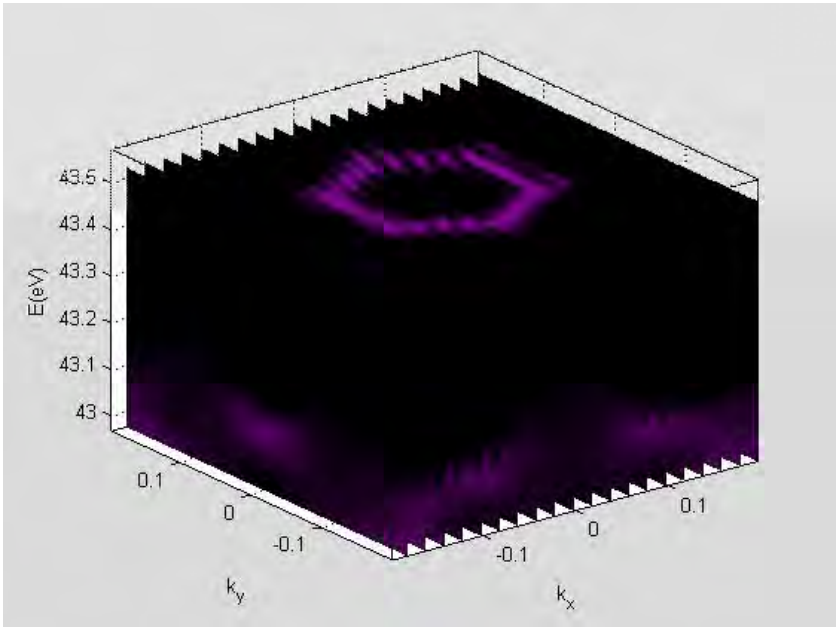


Or Alternatively…

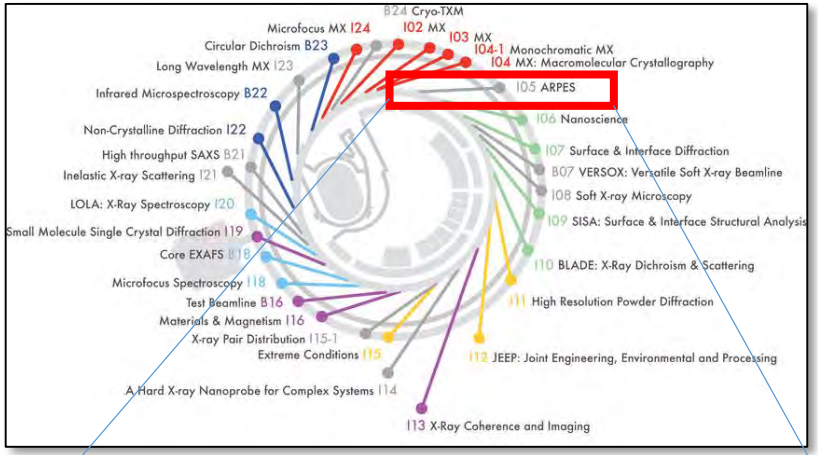
Experimental setup

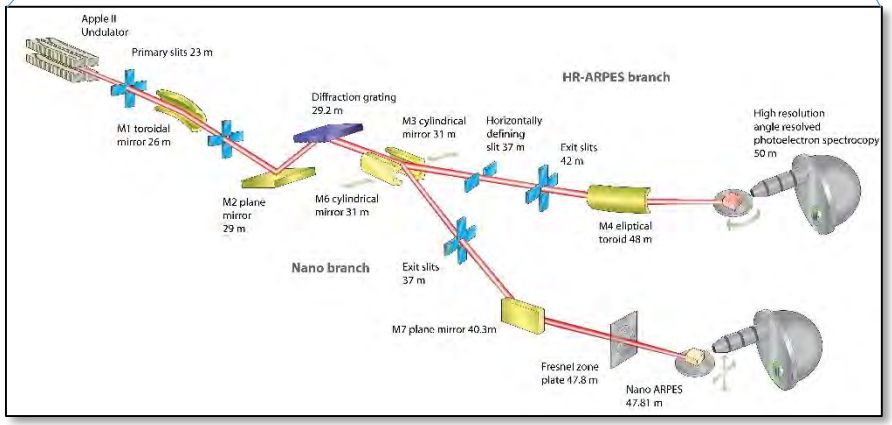
Data acquired



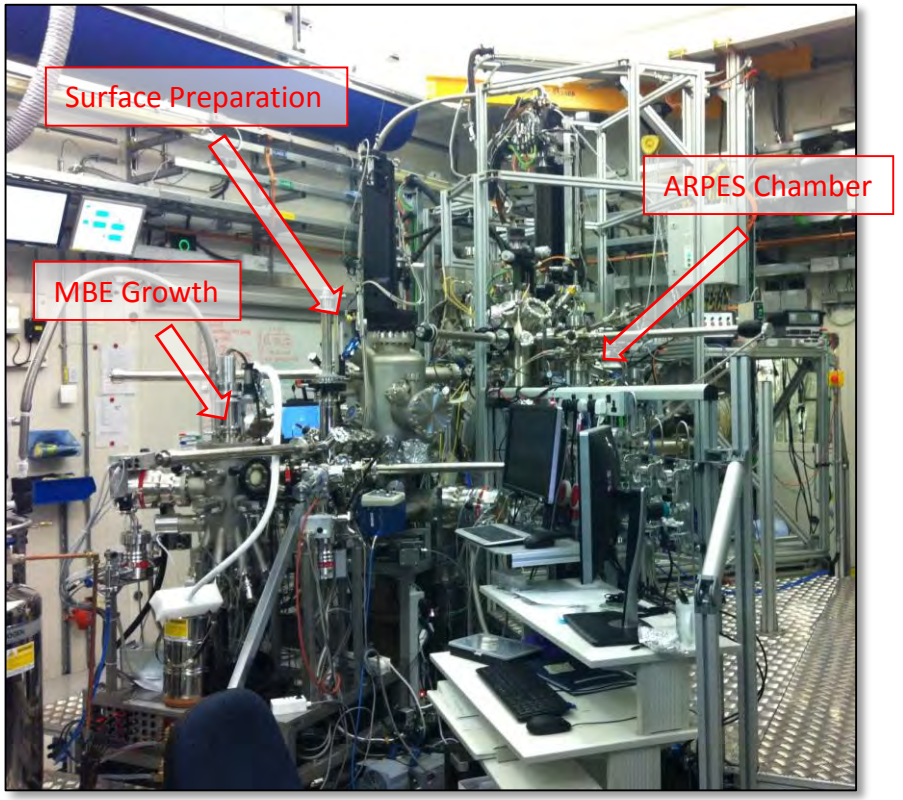


Synchrotron based ARPES station





BL I05

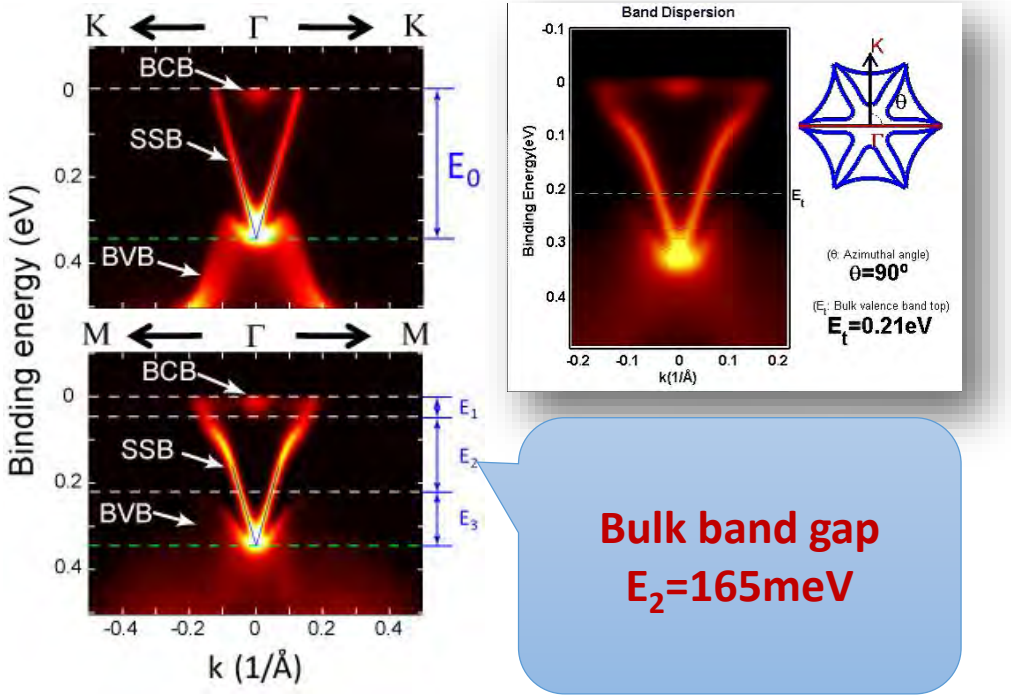


hv range: 18~240eV ΔE=2~10meV (hv: 18~80eV)
Temperature: 6K~RT
6 axis manipulator
Beamspot 50x50 um^2

Realization of TI state in Bi_2Te_3

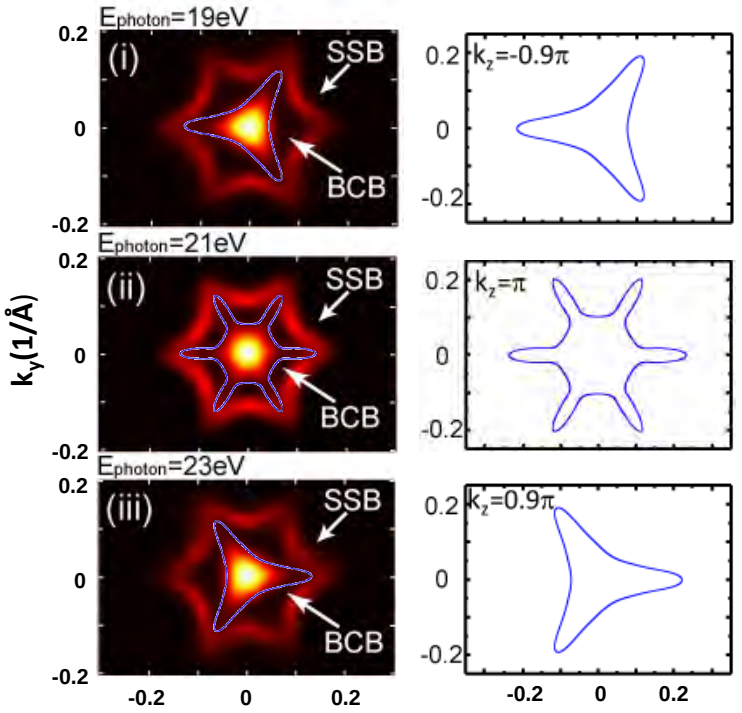
Y. L. Chen, *et. al.*, *Science* 325, 178 (2009)

Dirac fermion



Bulk band gap
E_2=165meV

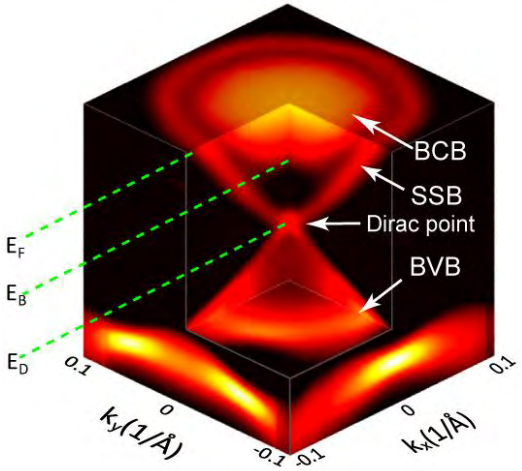
Dirac Fermion's Surface nature



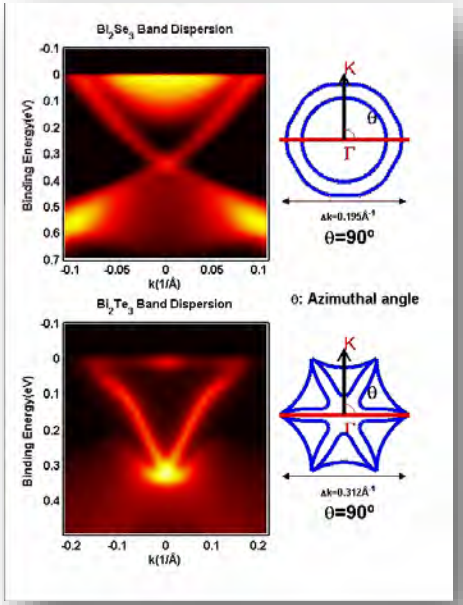
TRS protection – bulk doping

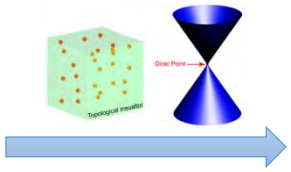
Y. L. Chen, *et. al.*, *Science* 329, 659 (2010)

In gap Dirac point of Bi_2Se_3



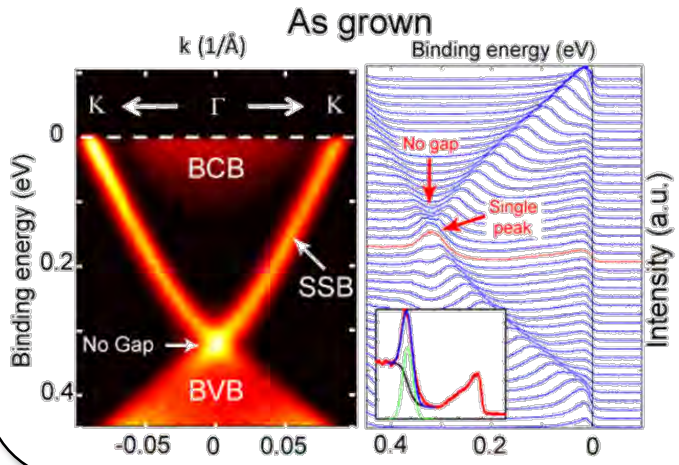
Compare to Bi_2Te_3

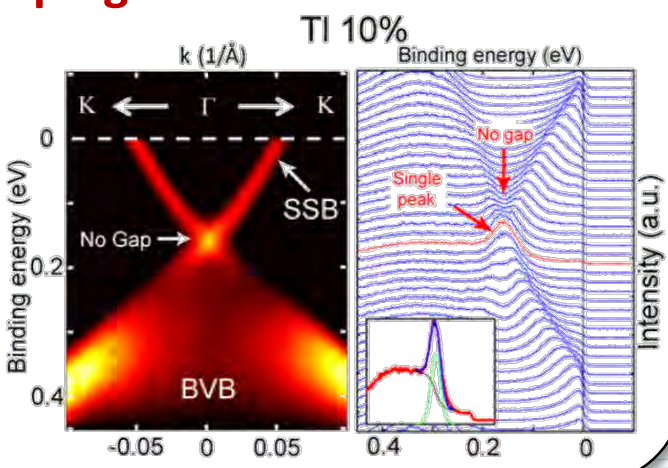




Non-magnetic impurities

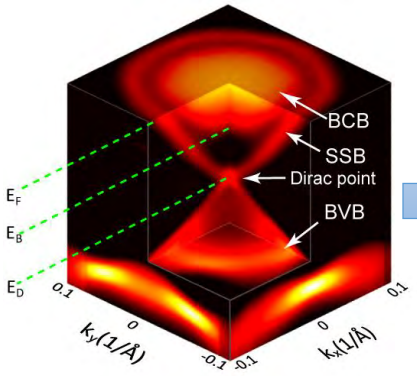
Bulk doping





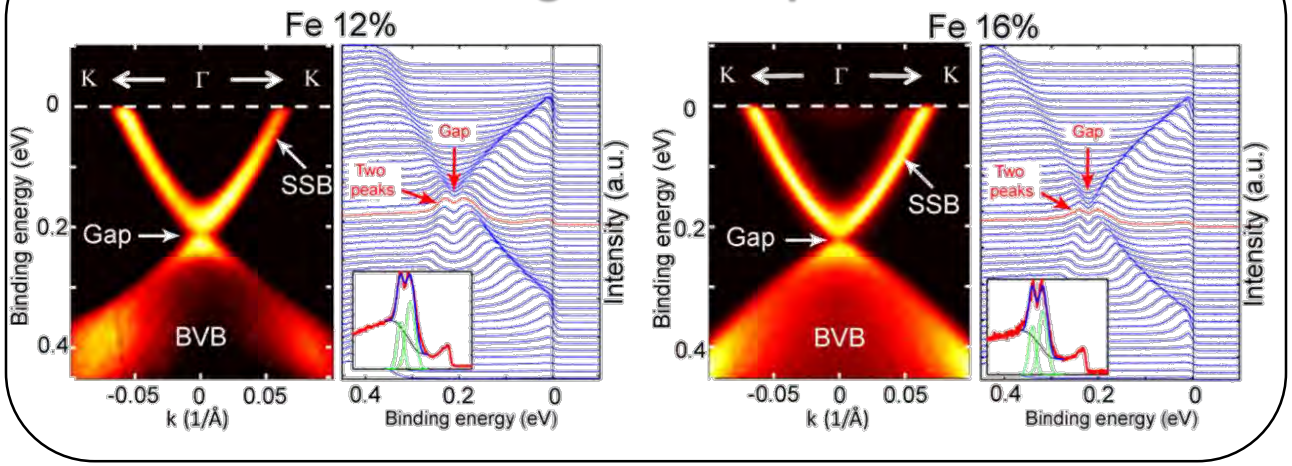
Dirac fermion becomes massive

Y. L. Chen, *et. al.*, *Science* 329, 659 (2010)



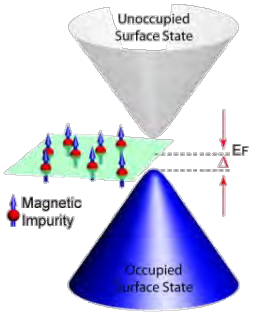
Magnetic impurities

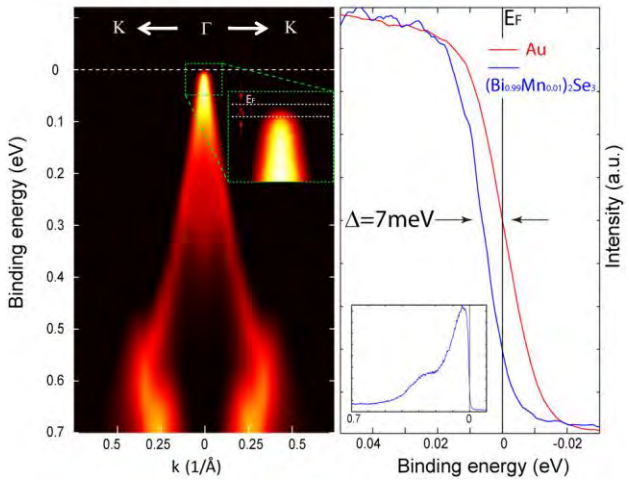
Braking the Dirac point



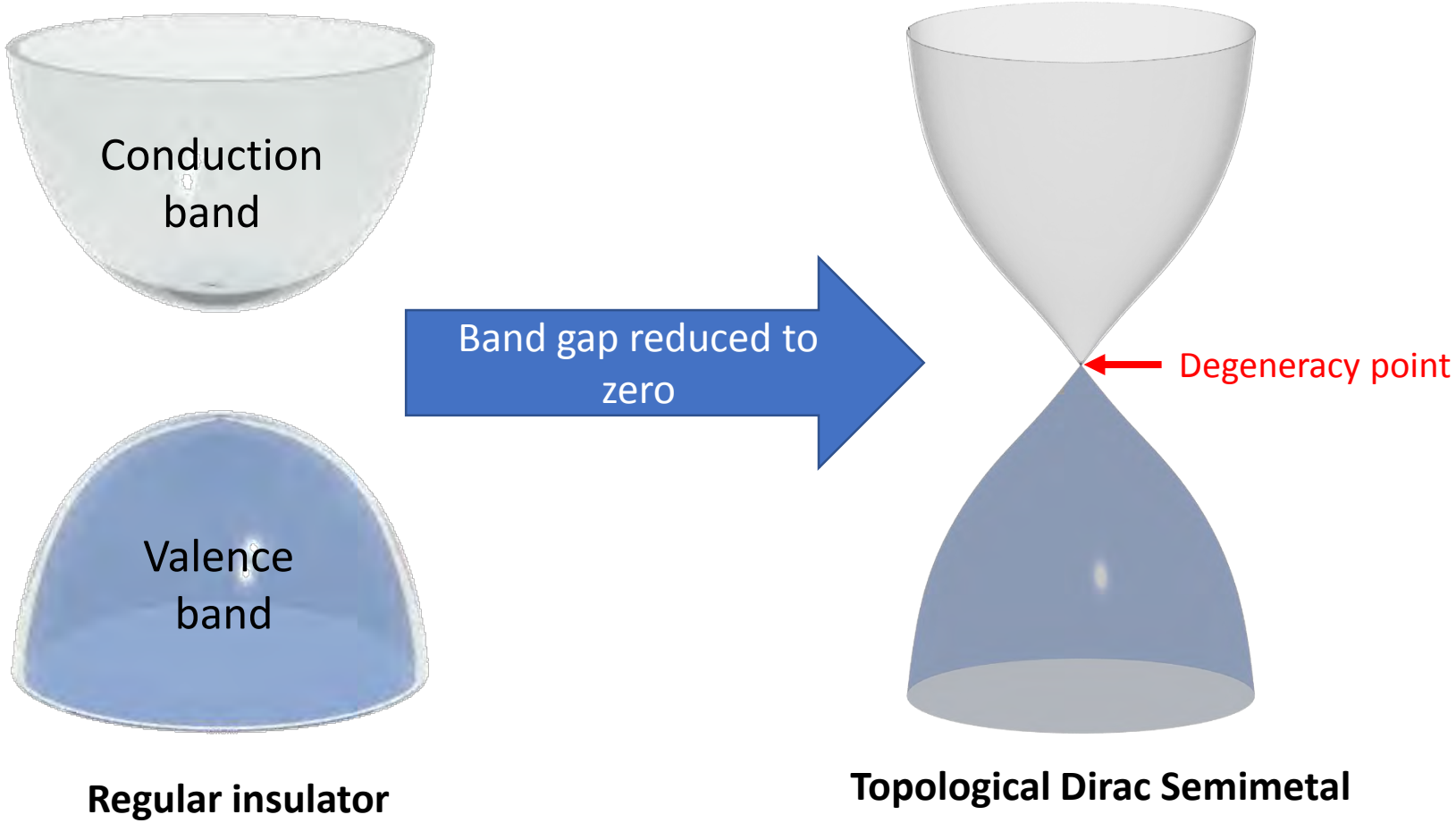
Charge tuning:
Move E_F into Dirac gap

Insulating massive Dirac fermion state





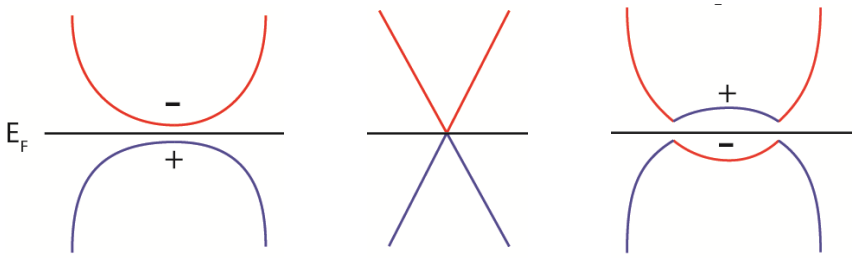
Topological Dirac Semimetals



Formation of 3D Topological Dirac Semimetal

Extrinsic 3D TDS:

Doping: x=a x=x_c x=b

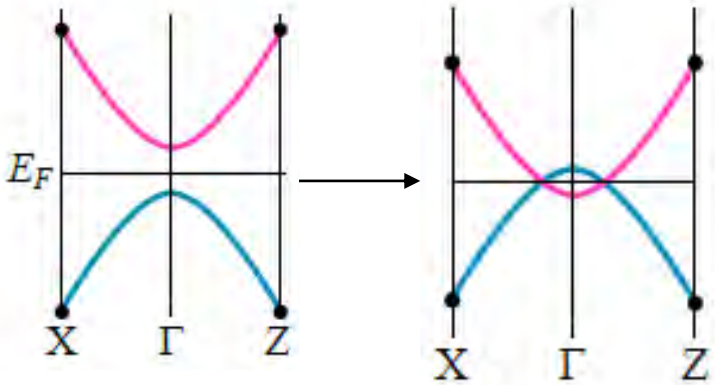


Normal insulator 3D TDS Topological insulator

Topological critical point between topological and normal insulator:

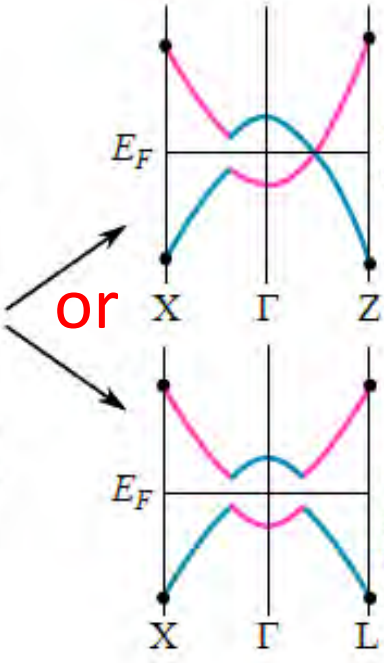
- Fine tuning of chemical composition required
- Not necessarily protected by crystal symmetry
- Very sensitive to temperature, pressure and composition homogeneity

Intrinsic 3D TDS:



Normal insulator Band inversion

Q.D.Gibson, PRB 91, 205128(2015)



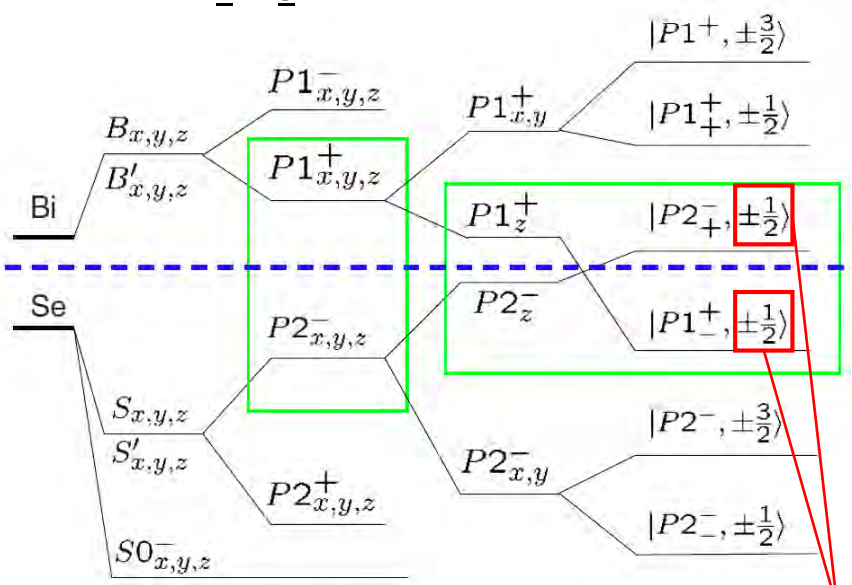
Node preserved: 3D TDS

- The crossing bands are orthogonal so that perturbation would not open a gap
- Crystal symmetry allows such orthogonal bands, even at the presence of SOC

Gap opening: Topological insulator

- SOC helps to increase the band inversion magnitude, at the same time, it would mix-up bands and make them non-orthogonal. So that an inversion gap usually persists

Bi_2Se_3, topological insulator



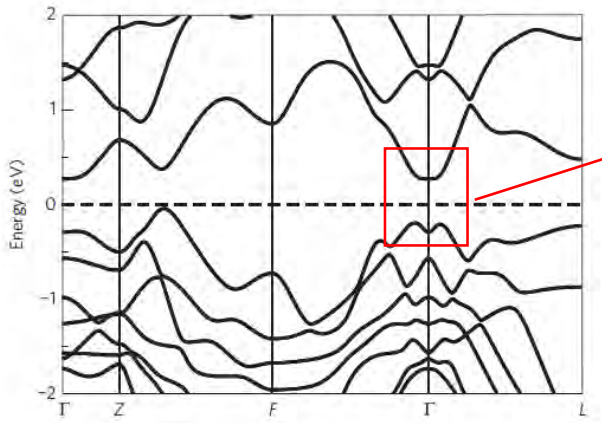
Orbital hybridization

Crystal field Splitting

Same |Jz|, Not Orthogonal

Chemical bounding

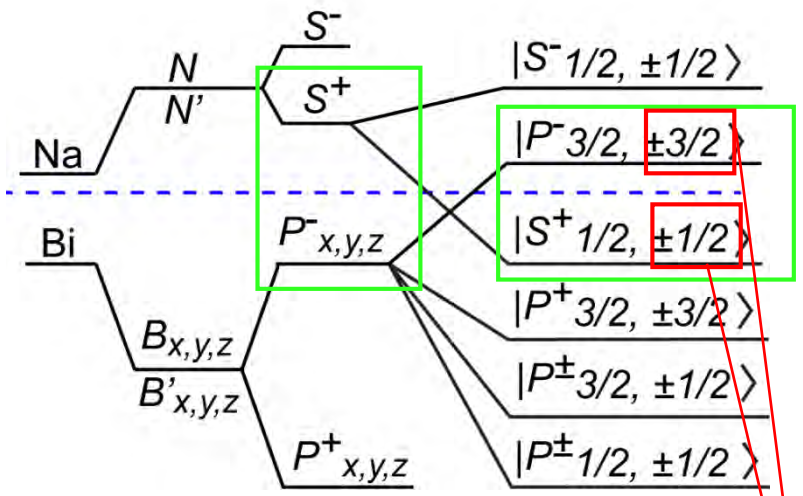
Spin-Orbit Coupling



Inverted Band gap From p-p Band inversion

H. J. Zhang *et al.*, *Nature Physics* **5**, 438 – 442(2009)
C. –X. Liu *et al.*, *Phys. Rev. B* **82**, 045122(2010)

Na_3Bi, 3D topological Dirac semimetal

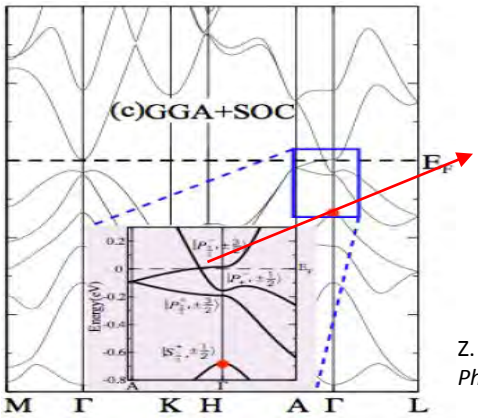


Orbital hybridization

Spin-Orbit Coupling

Different |Jz|, Orthogonal

Chemical bounding



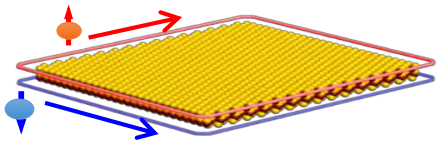
Band touching Point preserved From s-p Band inversion (at some Kz)

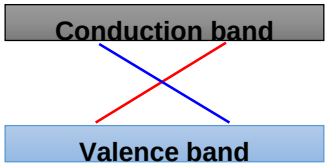
Z. J. Wang *et al.*, *Phys. Rev. B* **85**, 195320(2012)

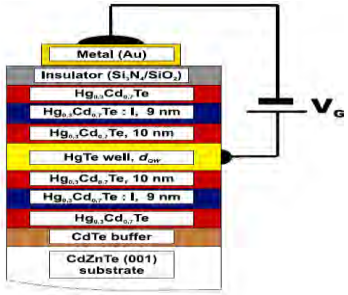
Dirac electron systems

1D Dirac fermions

Quantum spin Hall edge state

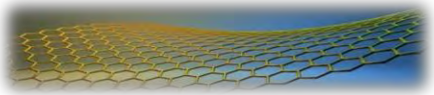


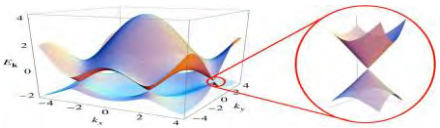




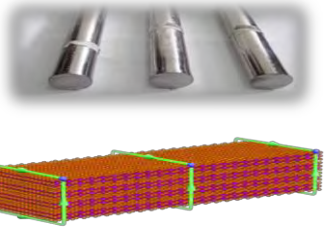
2D Dirac fermions

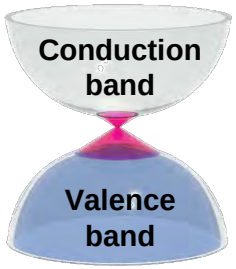
Graphene





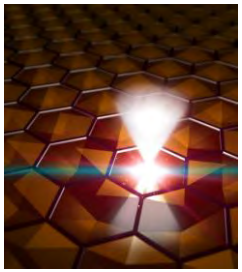
3D TI surface state

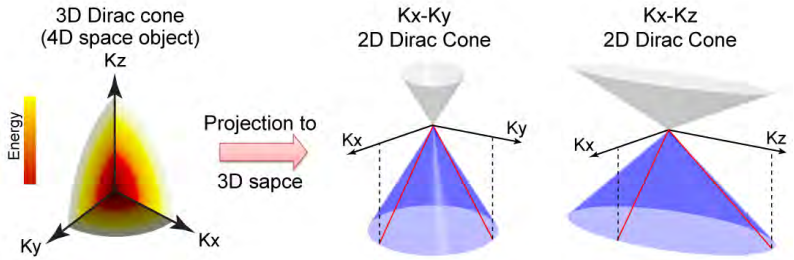




3D Dirac fermions

Topological Dirac Semimetal

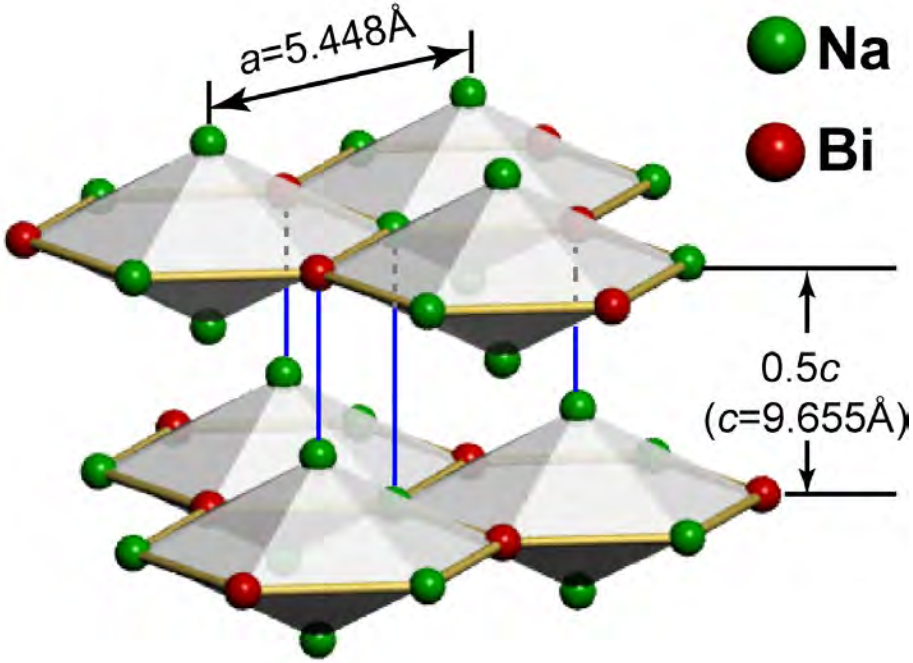




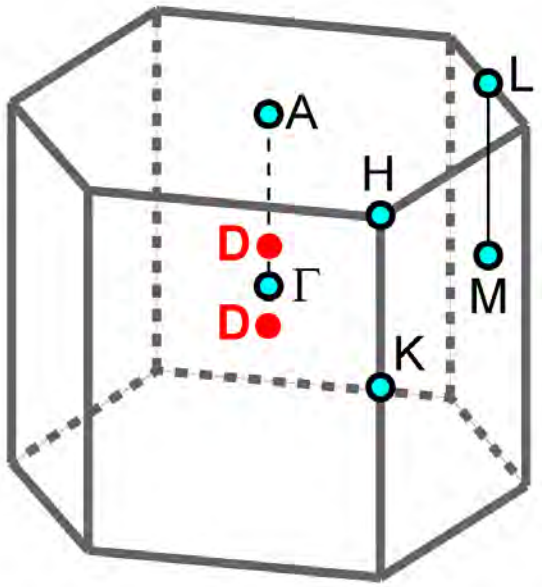
3D Topological Dirac Semi-metal (TDS)

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

Crystal structure

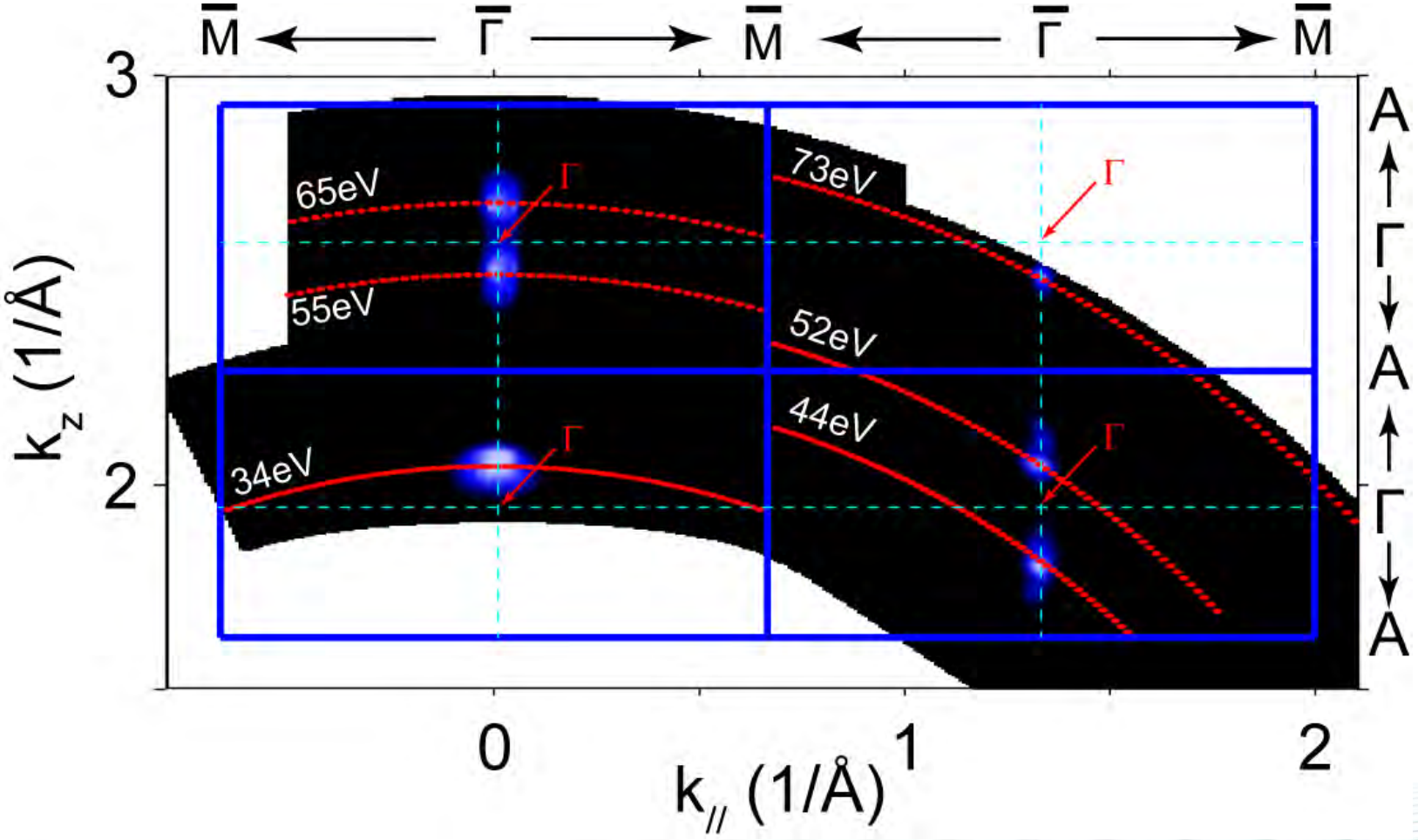


Brillouin Zone



Extracting *kz* dispersions

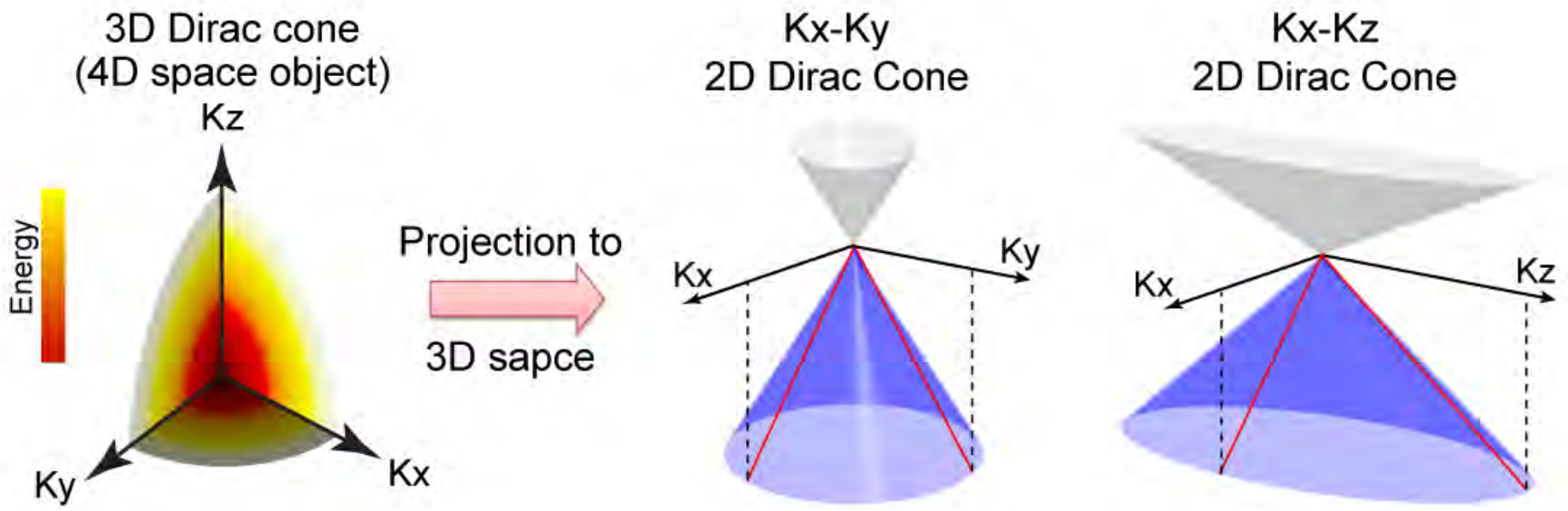
Multiple BZ mapping along kz



How to identify a 3D TDS?

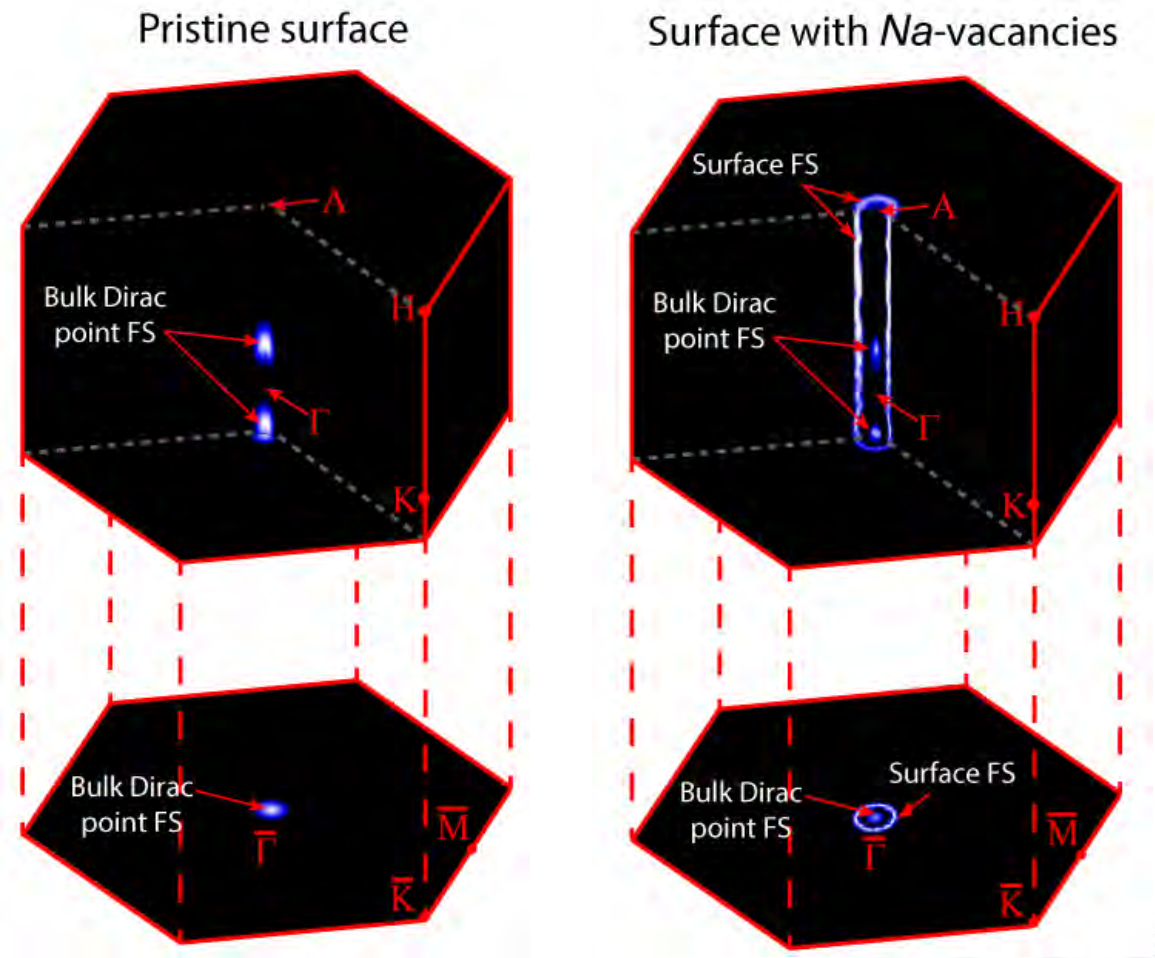
The 3D counterpart of graphene

Identify the band structure



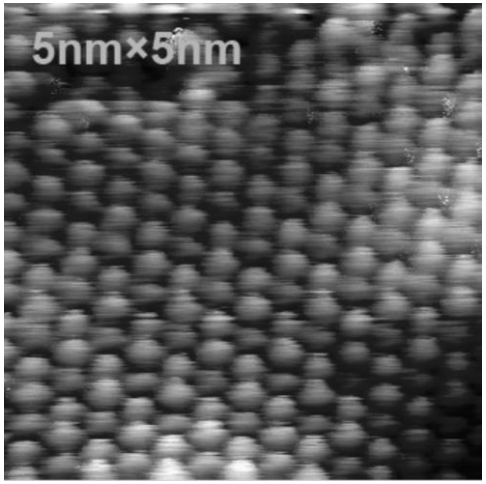
Fermi surface and Real surface

Complete 3D Fermi-surface mapping



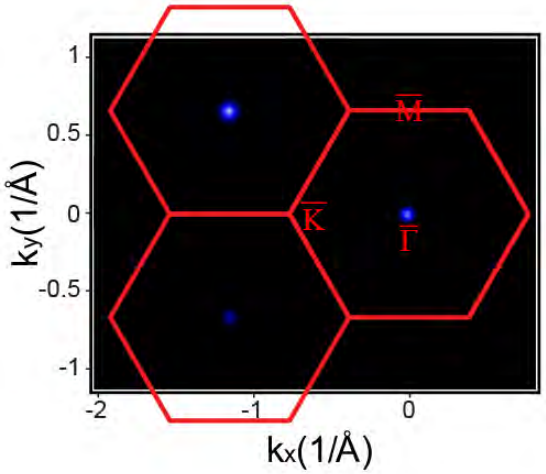
Real surface

(Courtesy of X. Chen Tsinghua Univ., China)

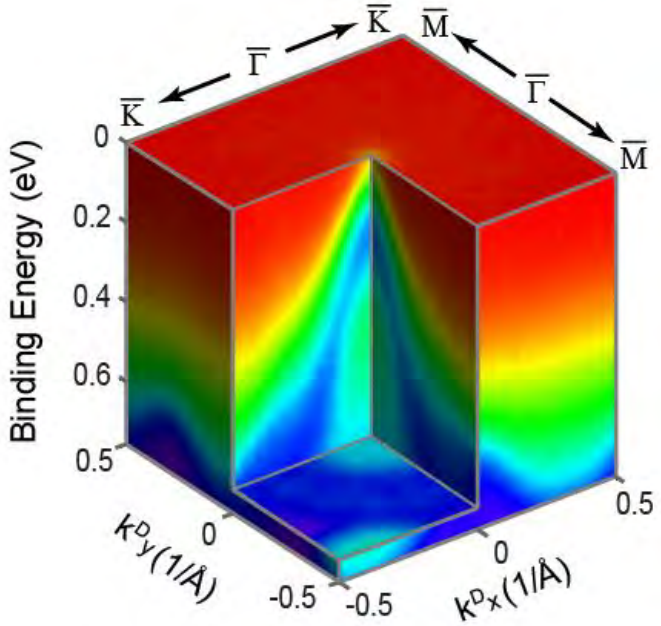


Projections to (*kx, ky, E*) space

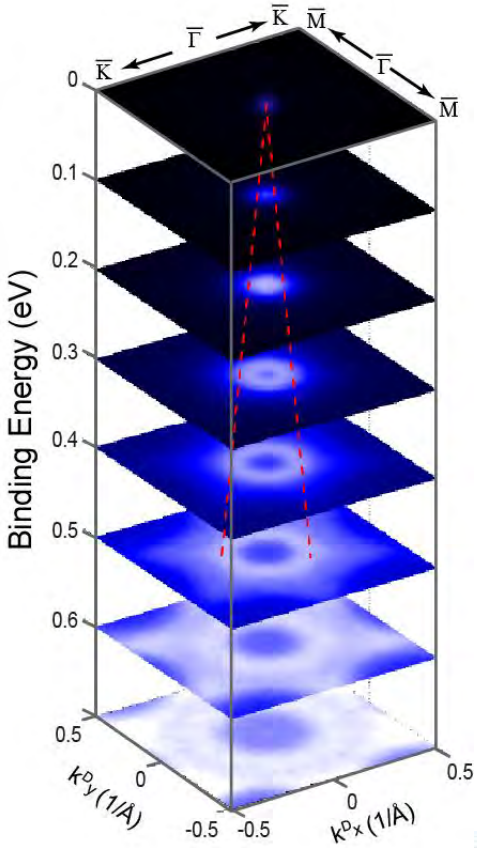
Fermi-surface



Band dispersion



Constant energy contours

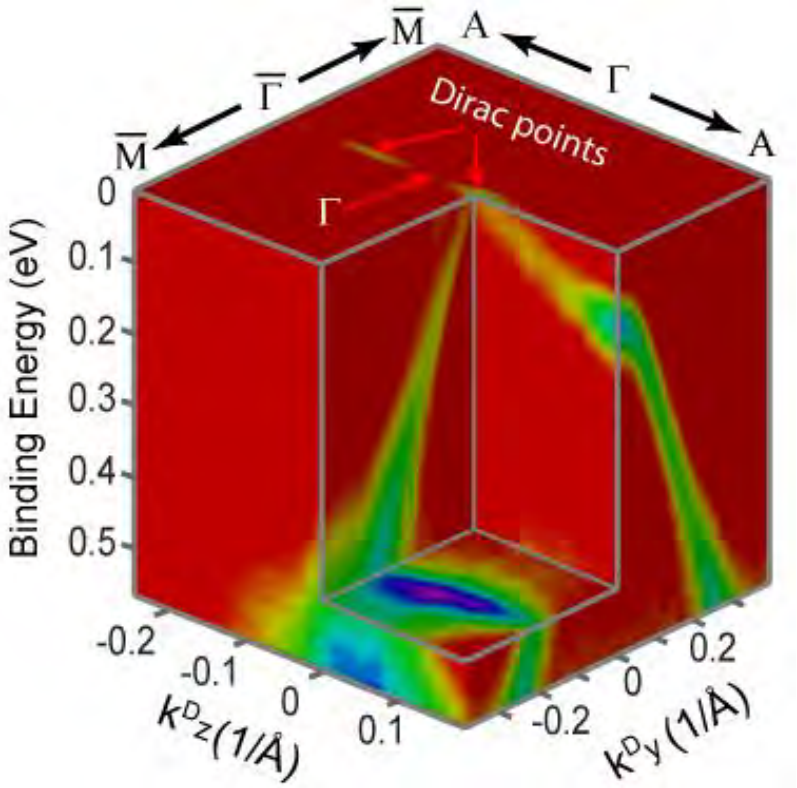


Vx = 2.75 eV•A or 4.17×10^5m/s

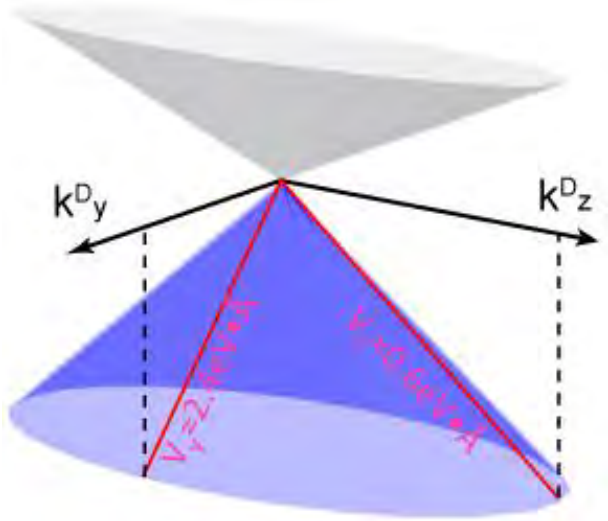
Vy = 2.39 eV•A or 3.63×10^5m/s

Projection to (ky, kz, E) space

Band dispersions

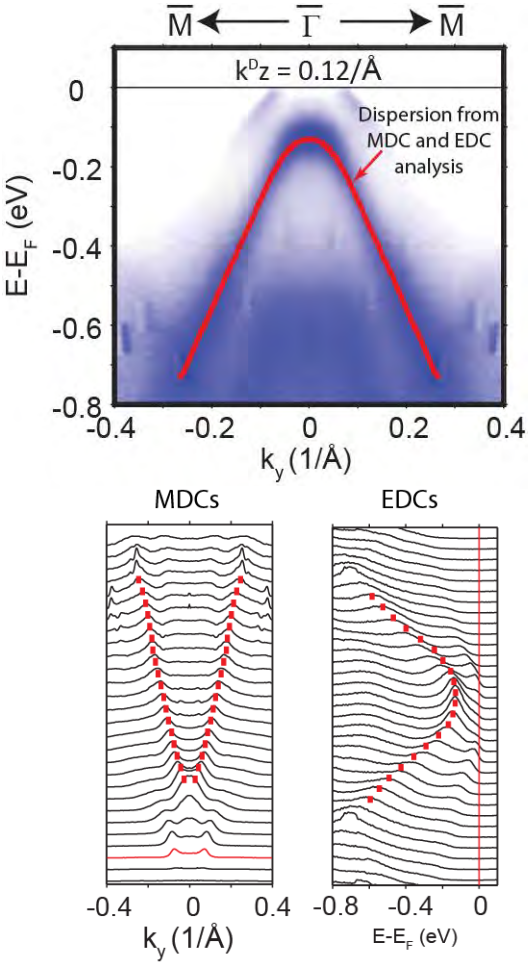


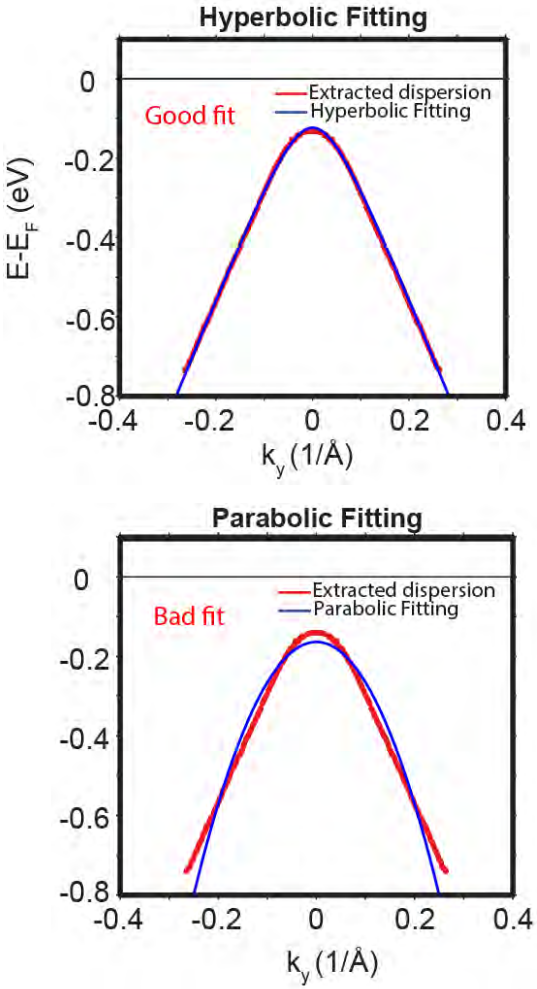
Strong anisotropy



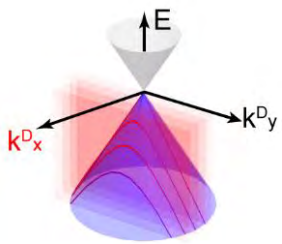
Vx = 2.75 eV•A	or	4.17×10^5m/s
Vy = 2.39 eV•A	or	3.63×10^5m/s
Vz = 0.6 eV•A	or	0.95×10^5m/s

Unusual hyperbolic dispersion

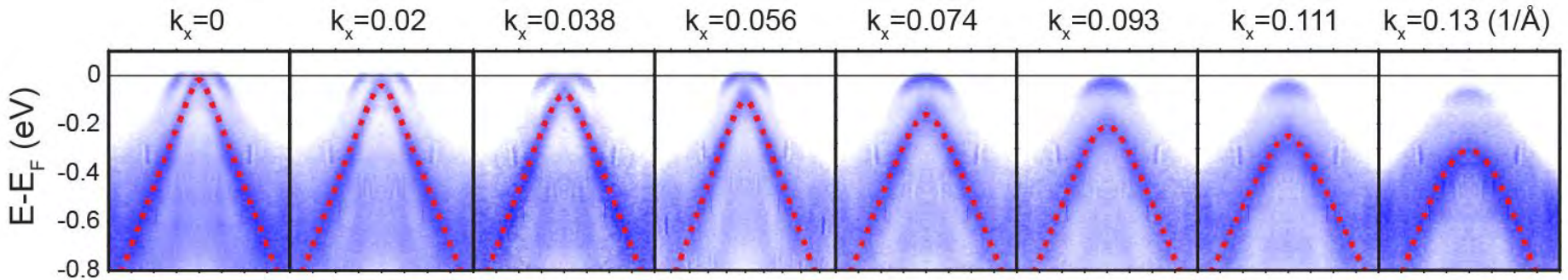


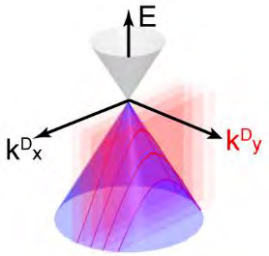


Dispersions at different *kx, ky* values

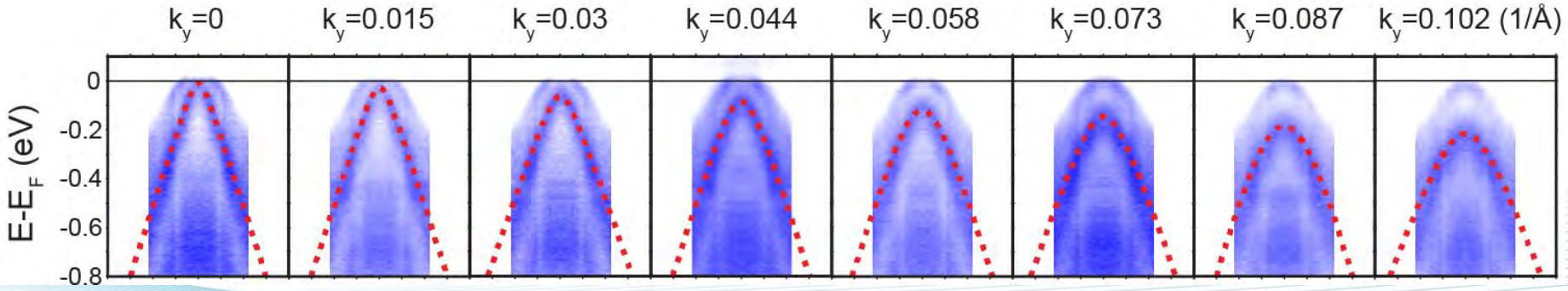


kx = 2.75 eV•A or 4.17×10^5m/s

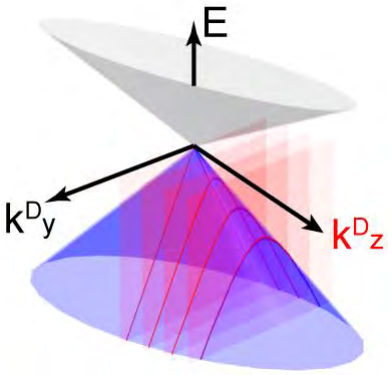




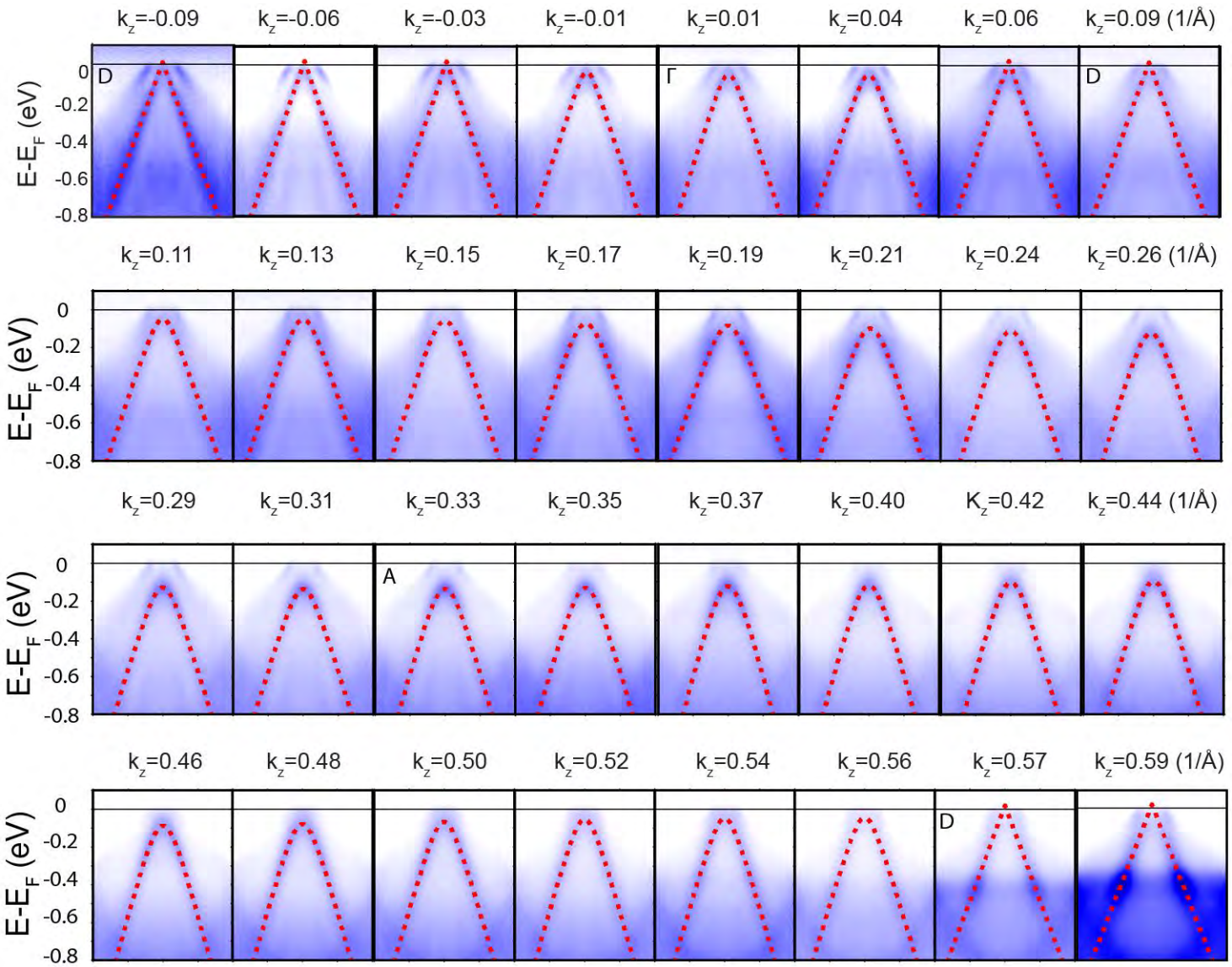
ky = 2.39 eV•A or 3.63×10^5m/s



Dispersions at different *kz* values

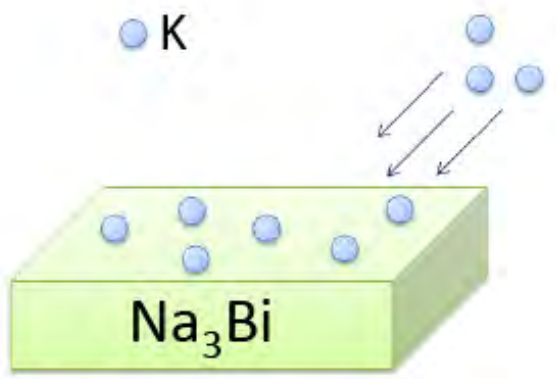


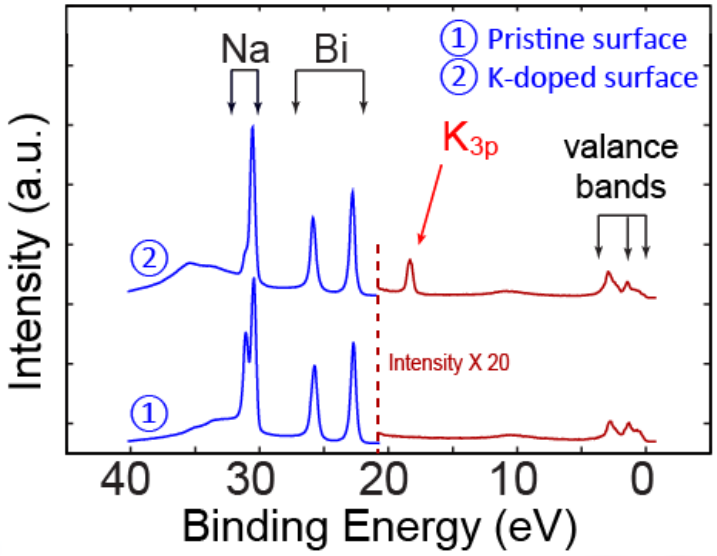
kz = 0.6 eV•A
or 0.95×10^5m/s

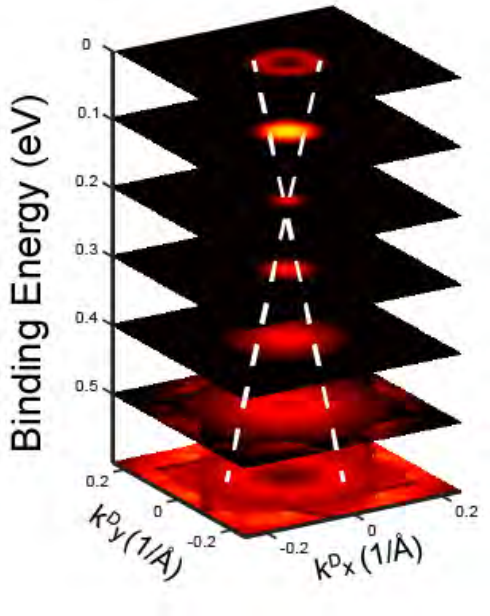


Observing the Dirac point and upper cone

***In-situ K*-doping**



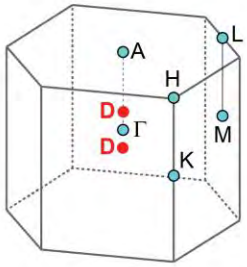




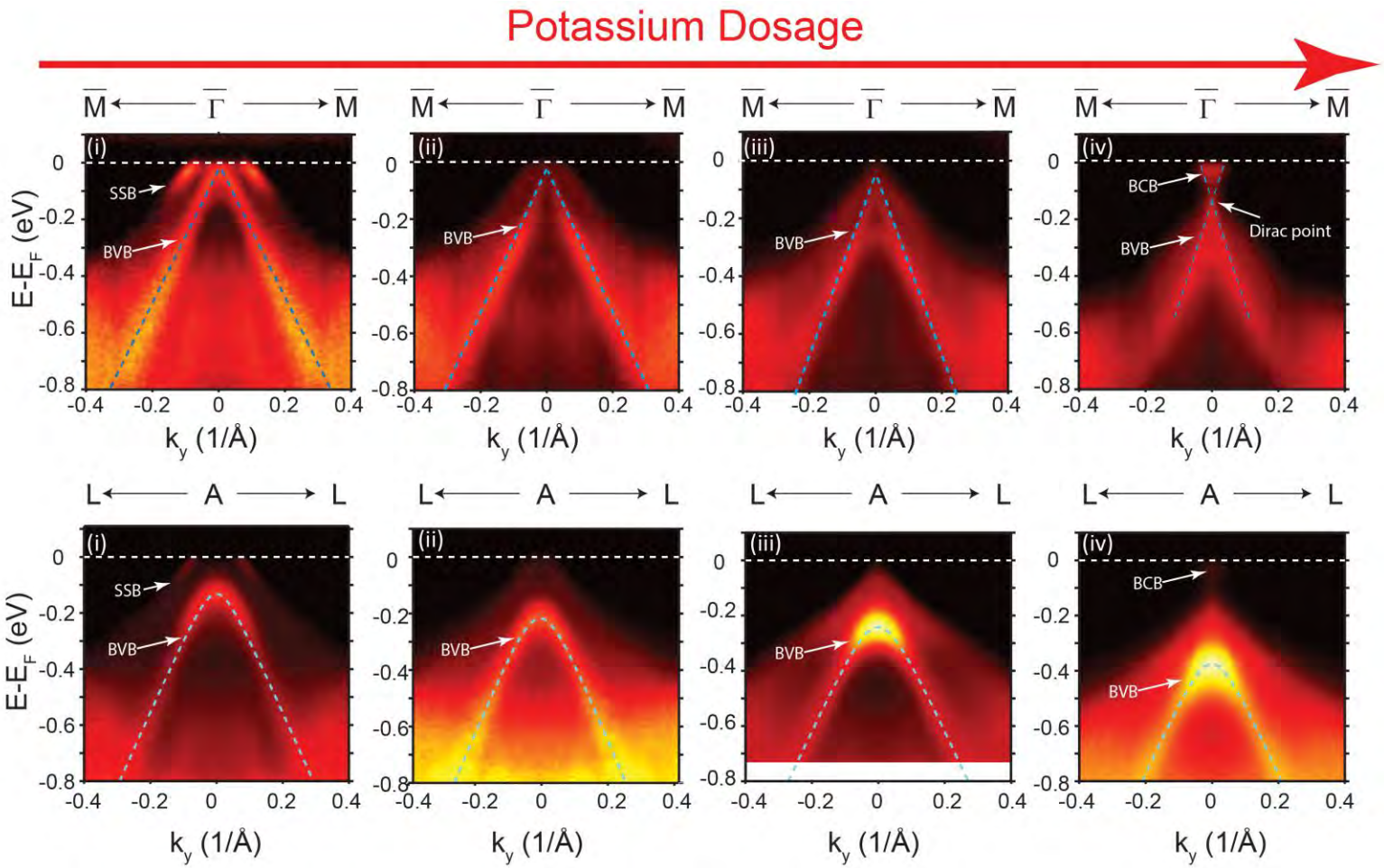
Protection of the crystalline symmetry

Disrupted surface state but intact bulk

kz=-0.09/Å
(Cut across the bulk Dirac point)

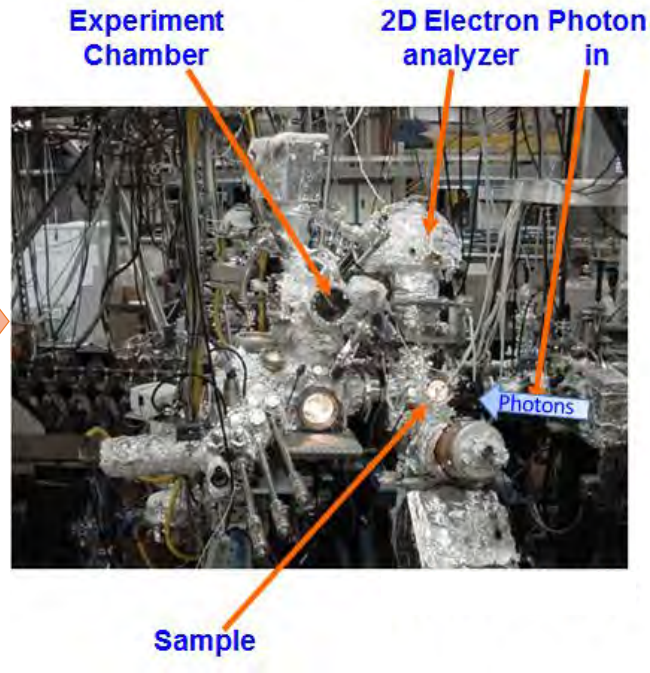


kz=0.327/Å
(Cut across the "A" point at the top of the BZ)



The problem of Na_3Bi

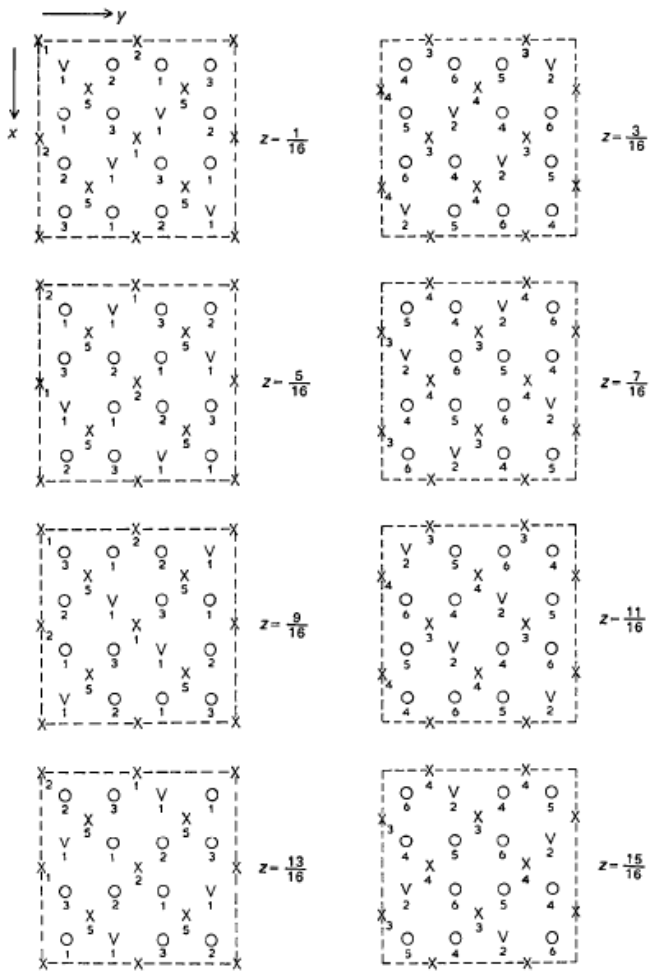
Too reactive in ambient environment …

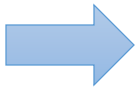


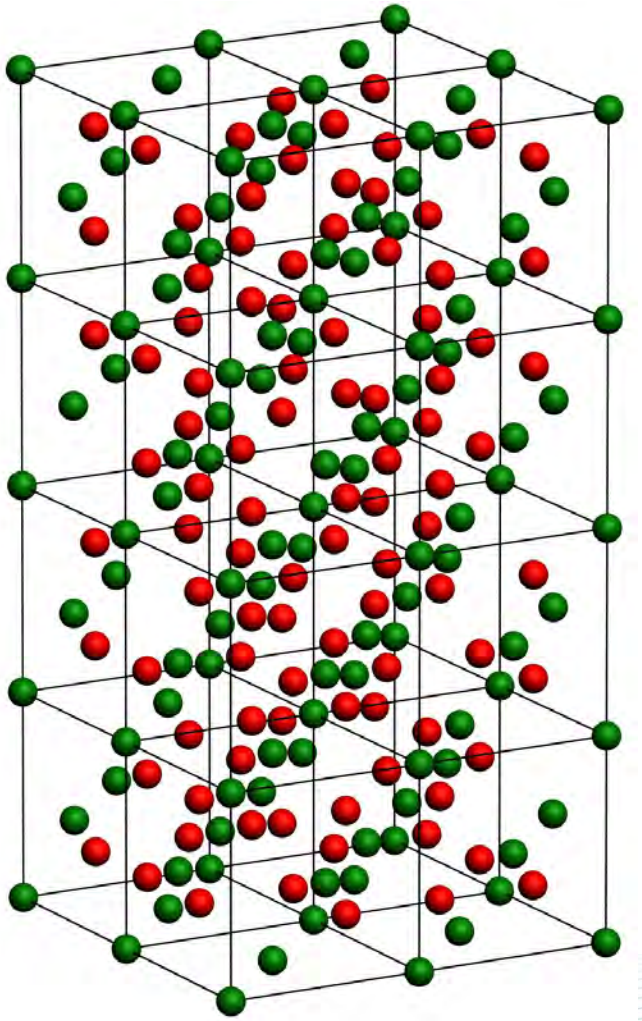
Hard to handle and used in functional devices

A stable 3D TDS, Cd_3As_2

Dizzying crystal structure…





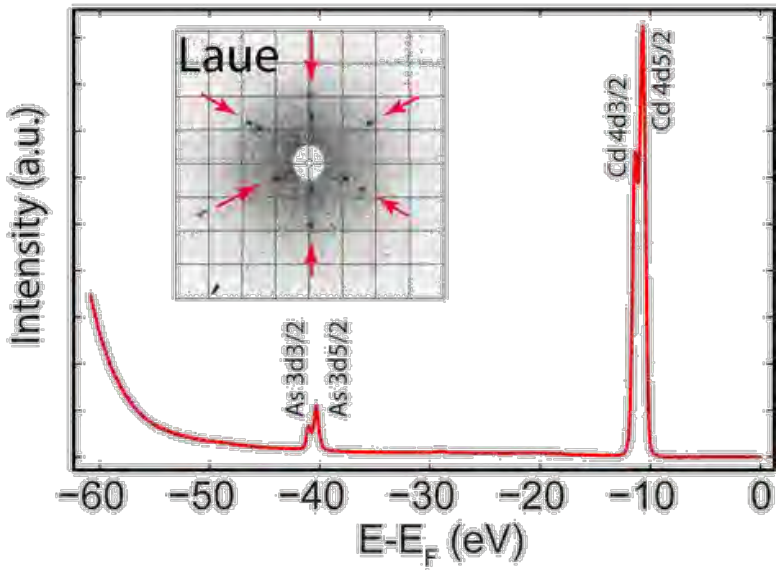


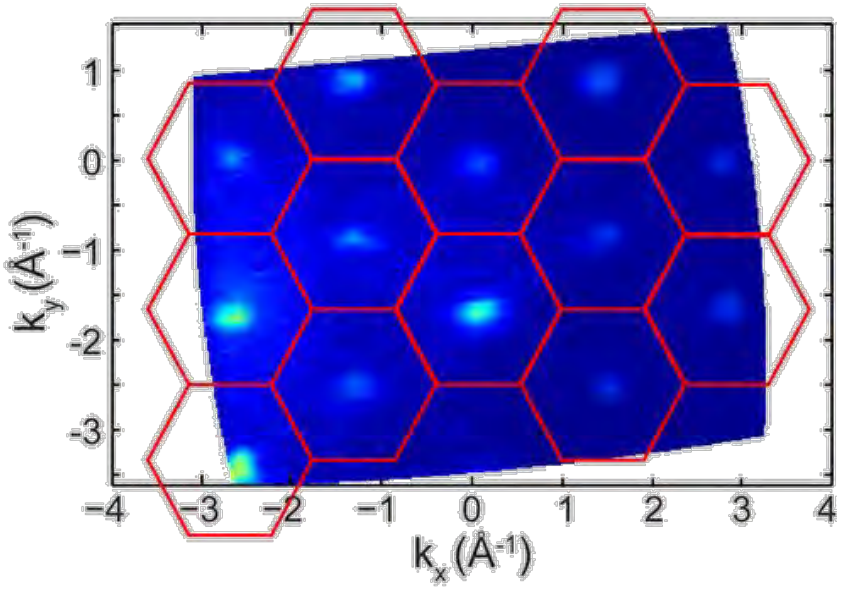
Steigmann and Goodyear
Acta Crystallographica Section B **24**(8): 1062 (1968)

A stable 3D TDS, Cd_3As_2

Z. K. Liu. *et. al.,* Nature Materials, 13, 677 (2014)

Laue, corelevel and broad FS mapping

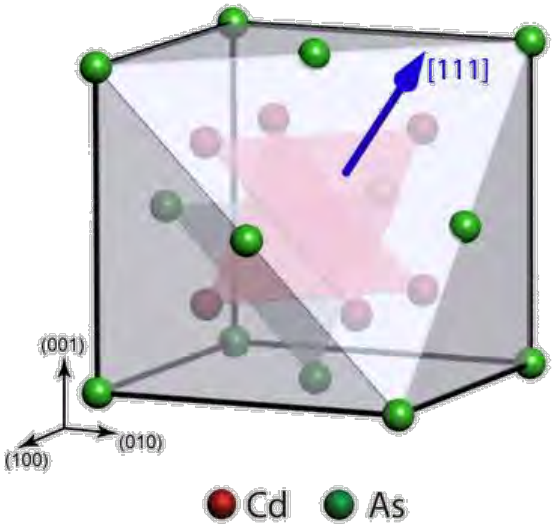


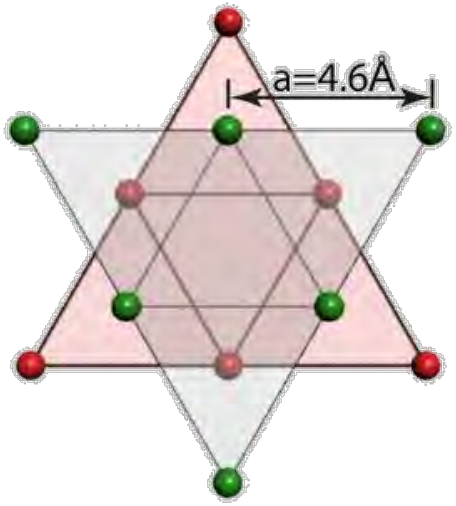


A stable 3D TDS, Cd_3As_2

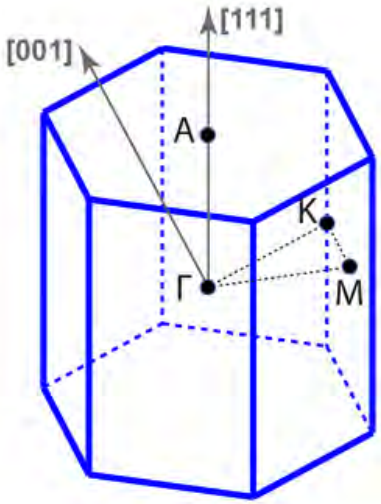
Z. K. Liu. *et. al.,* Nature Materials, 13, 677 (2014)

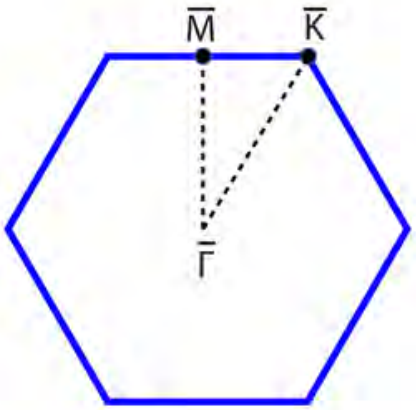
Crystal structure





Brillouin Zone

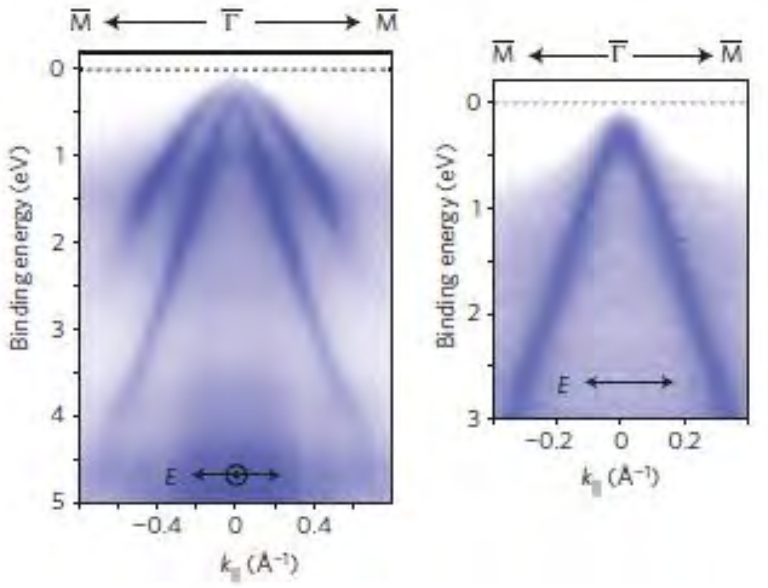




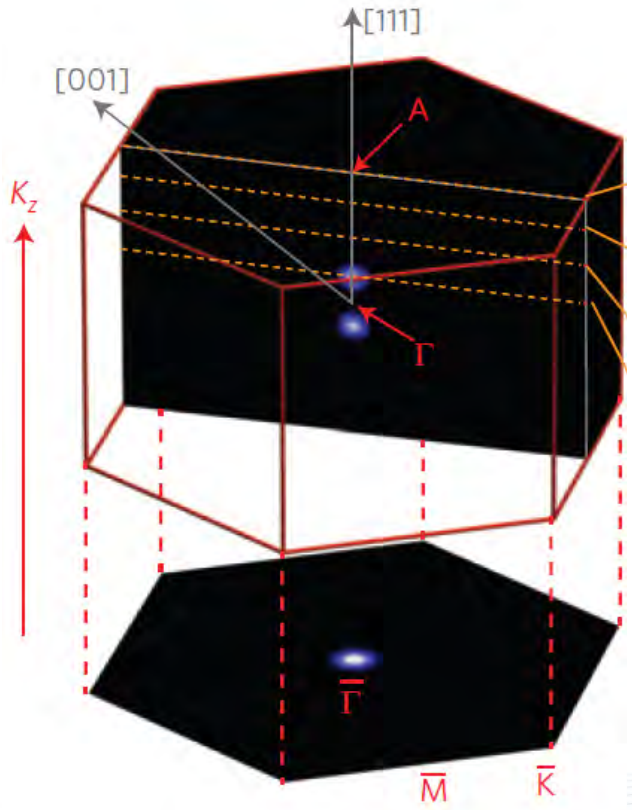
A stable 3D TDS, Cd_3As_2

Z. K. Liu. *et. al.,* Nature Materials, 13, 677 (2014)

Bands at different geometry

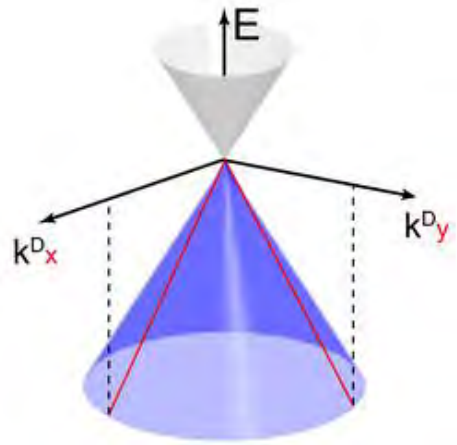


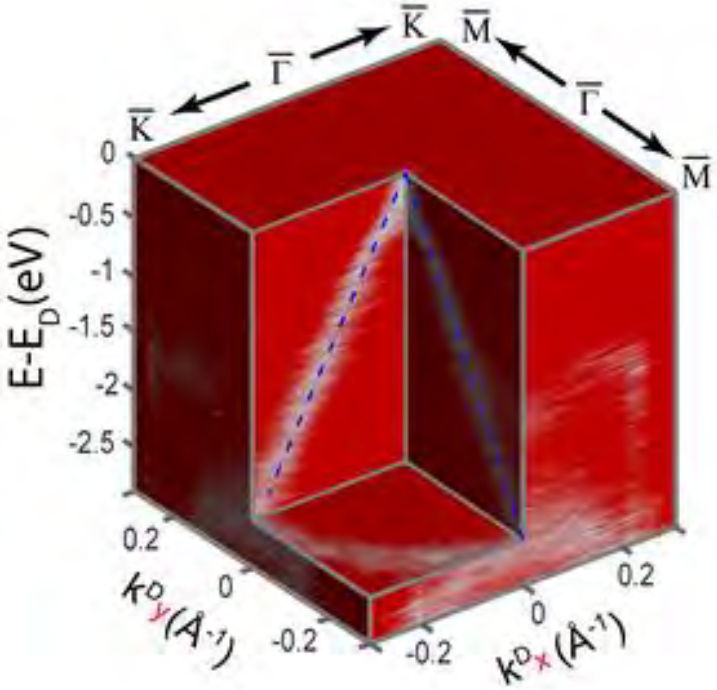
3D Fermi-Surface

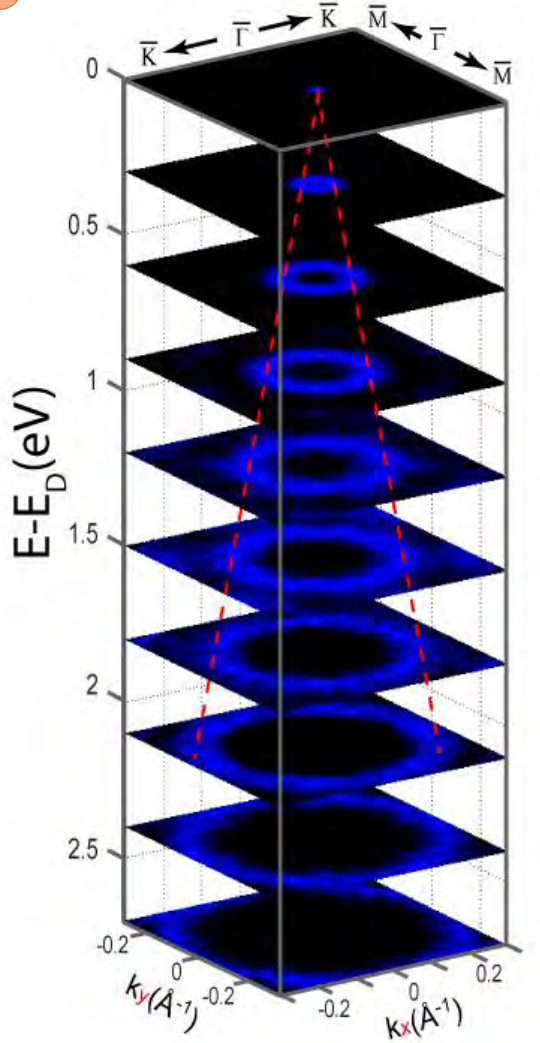


A stable 3D TDS, Cd_3As_2

Projection to (K_x,k_y,E)

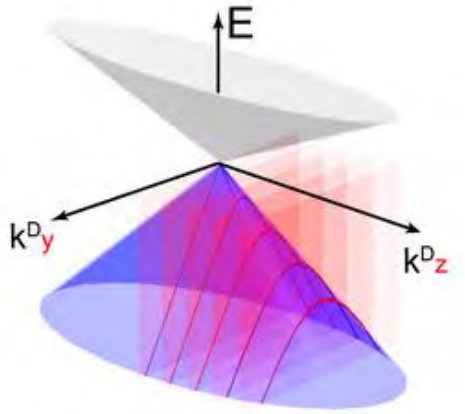


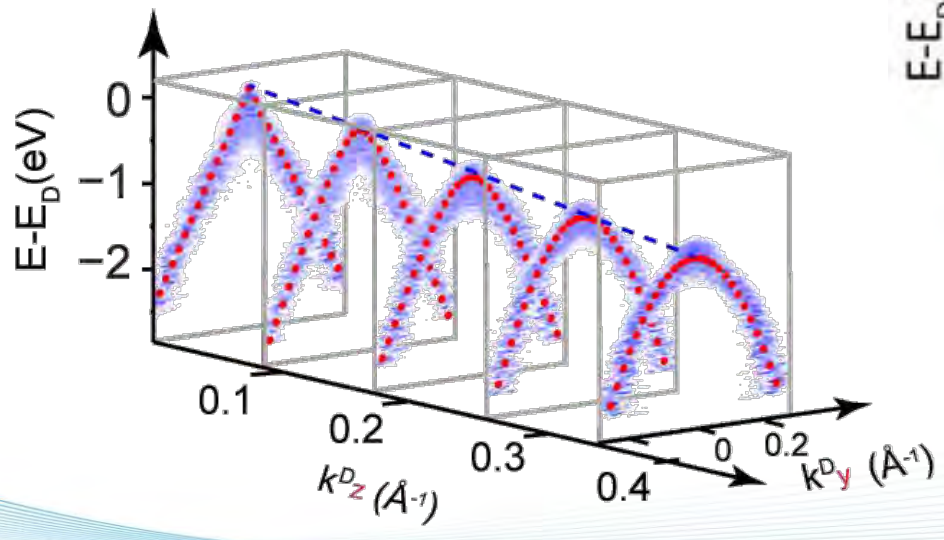


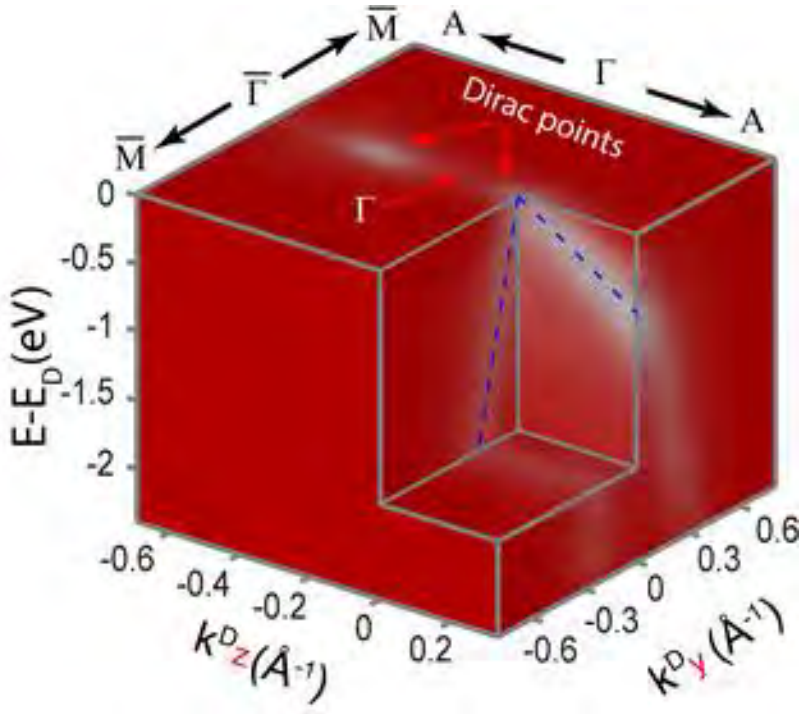


A stable 3D TDS, Cd_3As_2

Projection to (k_y,k_z,E)

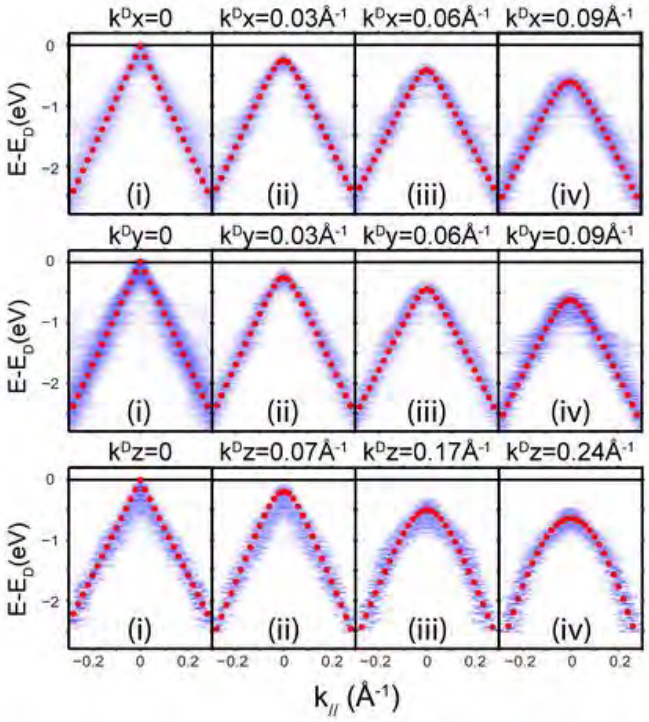






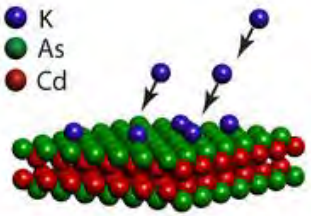
A stable 3D TDS, Cd_3As_2

Valence band

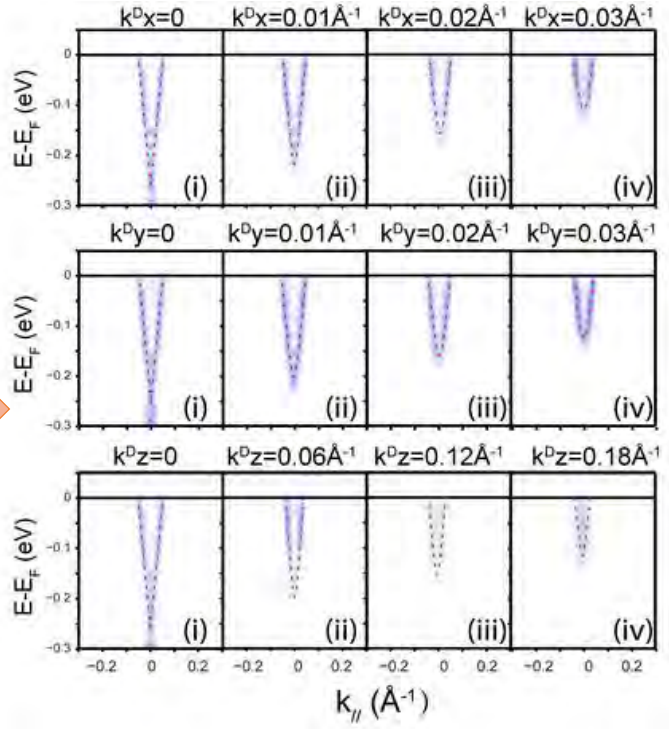


$V_x = 8.47$ eV•Å or 1.28×10^6 m/s
$V_y = 8.56$ eV•Å or 1.3×10^6 m/s
$V_z = 2.16$ eV•Å or 3.27×10^5 m/s

***In-situ K*-doping**

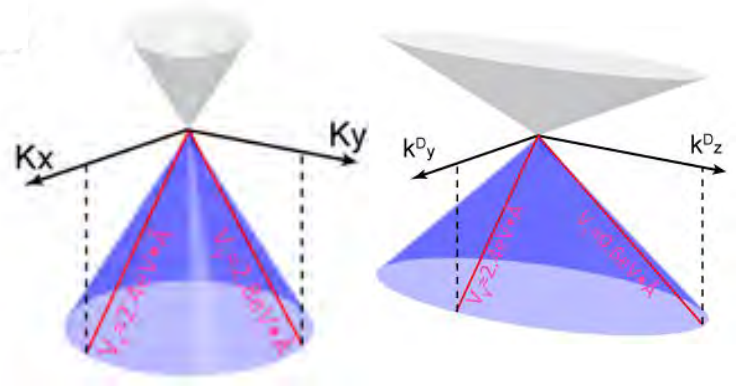


Conduction band



$V_x = 5$ eV•Å or 7.55×10^5 m/s
$V_y = 5.1$ eV•Å or 7.7×10^5 m/s
$V_z = 1.5$ eV•Å or 2.27×10^5 m/s

Parameter Extraction



- Discovery of a three-dimensional Dirac Fermion in Three-dimensional Dirac semimetal Na_3Bi and Cd_3As_2
- Stable objects, protected by topology

Fermi Velocity Comparison:

Na_3Bi: $V_x=4.17\times10^5$m/s, $V_y=3.63\times10^5$m/s, and $V_z=0.95\times10^5$m/s;

Cd_3As_2: $V_x=1.28\times10^6$m/s, $V_y=1.3\times10^6$m/s, and $V_z=3.27\times10^5$m/s;

Mobility $>4\times10^4$ $cm^2V^{-1}s^{-1}$ (T. Liang et al., Nat Mater 2014)

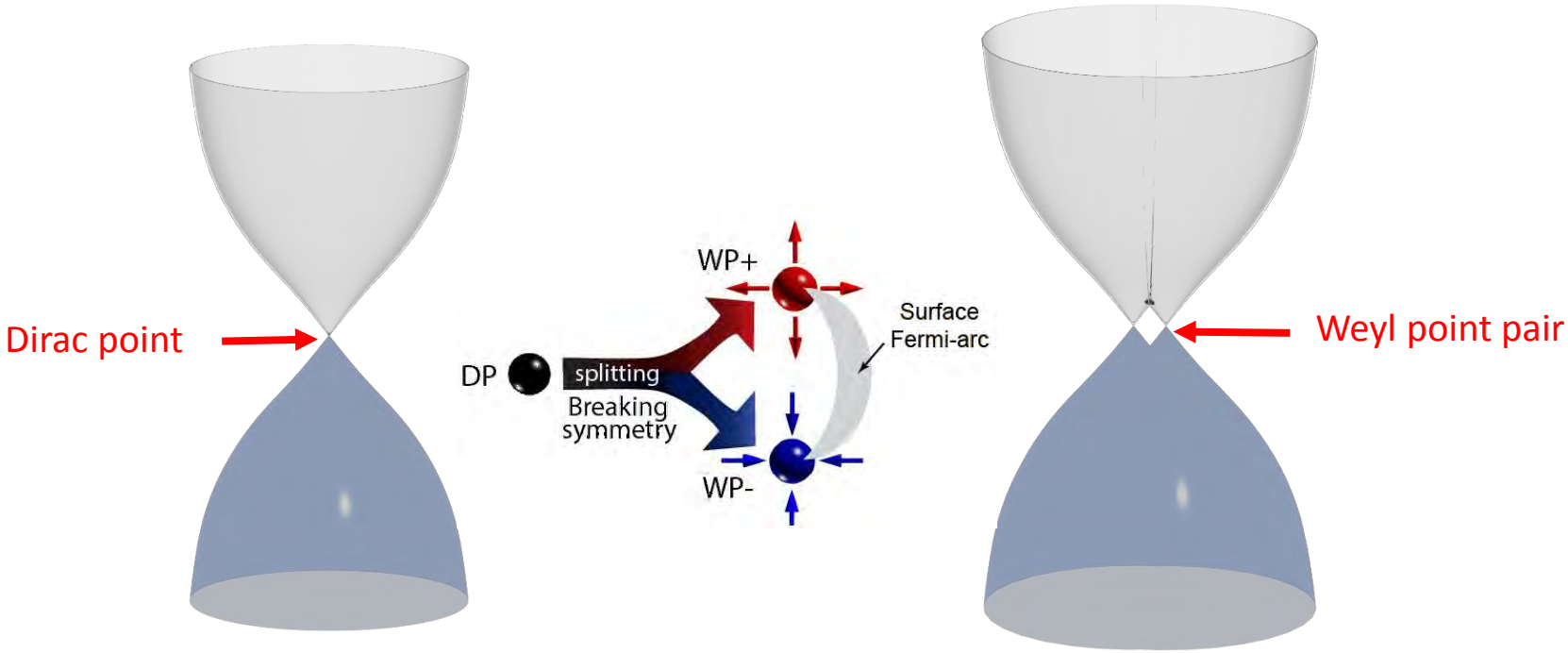
Bi_2Te_3: $V_{surface}=4\times10^5$m/s;

Graphene: $V_{Dirac}=1.1\times10^6$m/s;

Mobility $>1.5\times10^4$ $cm^2V^{-1}s^{-1}$ (Geim, A. K. & Novoselov, K. S. Nat Mater 2007)

High mobility & large amount of bulk electrons make TDS a promising material for electronic applications.

From Dirac to Weyl Semimetal



Topological Dirac Semimetal

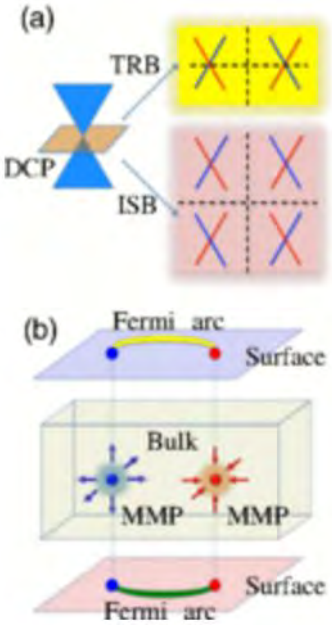
Electron as Dirac Fermions

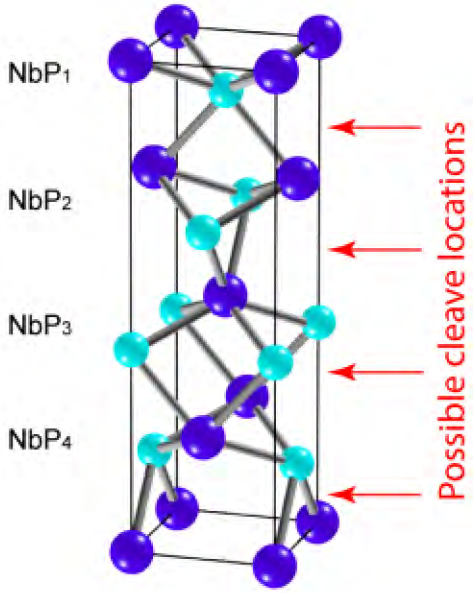
Topological Weyl Semimetal

Electron as Weyl Fermions:
½ of the Dirac Fermion

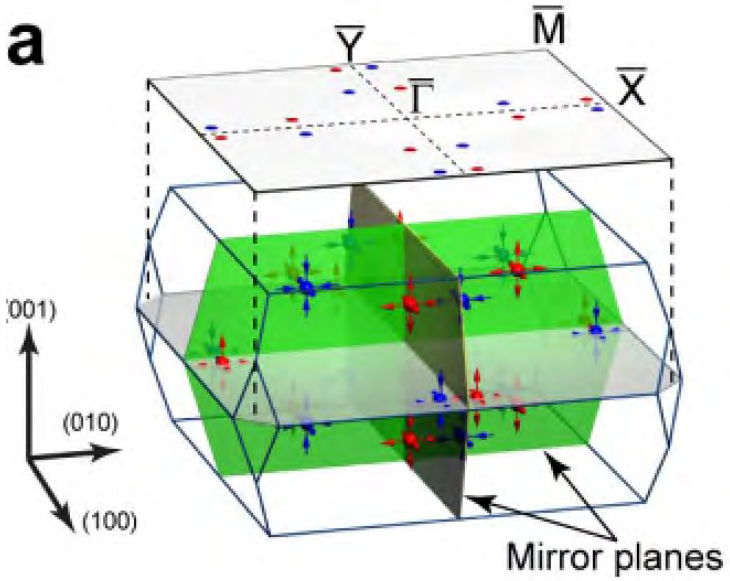
Model Materials:
Time reversal symmetry breaking: $HgCr_2Se_4$, $Y_2Ir_2O_7$,XCO_2Z, VCo_2Ga…
Inversion symmetry breaking: Ta(Nb)As(P), $SrSi_2$…

TWS in Inversion symmetry breaking transition metal monophosphide family





(BCT)



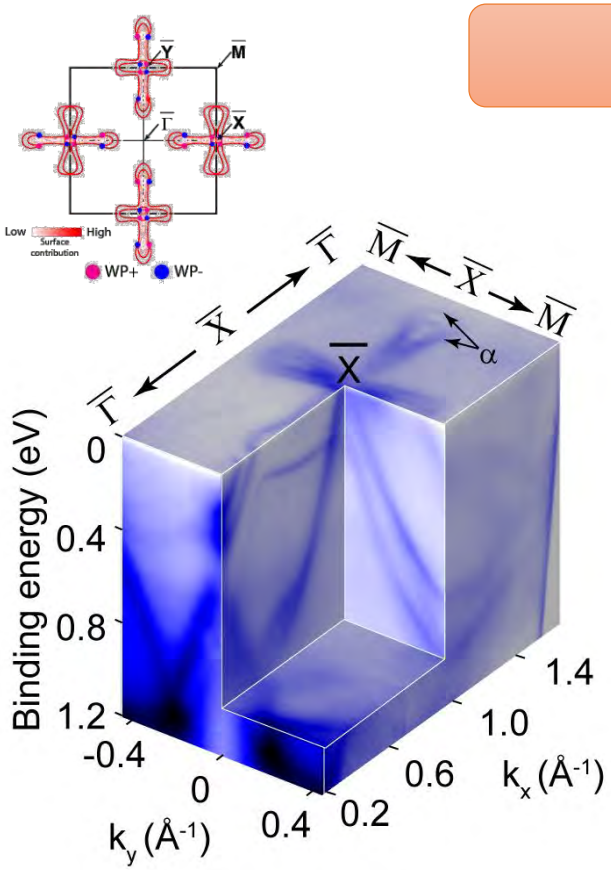
ARPES:

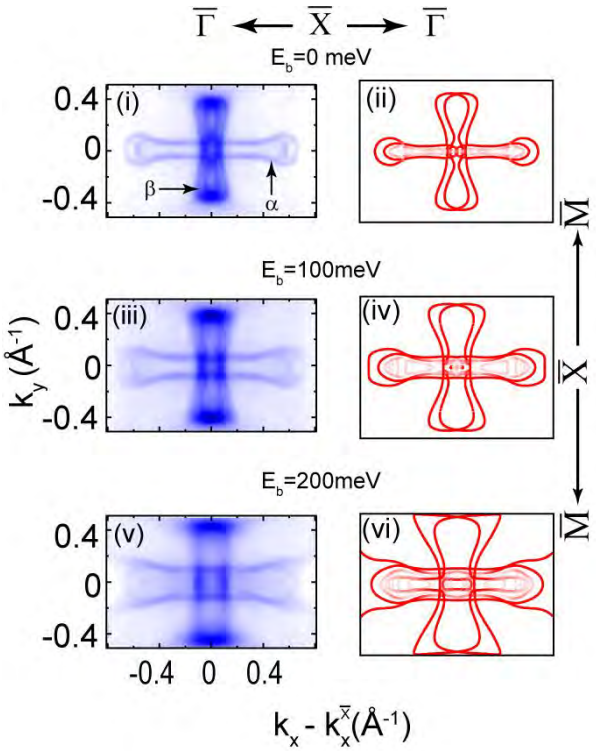
B. Q. Lv, et al., Phys. Rev. X 5, 031013 (2015)
B. Q. Lv, et al., Nature Physics 11, 724–727 (2015)
B. Q. Lv, et al., Phys. Rev. Lett. 115, 217601 (2015)
S.-Y. Xu, et al., Science 349, 613 (2015).
S.-M. Huang, et al., Nature Commun. 6:7373 (2015).
S.-Y. Xu, et al., Nature Physics 11, 748 (2015).
S.-Y. Xu, et al., Phys. Rev. Lett. 116, 096801 (2016)

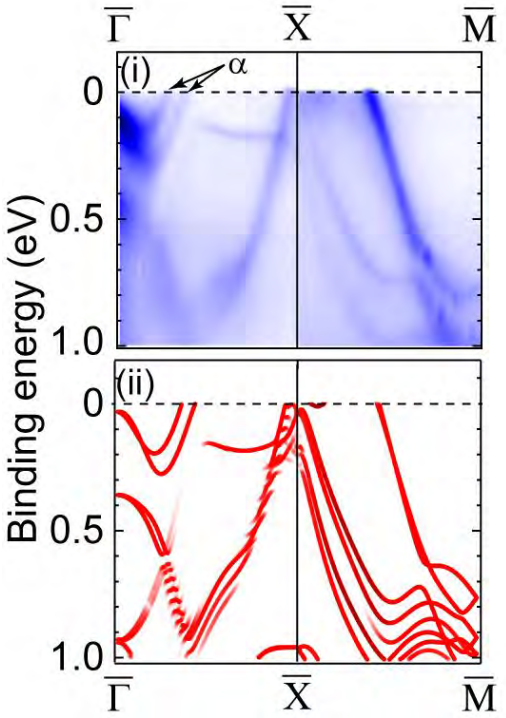
3D Topological Weyl Semimetal TaAs

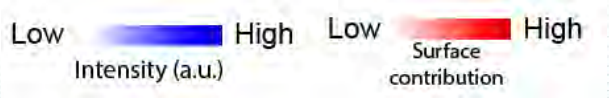
L. X. Yang, *et. al.*, *Nature Physics, 11, 728 (2015)*

Fermi-surface & band structures





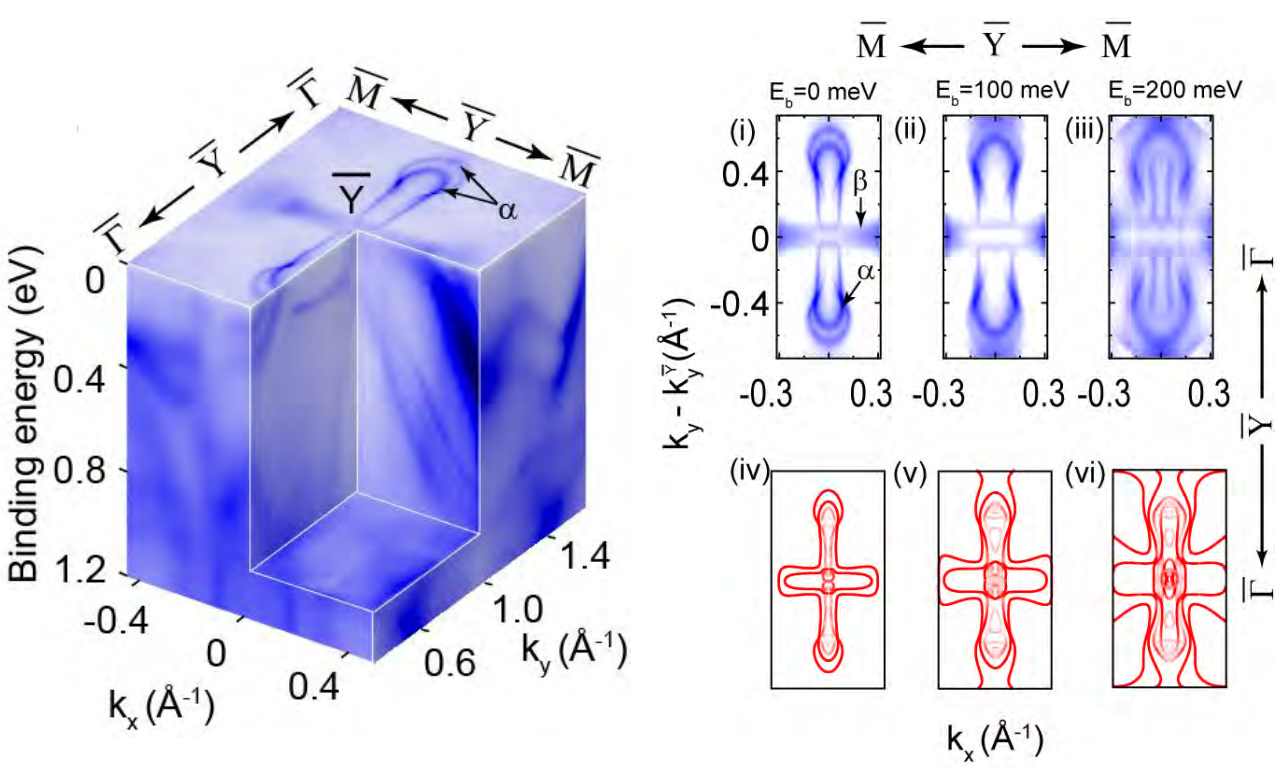


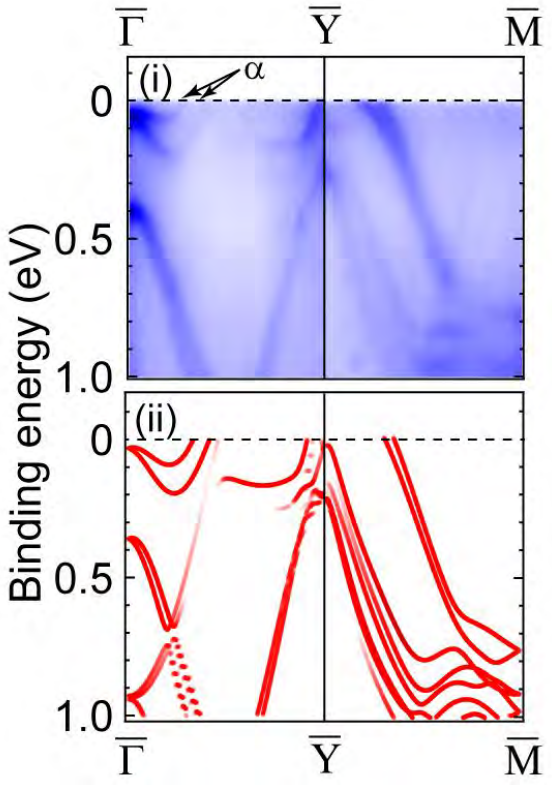


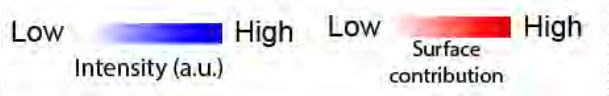
3D Topological Weyl Semimetal TaAs

L. X. Yang, *et. al.*, *Nature Physics, 11, 728 (2015)*

Rich texture of the band structure

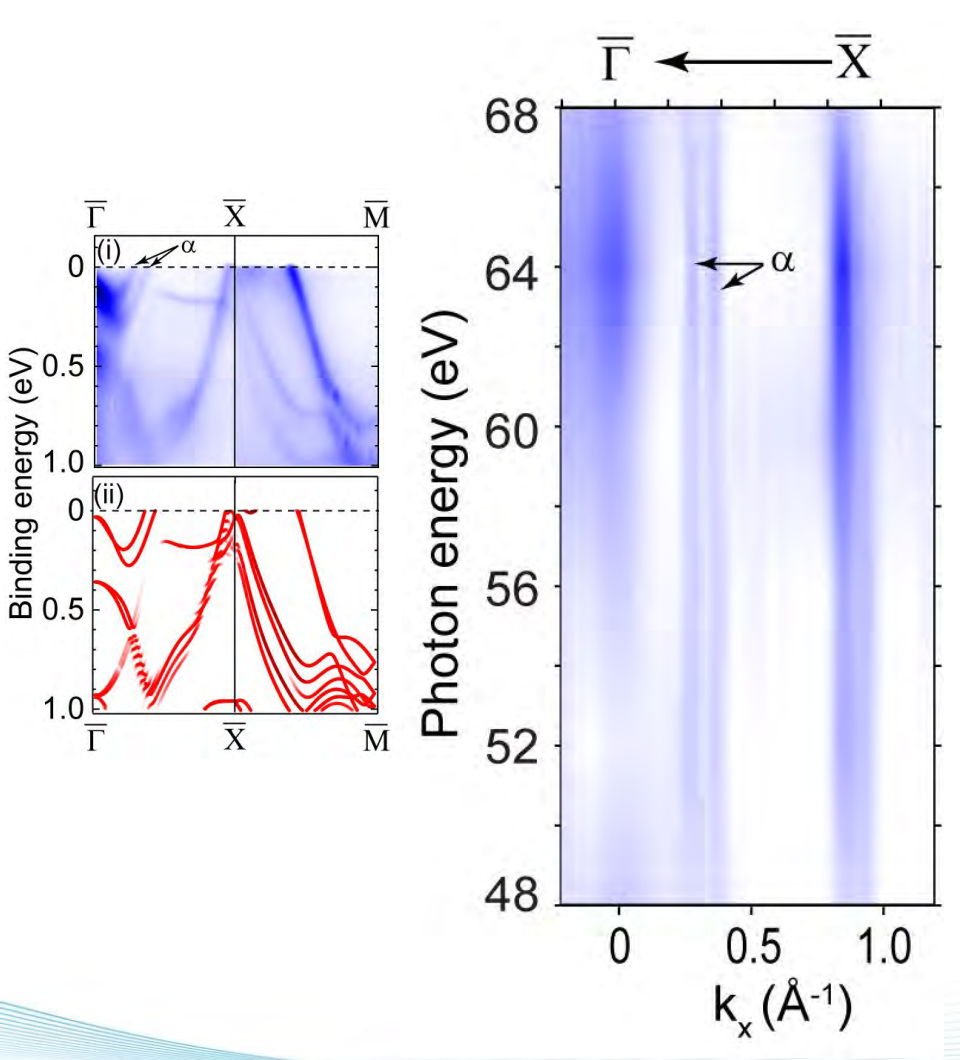


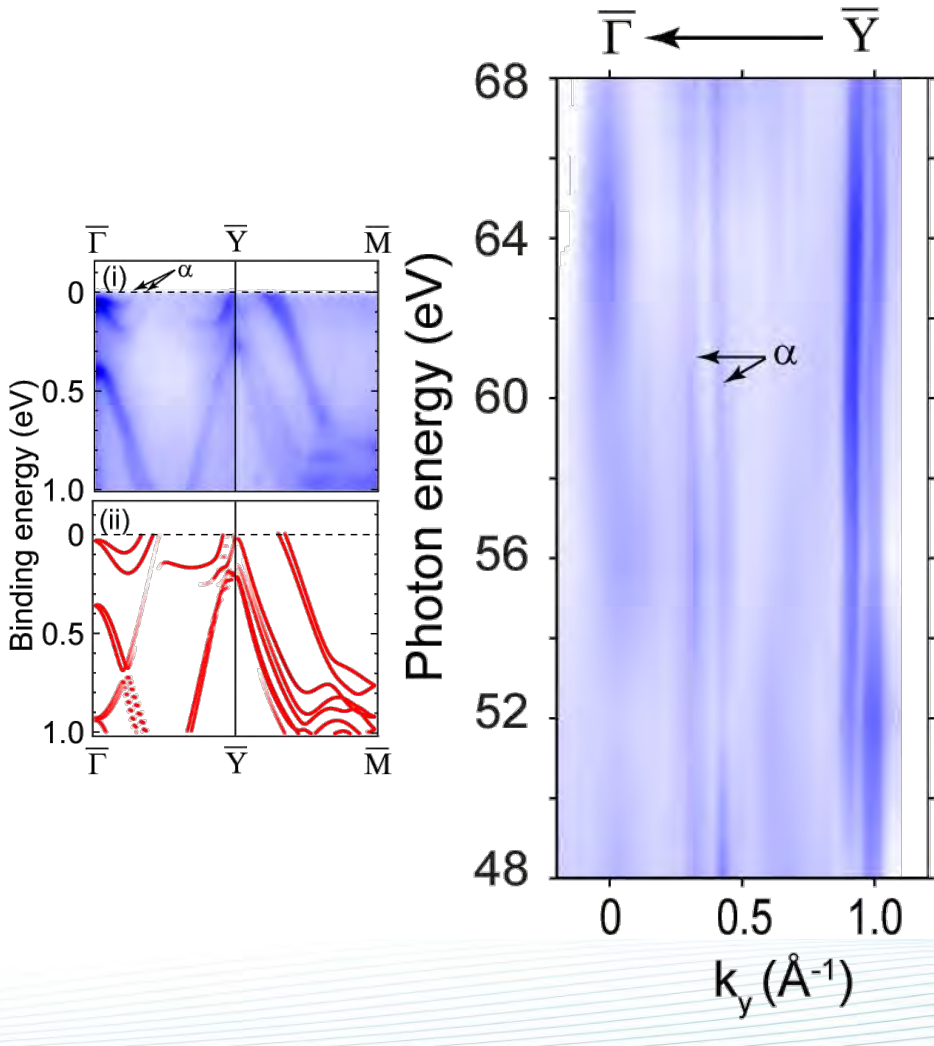




3D Topological Weyl Semimetal TaAs

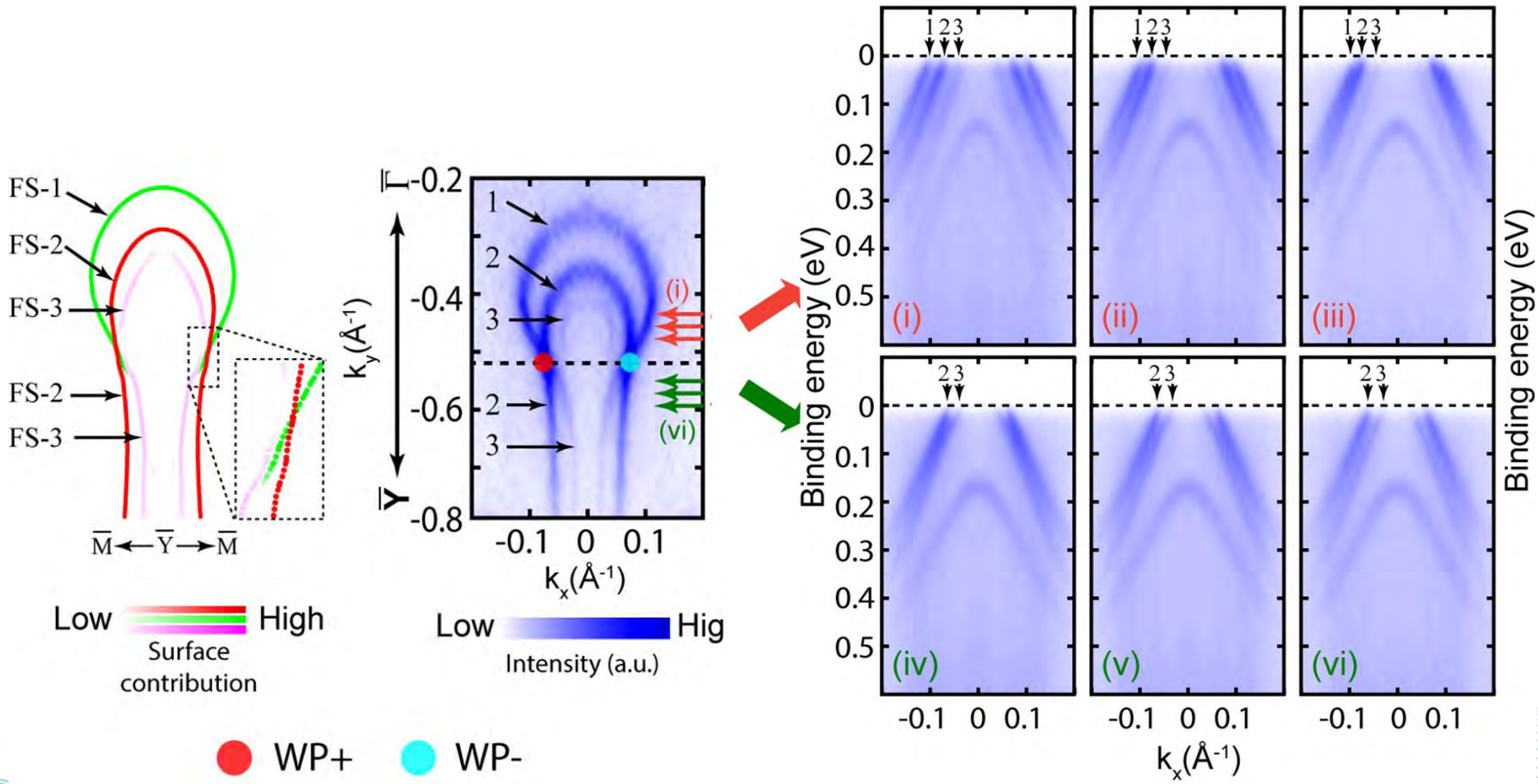
Surface or bulk state?





3D Topological Weyl Semimetal TaAs

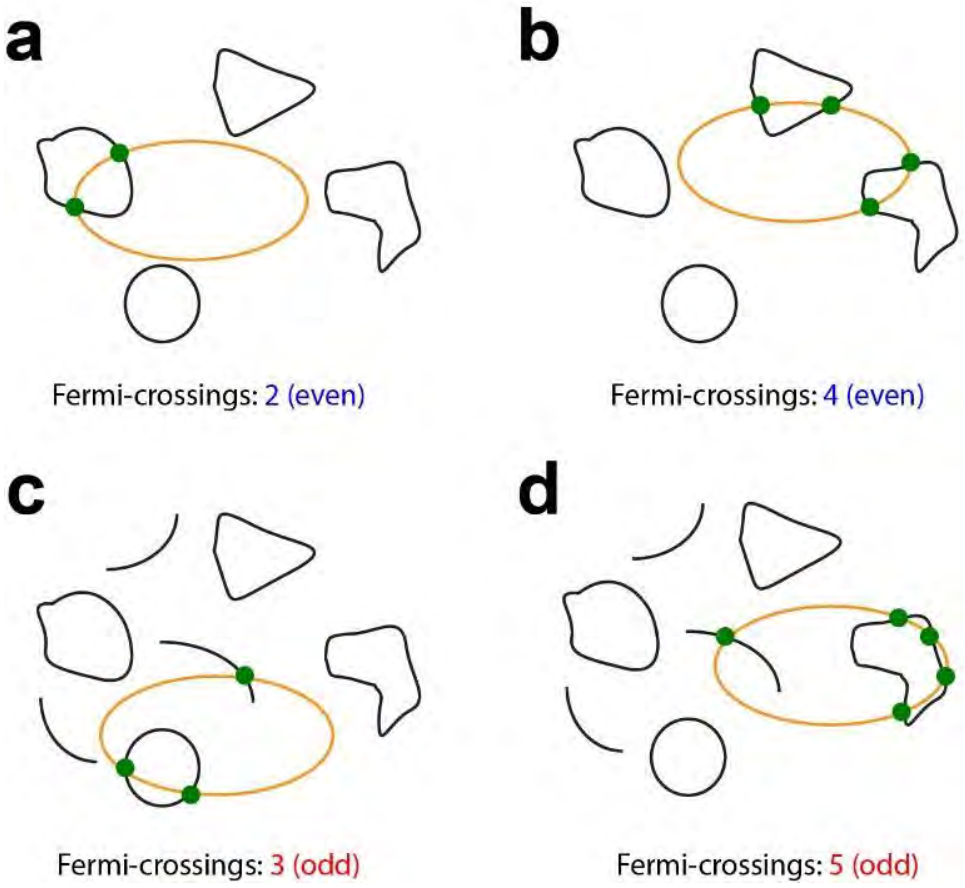
Identify the Fermi-arcs

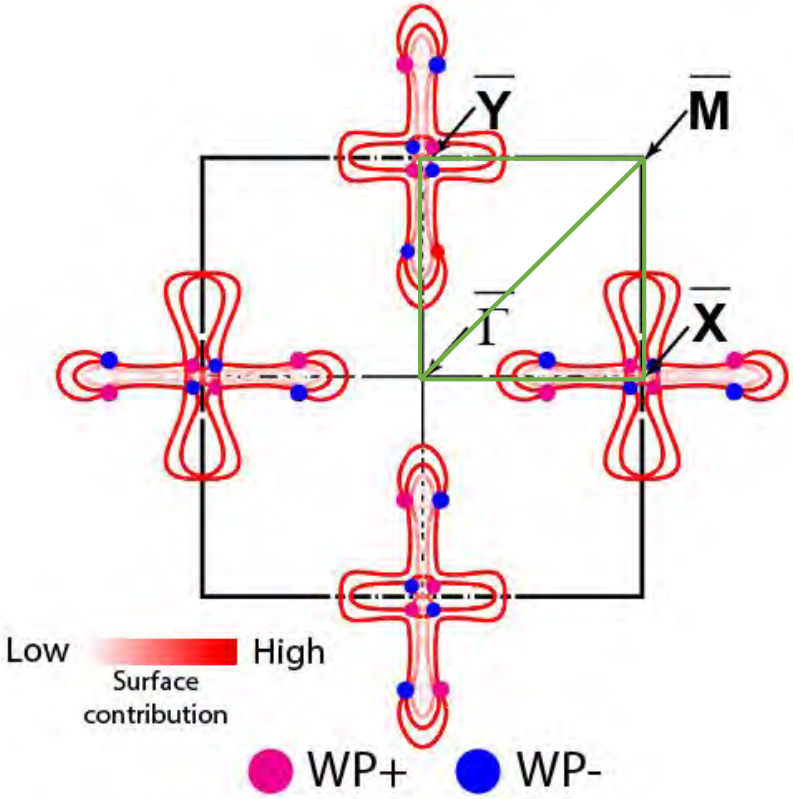


3D Topological Weyl Semimetal TaAs

L. X. Yang, *et. al., Nature Physics, 11, 728 (2015)*

Other Method to identify Fermi-arcs?

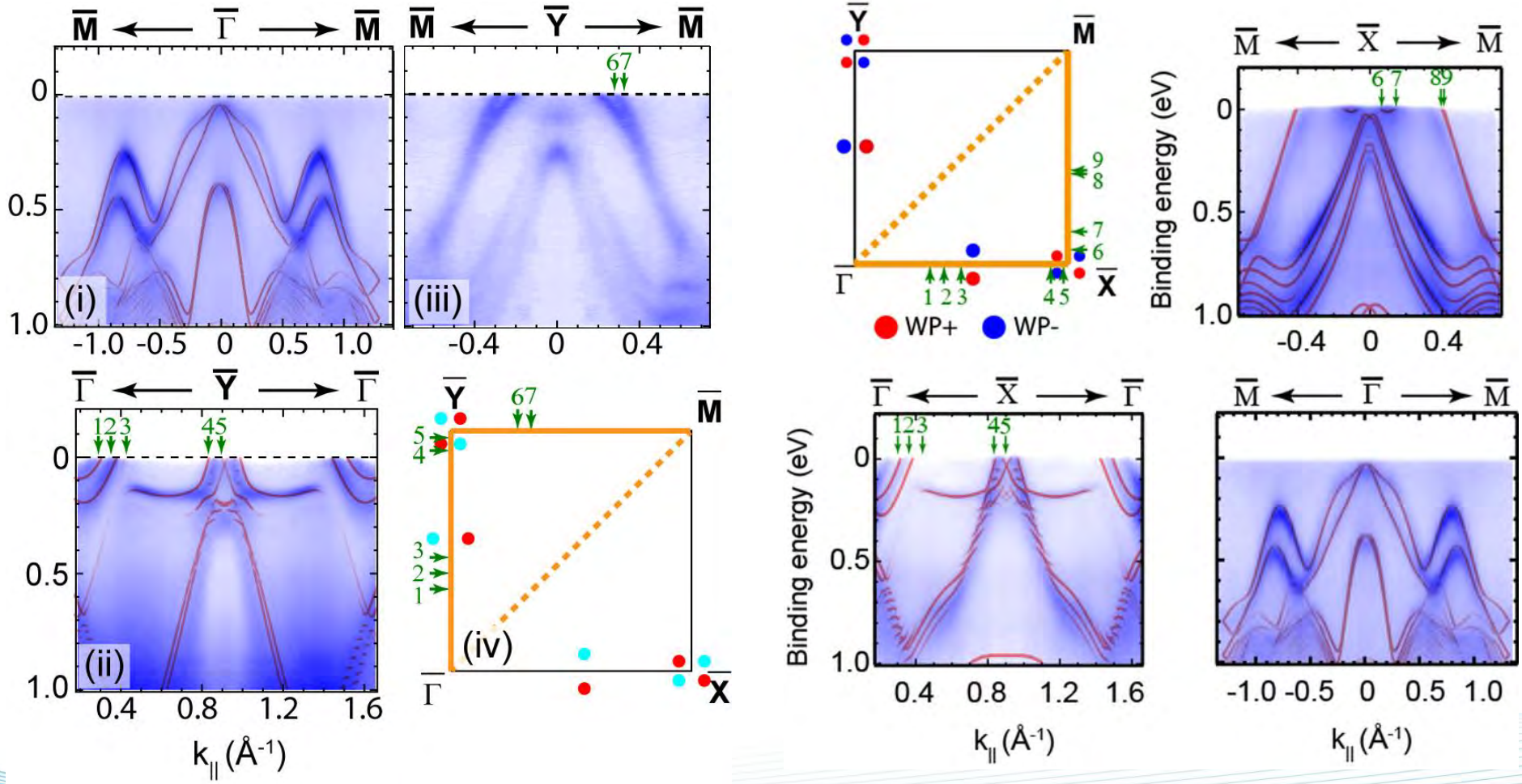




3D Topological Weyl Semimetal TaAs

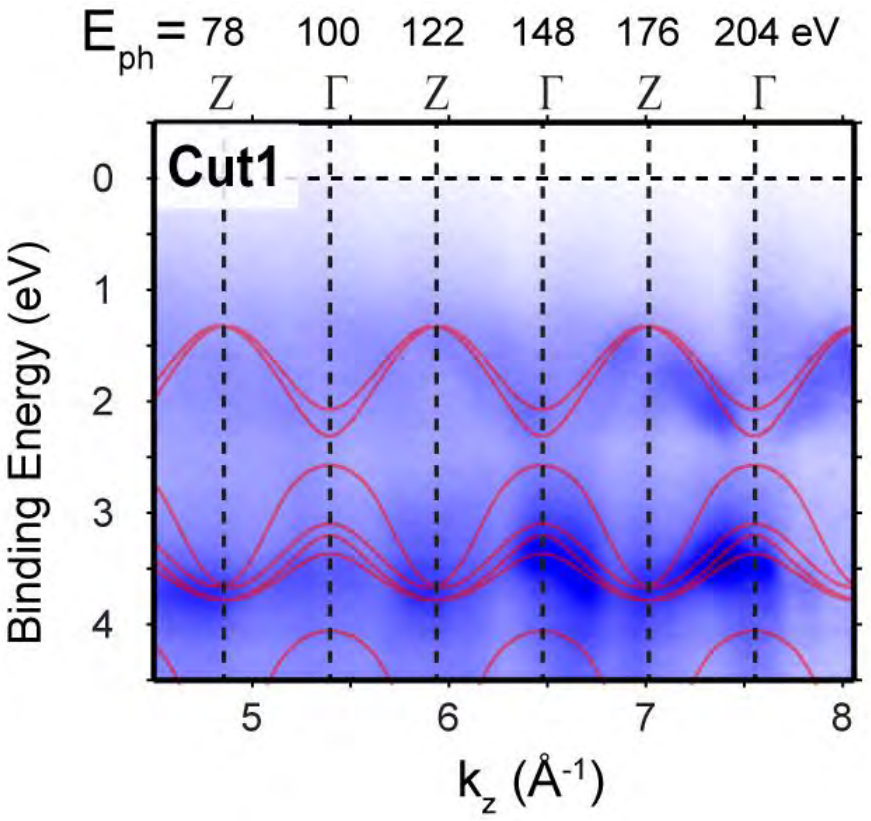
L. X. Yang, *et. al.*, *Nature Physics, 11, 728 (2015)*

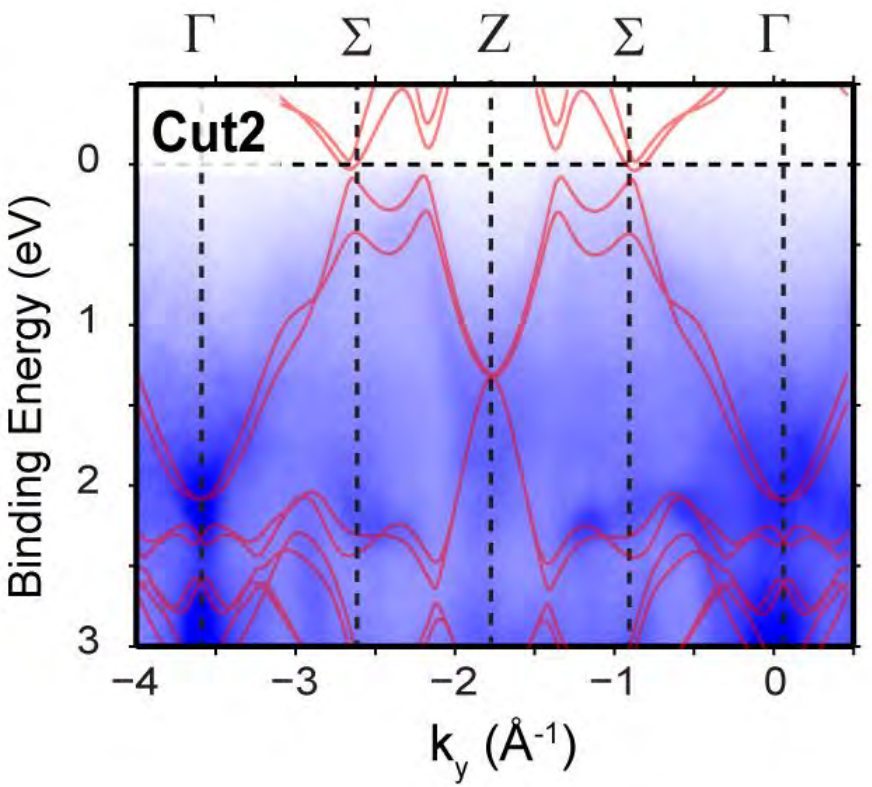
Fermi-crossings from two closed loops



3D Topological Weyl Semimetal TaAs

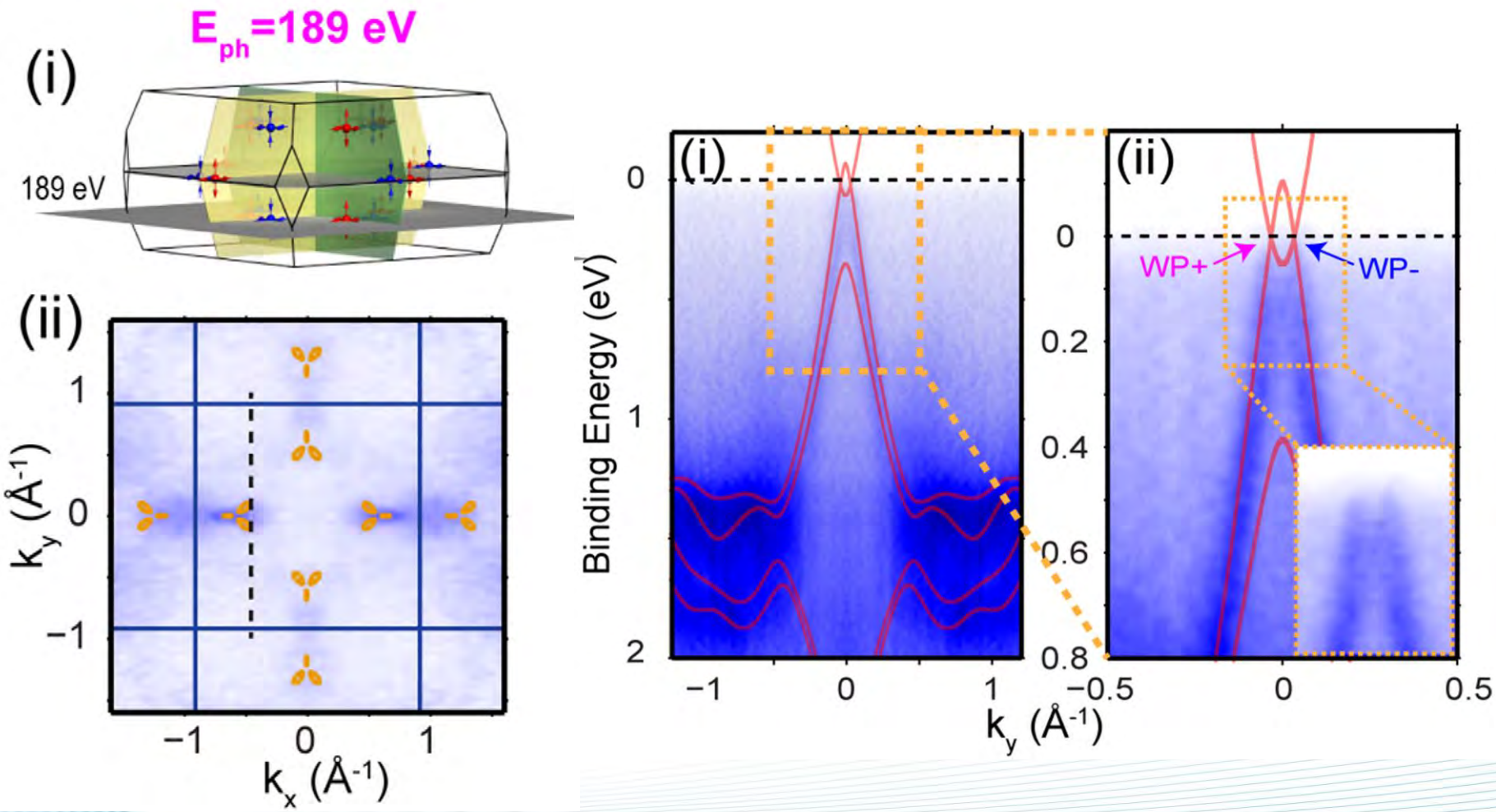
Dispersions along k_z direction





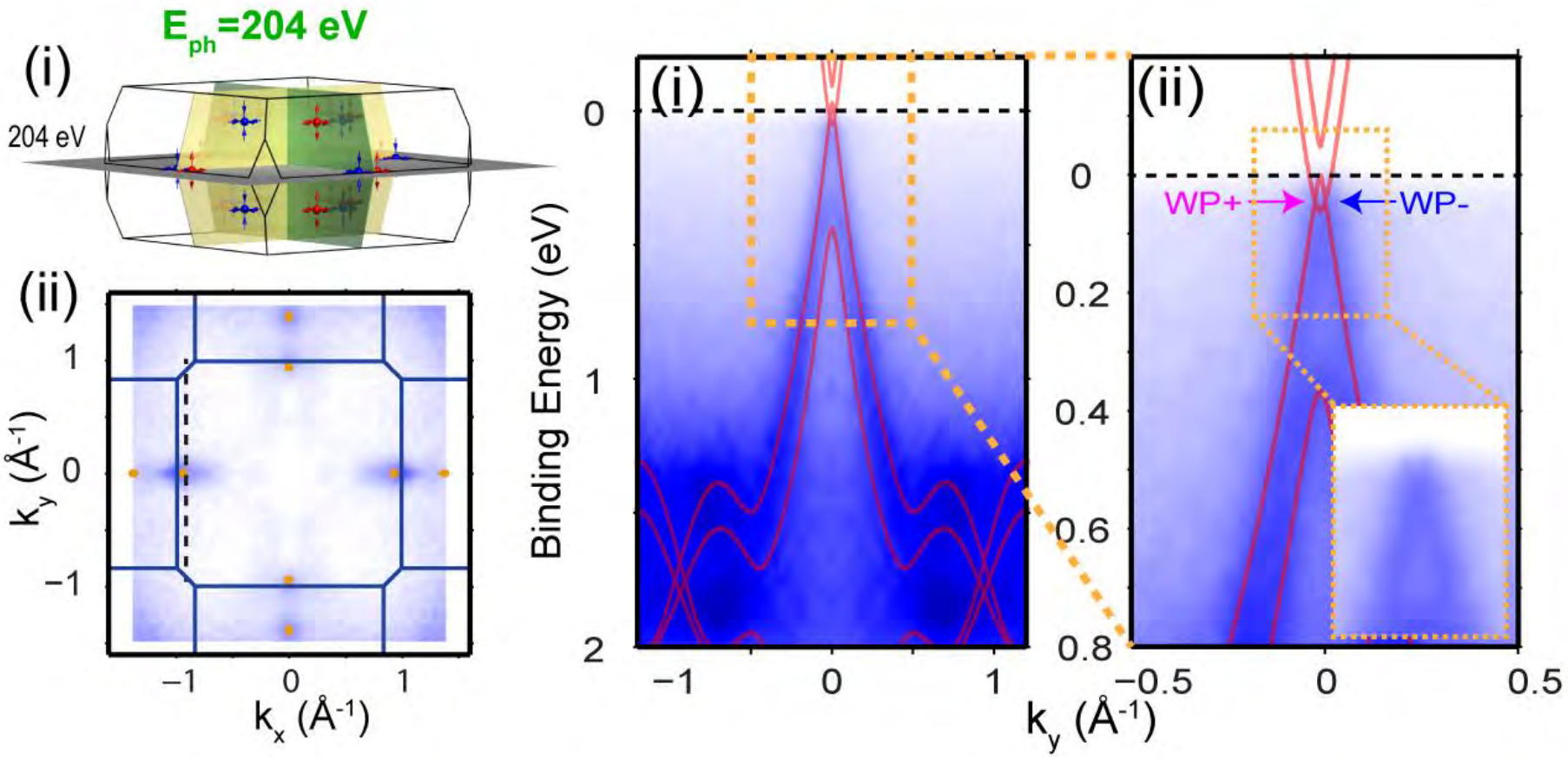
3D Topological Weyl Semimetal TaAs

Bulk dispersions near the Weyl points



3D Topological Weyl Semimetal TaAs

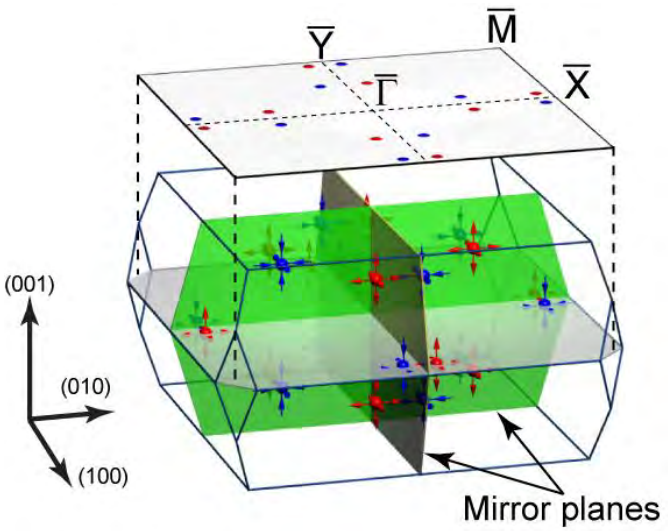
Bulk dispersions near the Weyl points

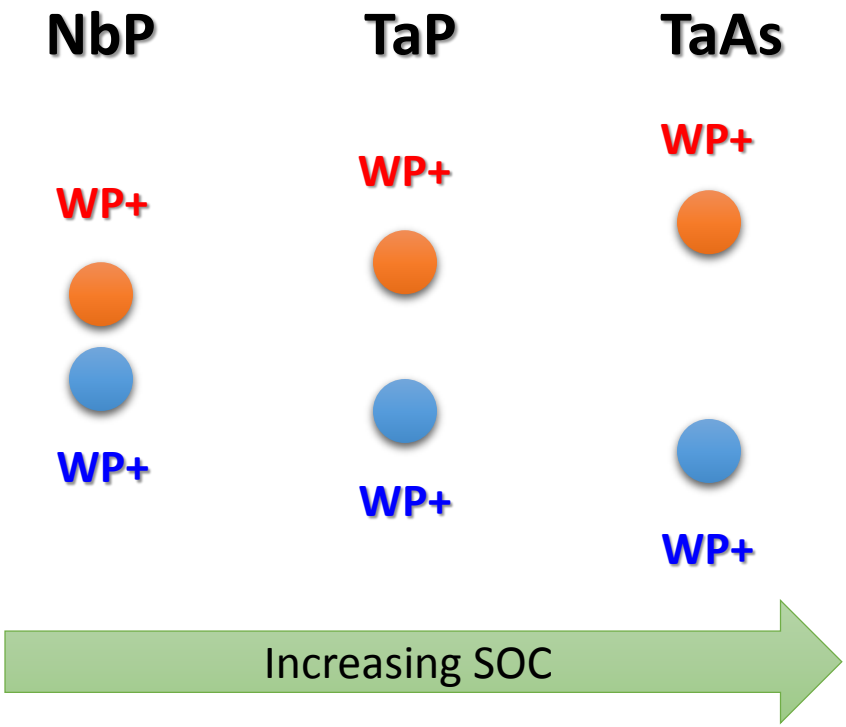


Fermiology Evolution of Weyl Semimetals

Z. K. Liu, *et. al., Nature Materials, 15, 27 (2016)*

Evolution of band structure of different compounds

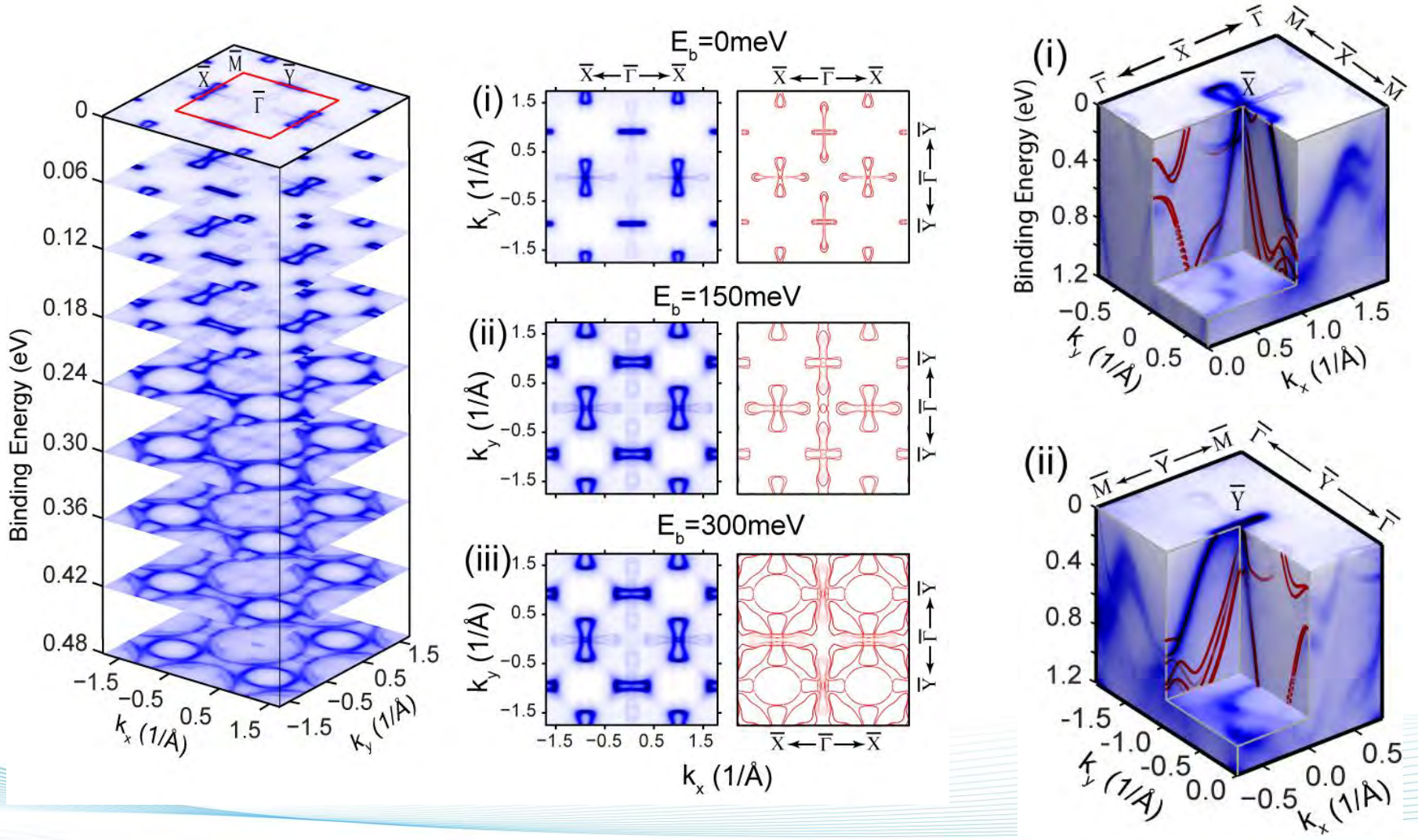




Fermiology Evolution of Weyl Semimetals

Z. K. Liu, *et. al., Nature Materials, 15, 27 (2016)*

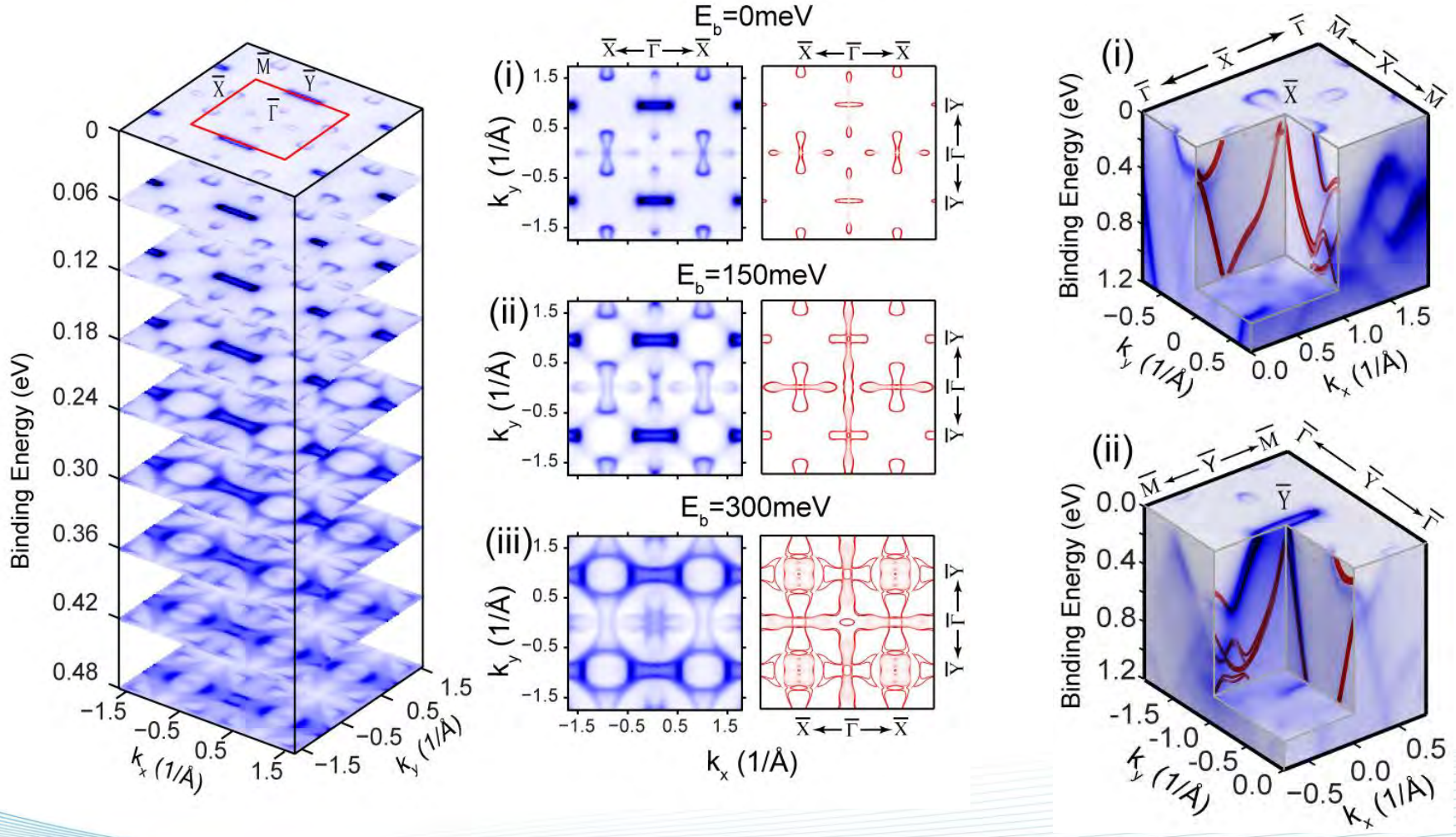
Rich texture of the band structure of TaP



Fermiology Evolution of Weyl Semimetals

Z. K. Liu, *et. al., Nature Materials, 15, 27 (2016)*

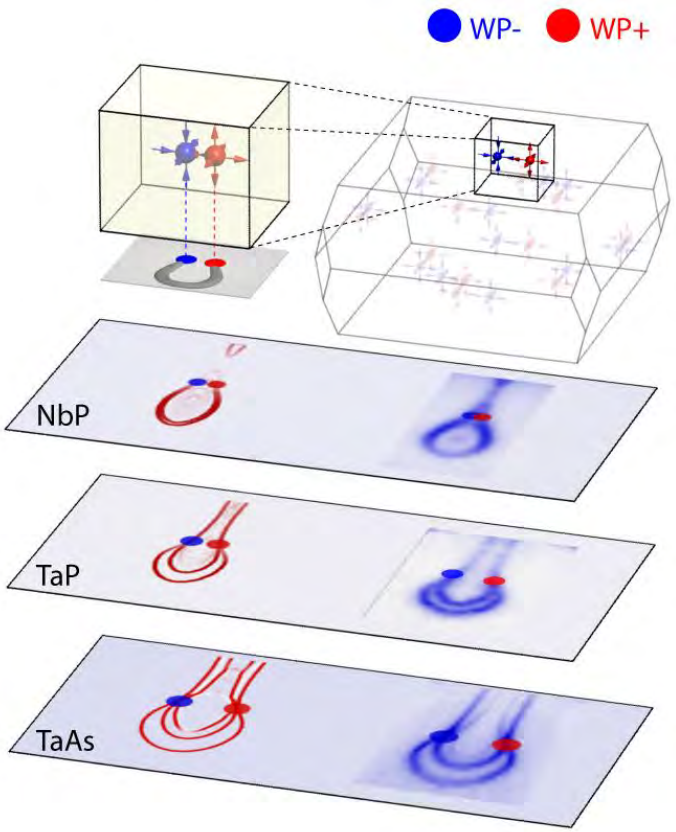
Rich texture of the band structure of NbP

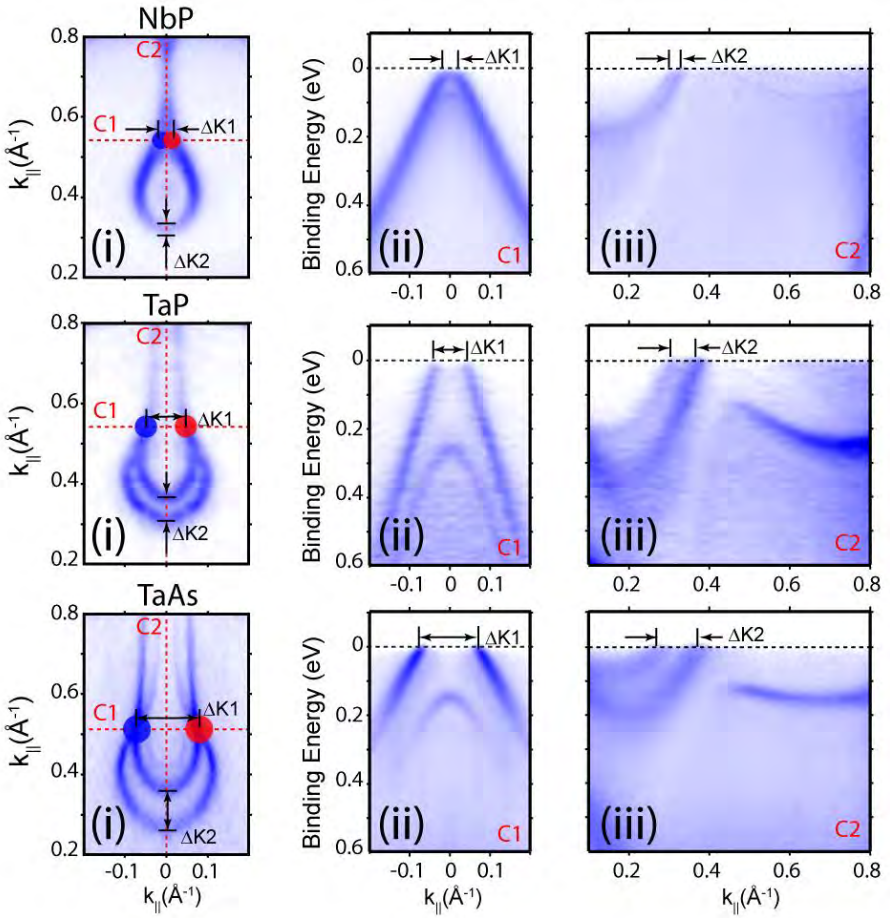


Fermiology Evolution of Weyl Semimetals

Z. K. Liu, *et. al., Nature Materials, 15, 27 (2016)*

Evolution of band structures with SOC

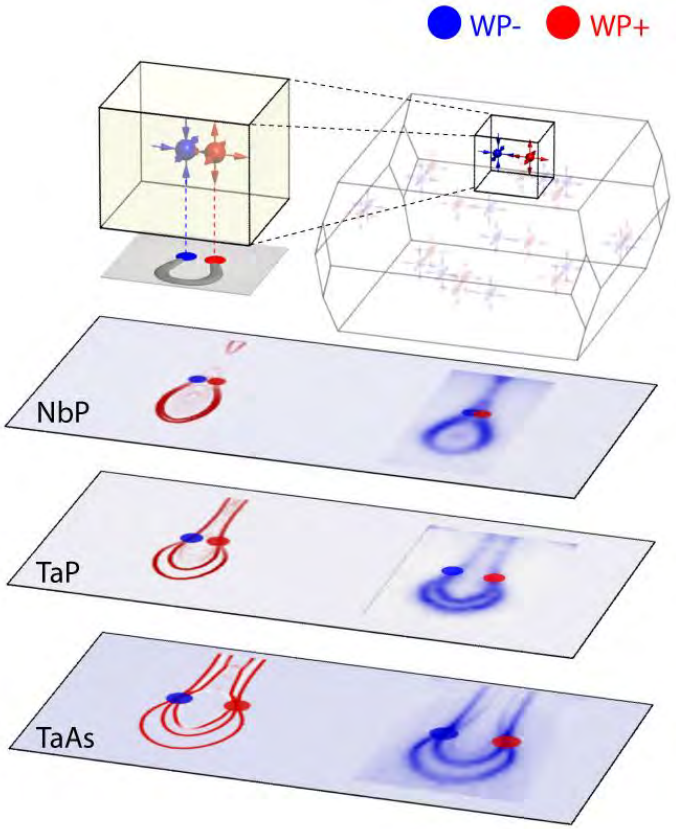


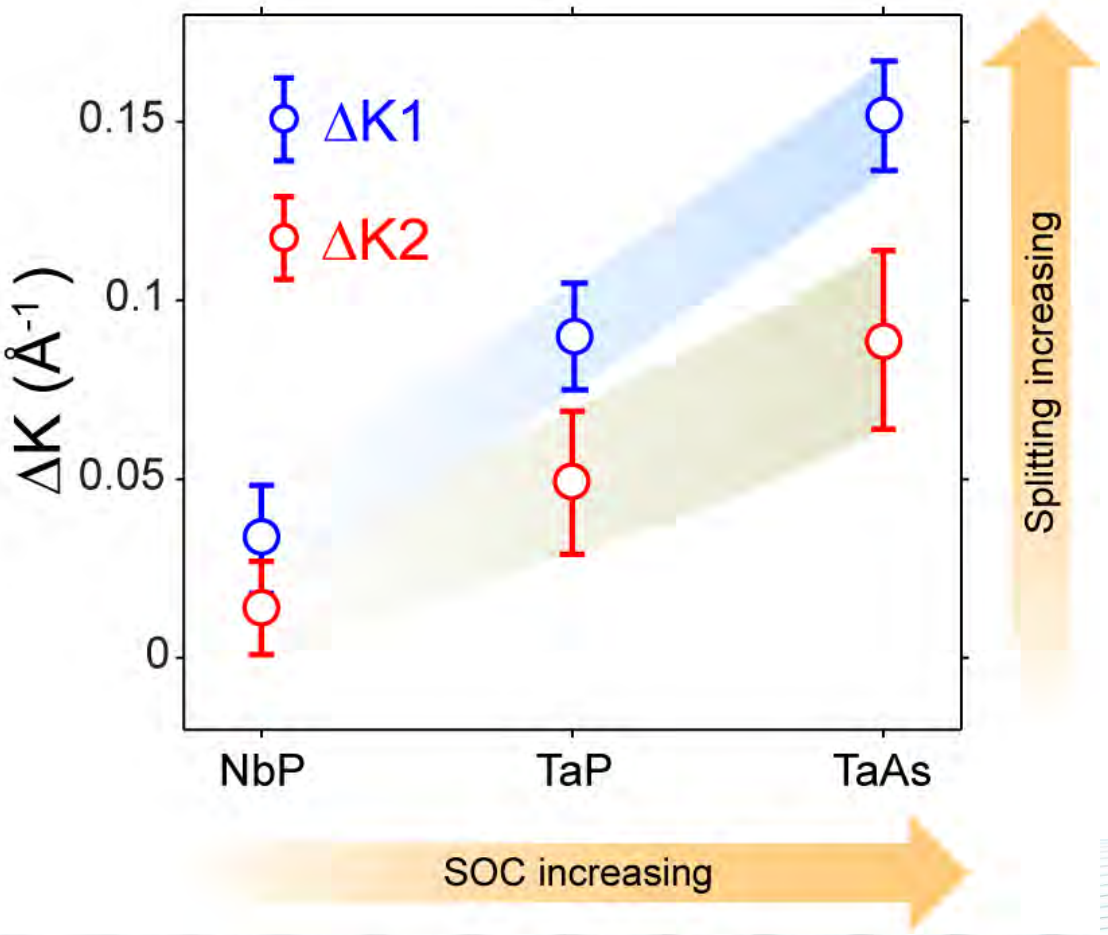


Fermiology Evolution of Weyl Semimetals

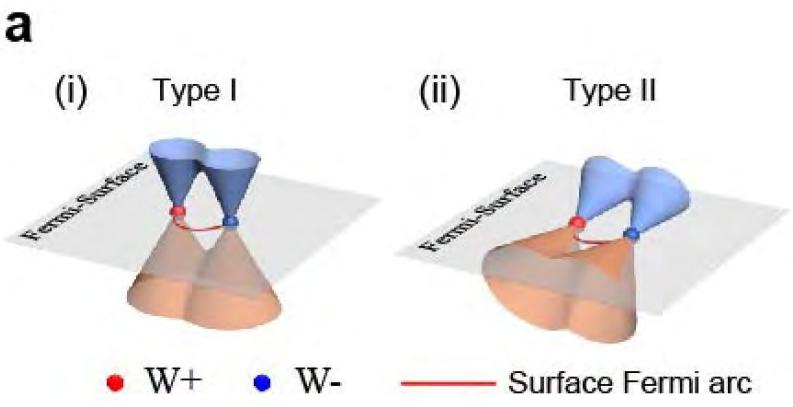
Z. K. Liu, *et. al., Nature Materials, 15, 27 (2016)*

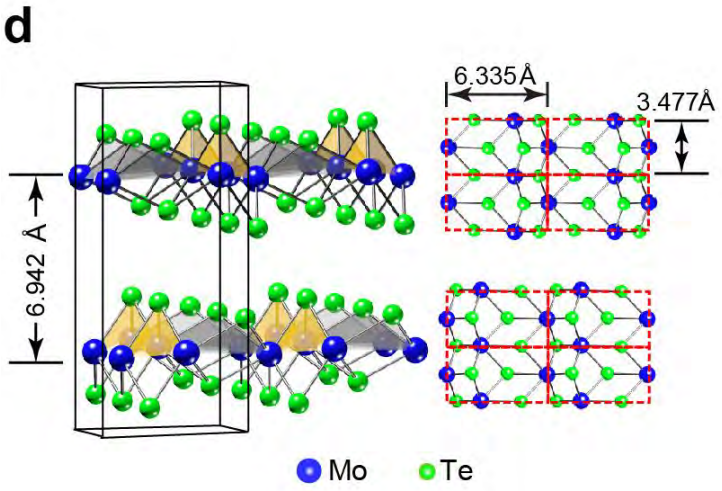
Evolution of band structures with SOC

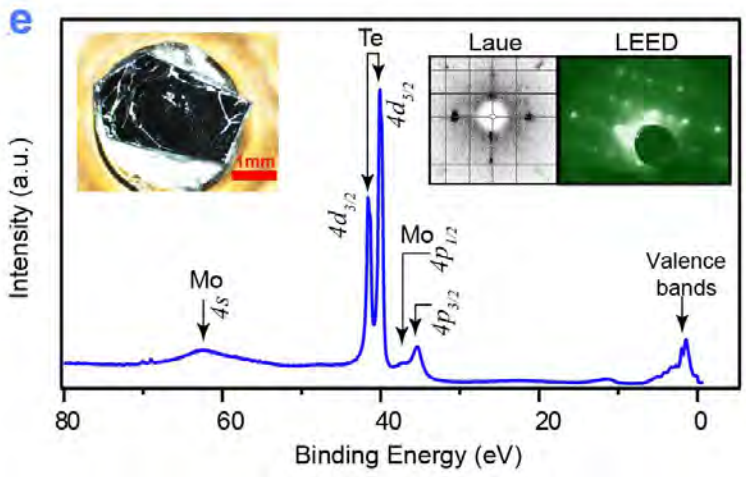


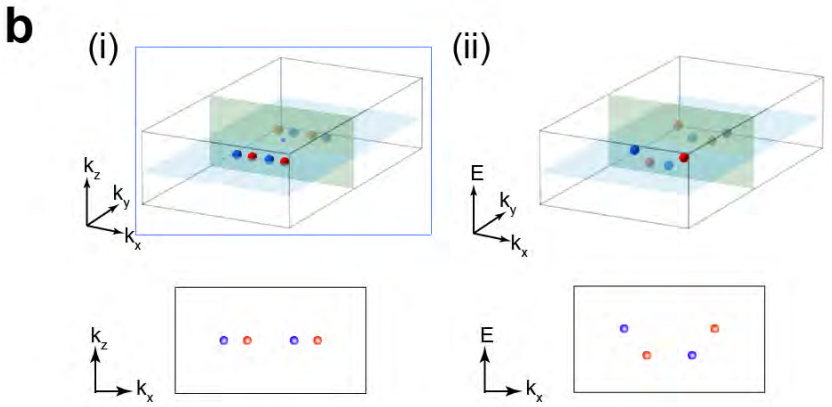


$MoTe_2$, a candidate for type II Weyl Fermion

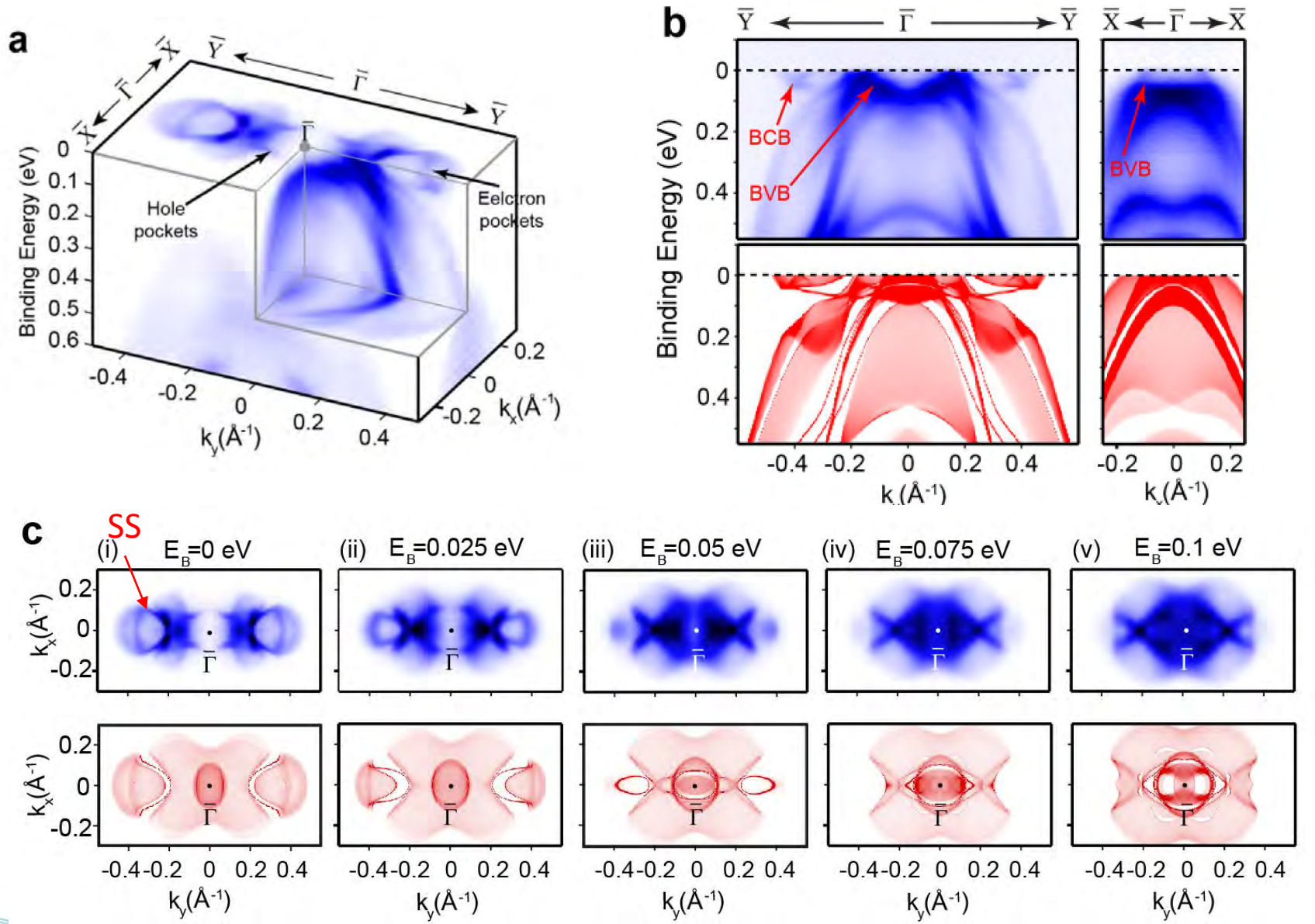




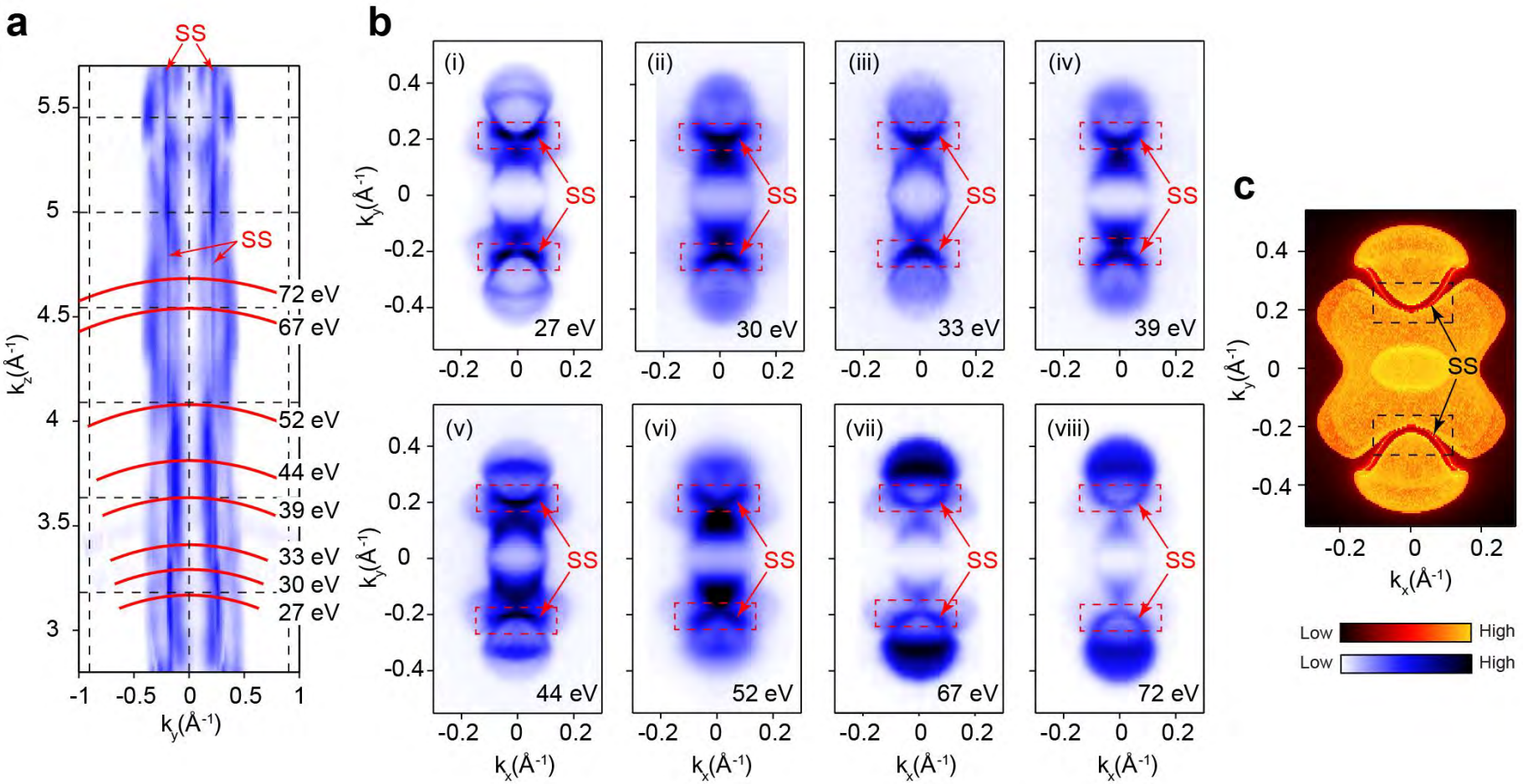




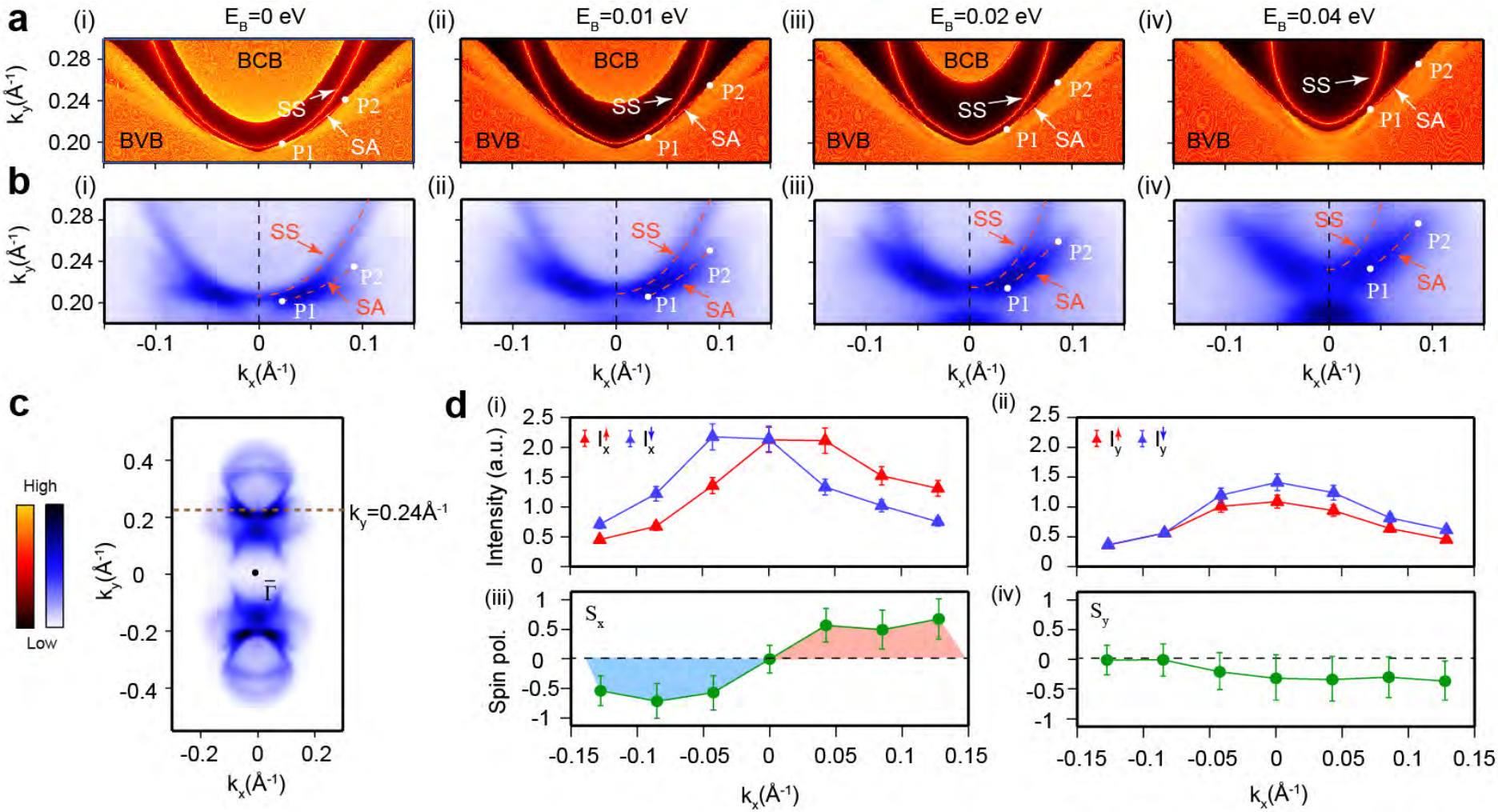
MoTe2, electronic structure



Identification of the SS

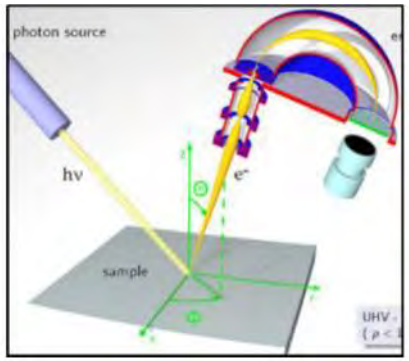


$MoTe_2$,Signature of the Fermi Arc feature

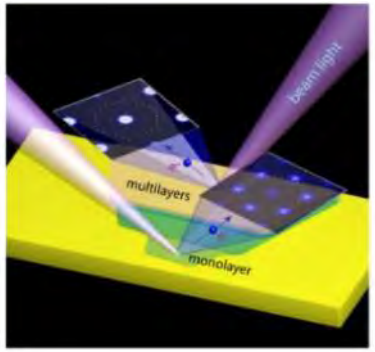


Multi-dimension ARPES technique

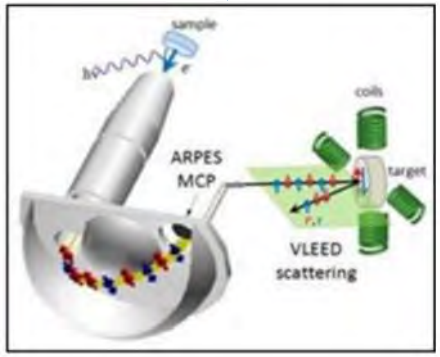
$$f(k,E,r,\sigma,t)$$



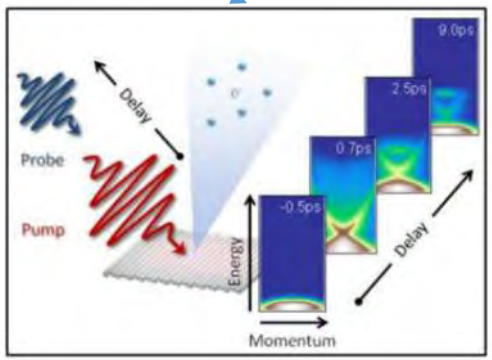
ARPES



Spatial Resolved ARPES



Spin Resolved ARPES



Time Resolved ARPES

Spatial Resolved Photoemission （NanoARPES）

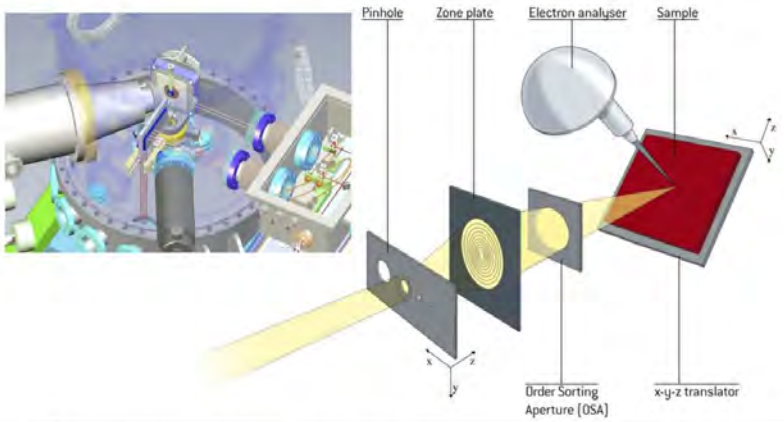
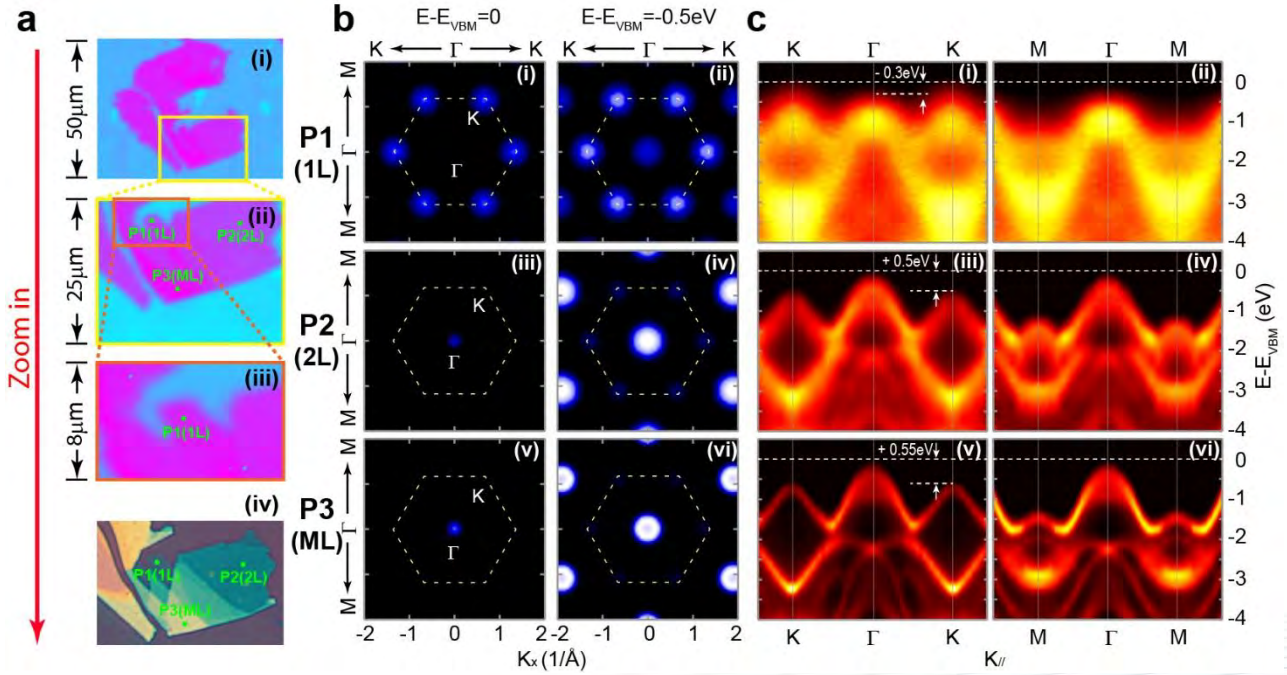


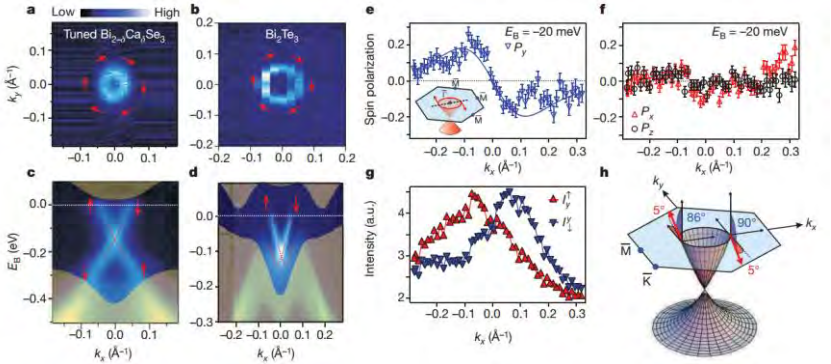
Figure 2: A schematic of the internal workings of the SOLEIL nanoARPES. The figure illustrates the general principles of ZP focusing.

A. Bostwick et al., Synchrotron radiation news, Vol. 25, No. 5, 2012



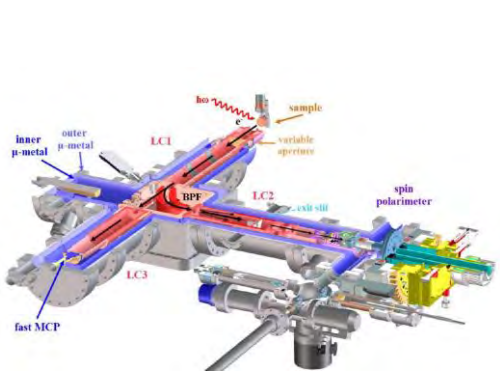
H. T. Yuan, et al., submitted

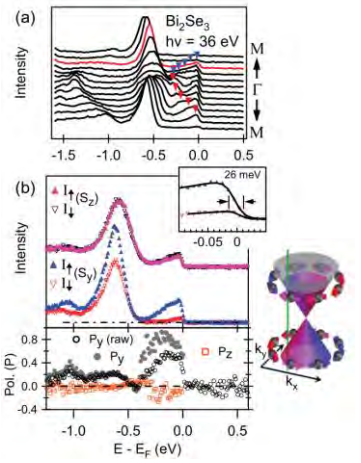
Spin Resolved Photoemission （SpinARPES）



D. Hsieh et al., Nature 460, 1101-1105 (2009)

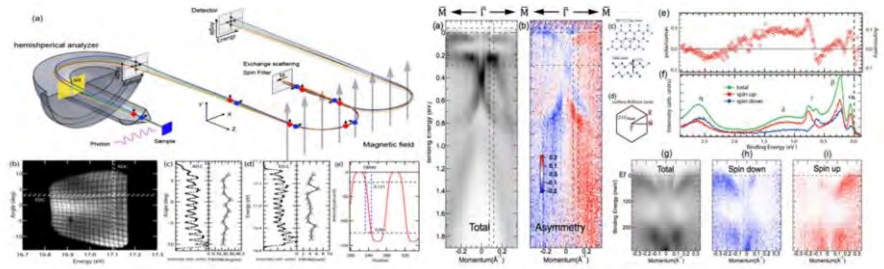
0D, Mott Detector





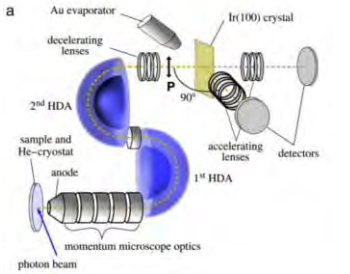
C. Jozwiak, et. al., Phys. Rev. B. 84, 165113 (2011)

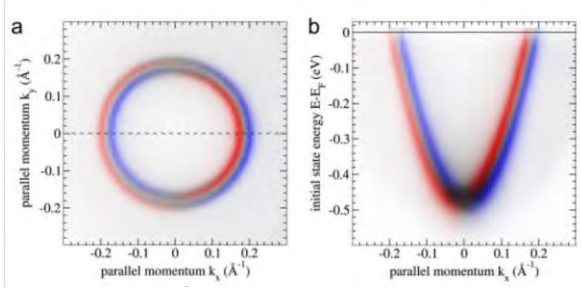
1D, Exchange scattering



2D, Multi-channel exchange scattering

F. Ji et al., Phys. Rev. Lett. 116, 177601 (2016)

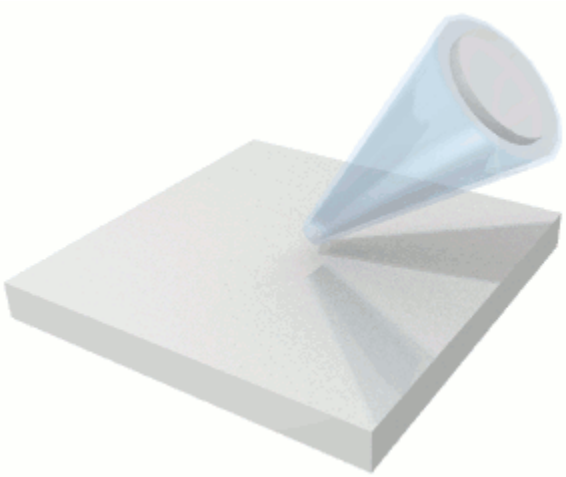




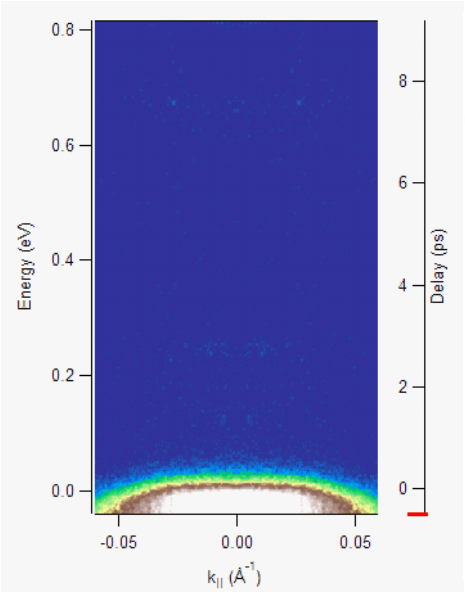
2D, PEEM+VLEED

C. Tusche, et al., Ultramicroscopy, 159, 520 (2015)

Time Resolved Photoemission

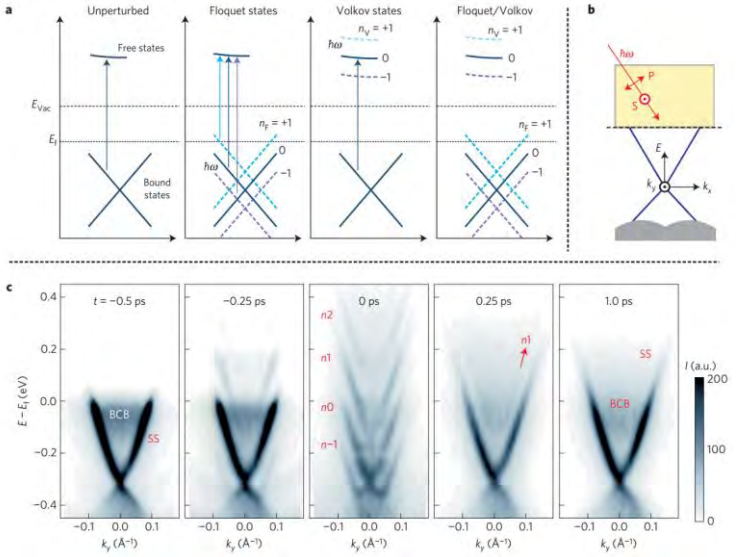


Ultrafast Dynamics of the Surface States in Bi_2Se_3



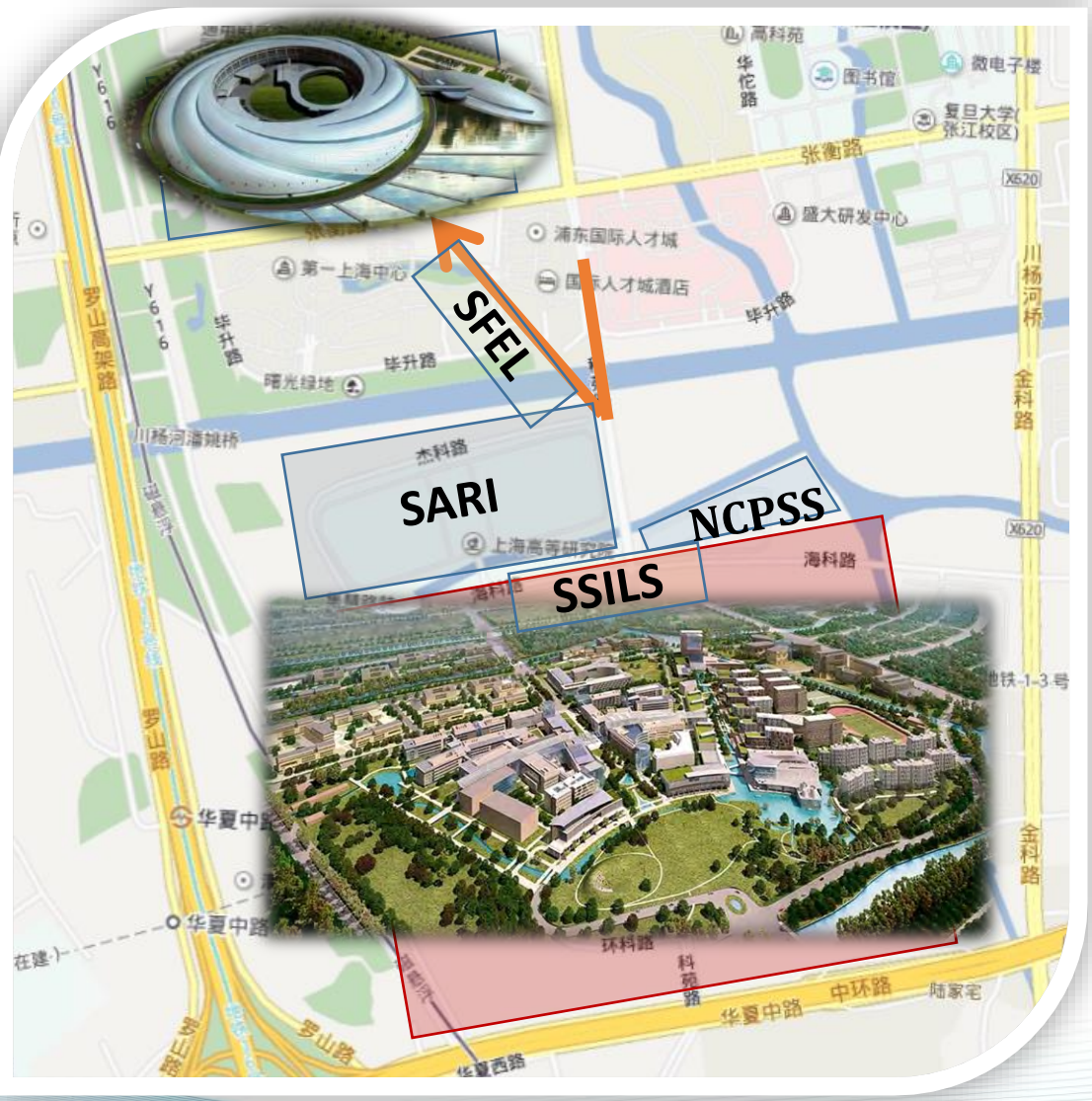
J. A. Sobota et al. ,Phys. Rev. Lett. 108, 117403 (2012)

Floquent Surface States in Bi_2Se_3



F. Mahmood et al., Nature Physics 12, 306–310 (2016)

ShanghaiTech University



- Located in Pudong, Shanghai
- 30 mins from Pudong International Airport
- 2 kms away from Shanghai Synchrotron
- At the heart of national science facilities

- Founded by the Shanghai Government and Chinese Academy of Science in 2013
- Small Scale, Research Oriented University

SSRF: Shanghai Synchrotron Radiation Facility
SFEL: Shanghai Free Electron Laser
SSILS: Shanghai Super Intense Laser Source
SARI: Shanghai Advanced Research Institute
NCPSS: National Center for Protein Science

Division of Condensed Matter Physics and Photon Science

Interface and Photon Science

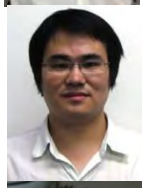



+ 6 Adj. Prof.

ME² BL

Quantum Material

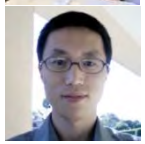





+ 1 Adj. Prof.

S² BL

Theory

Local Clusters, Super Comp. Center

Photon Sci. Joint Lab


王美晓

S-XFEL Detector Initiatives

SSILS Joint Lab


姜甲明

SSILS

SIMIT Joint Lab


宋艳汝

Detector Initiatives

Project Management

Lei Shi

SSILS
S² BL
S-XFEL

Current major projects

- **ME^2 (Materials for Energy and Environment) beamline project at SSRF**
- **S^2 beamline (Spatially and Spin resolved ARPES beamline) at SSRF**
- **Shanghai Super Intense Laser Source (SSILS) at ShanghaiTech University**
- **S-XFEL User Facility Upgrade**

ME^2beamline (SIMIT, SSRF)

S^2 beamline (SSRF)

SSILS

Shanghai - FEL

Thank you and Welcome to Shanghai