Chasing relativistic electrons in topological quantum materials

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Center for Emergent Materials

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Ames Laboratory, Iowa State University

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University of Tennessee, Center for Emergent Materials

Oak Ridge National Laboratory

Na Hyun Jo, Paul Canfield, Sergey Bud'ko,

Ames Laboratory, Iowa State University

Theory: **Nandini Trivedi, Tim McCormick**

Ohio State University, Center for Emergent Materials

Ryotaro Arita, Masayuki Ochi

RIKEN

Outline:

- Introduction to ARPES
- Introduction to topological materials

- Topological Insulators
- 3D Dirac semimetals
- Weyl semimetals
- Beyond what is known…

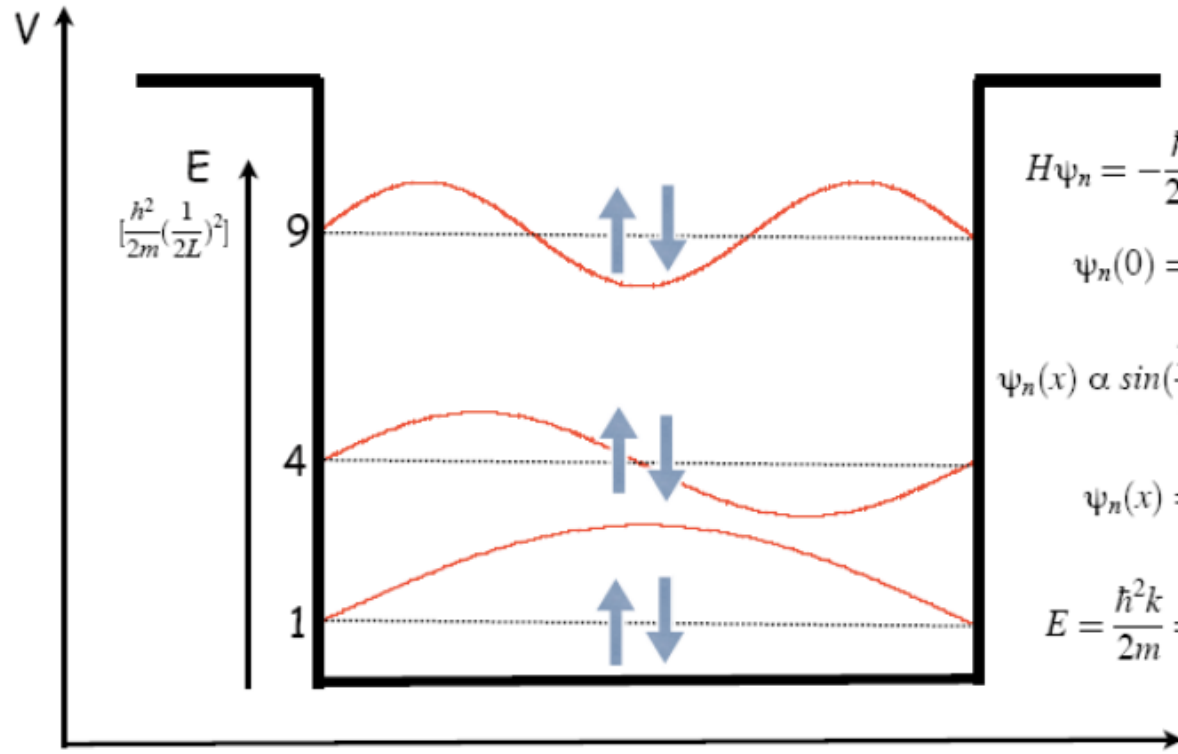
Complexity arising from large number of electrons leads to fascinating physics of solids

US penny: 3.1 grams of copper, 2.9×10^{22} electrons

DVD: 4×10^{10} bits

we would need some 7.25×10^{11} DVD's to store information just about spin of all electrons

Simplest quantum model: electrons in 1D box:



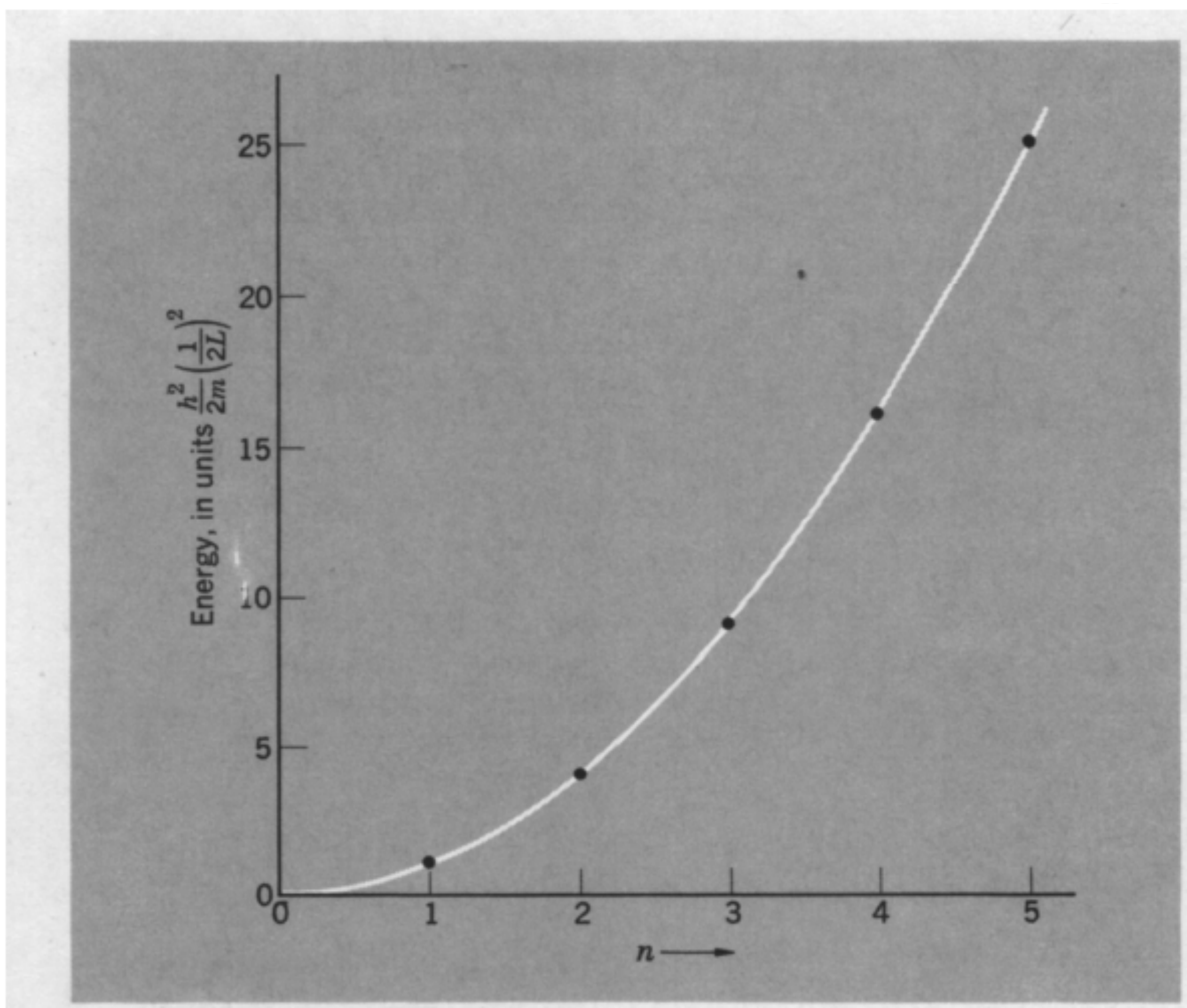
$$H\psi_n = -\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} = \varepsilon_n\psi_n$$

$$\psi_n(0) = \psi_n(L) = 0$$

$$\psi_n(x) \; \alpha \; sin(\frac{2\pi}{\lambda_n}x) \qquad \frac{1}{2}n\lambda_n = L$$

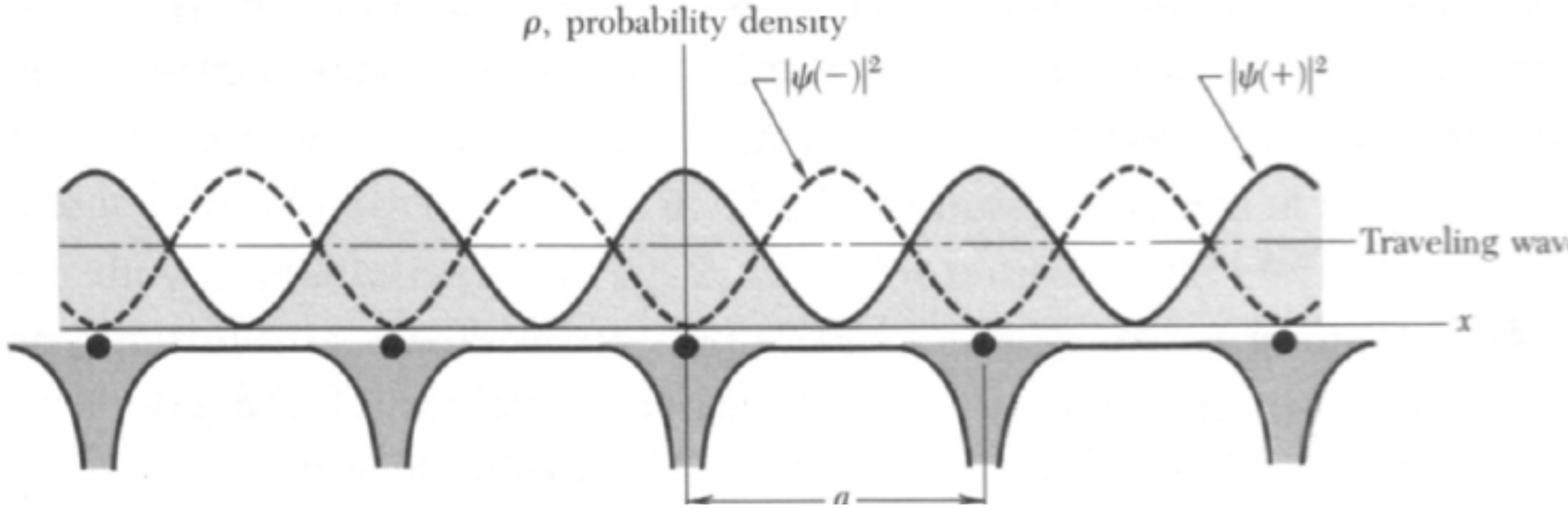
$$\psi_n(x) = sin(\frac{n\pi}{L}x)$$

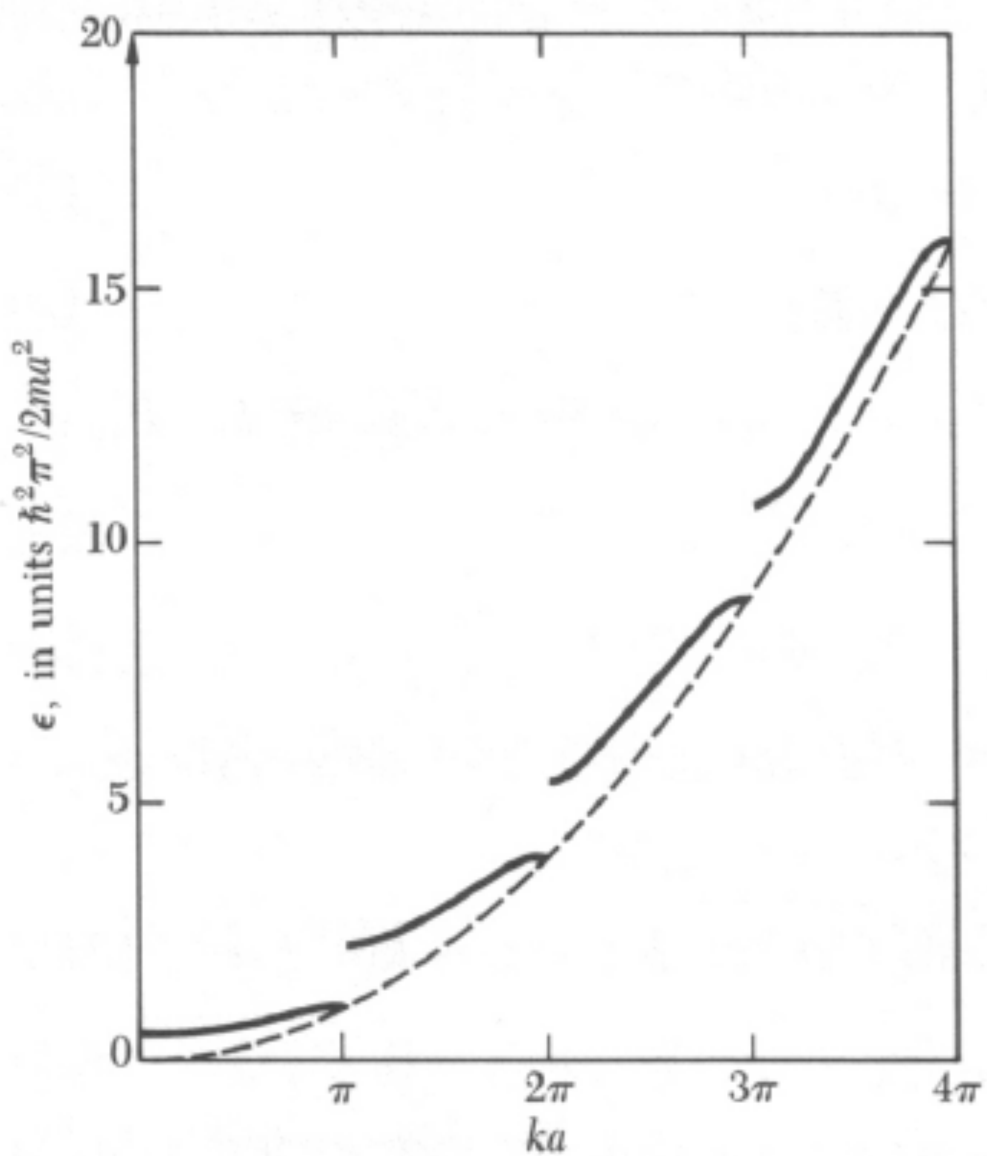
$$E = \frac{\hbar^2 k}{2m} = \frac{h^2}{2m}(\frac{n}{2L})^2$$



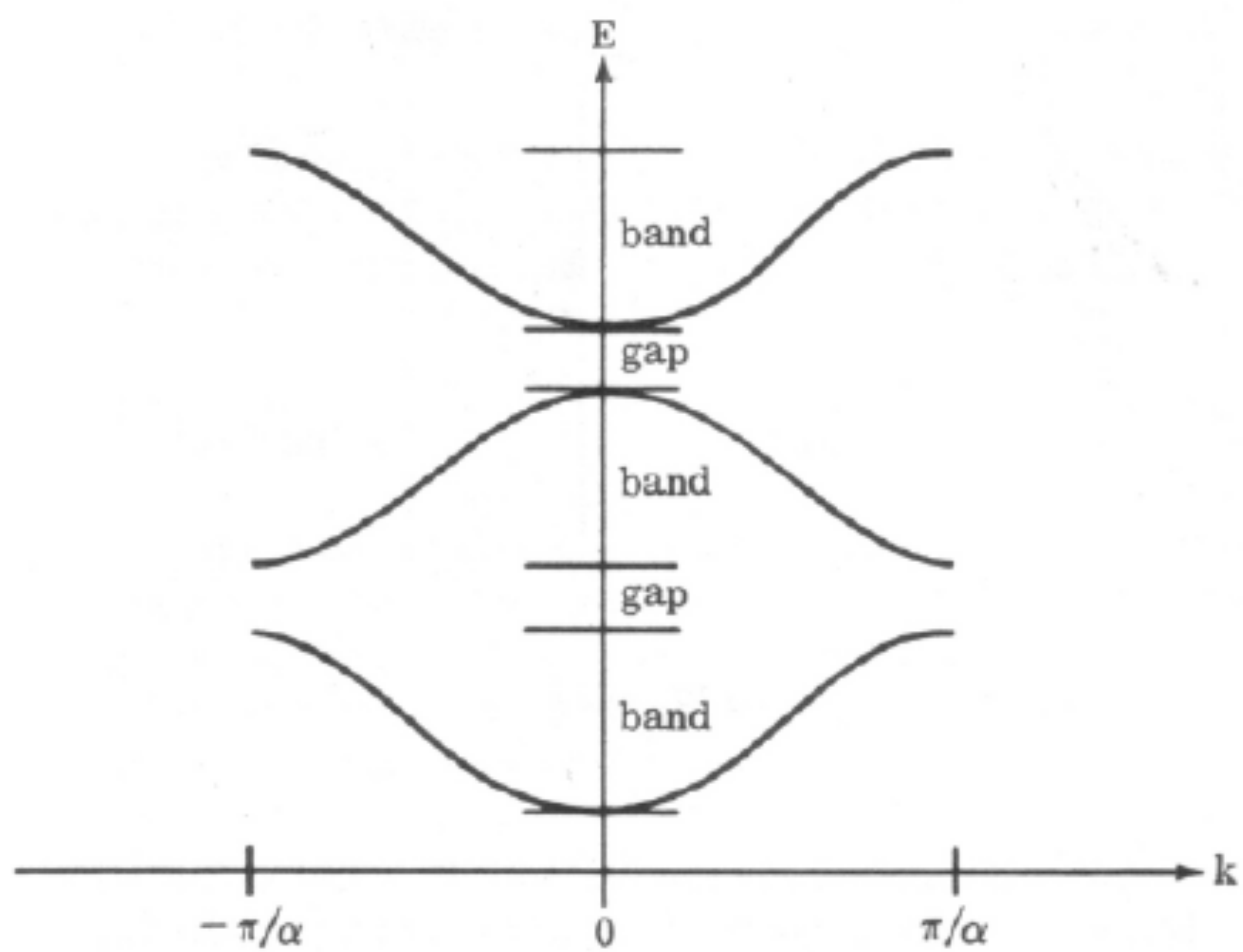
Kittel, Solid State Physics

Periodic ionic potential



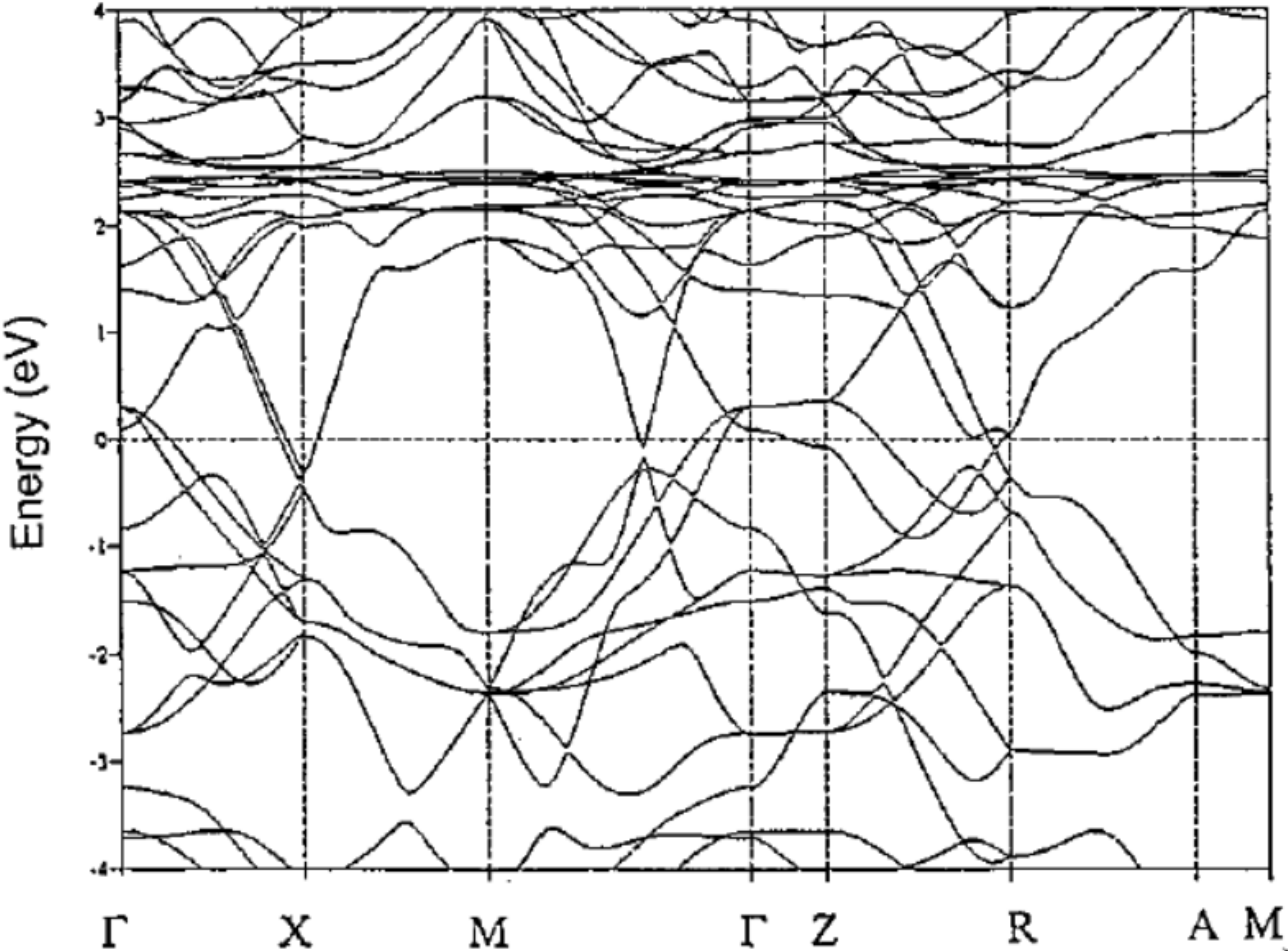


Reduced band scheme

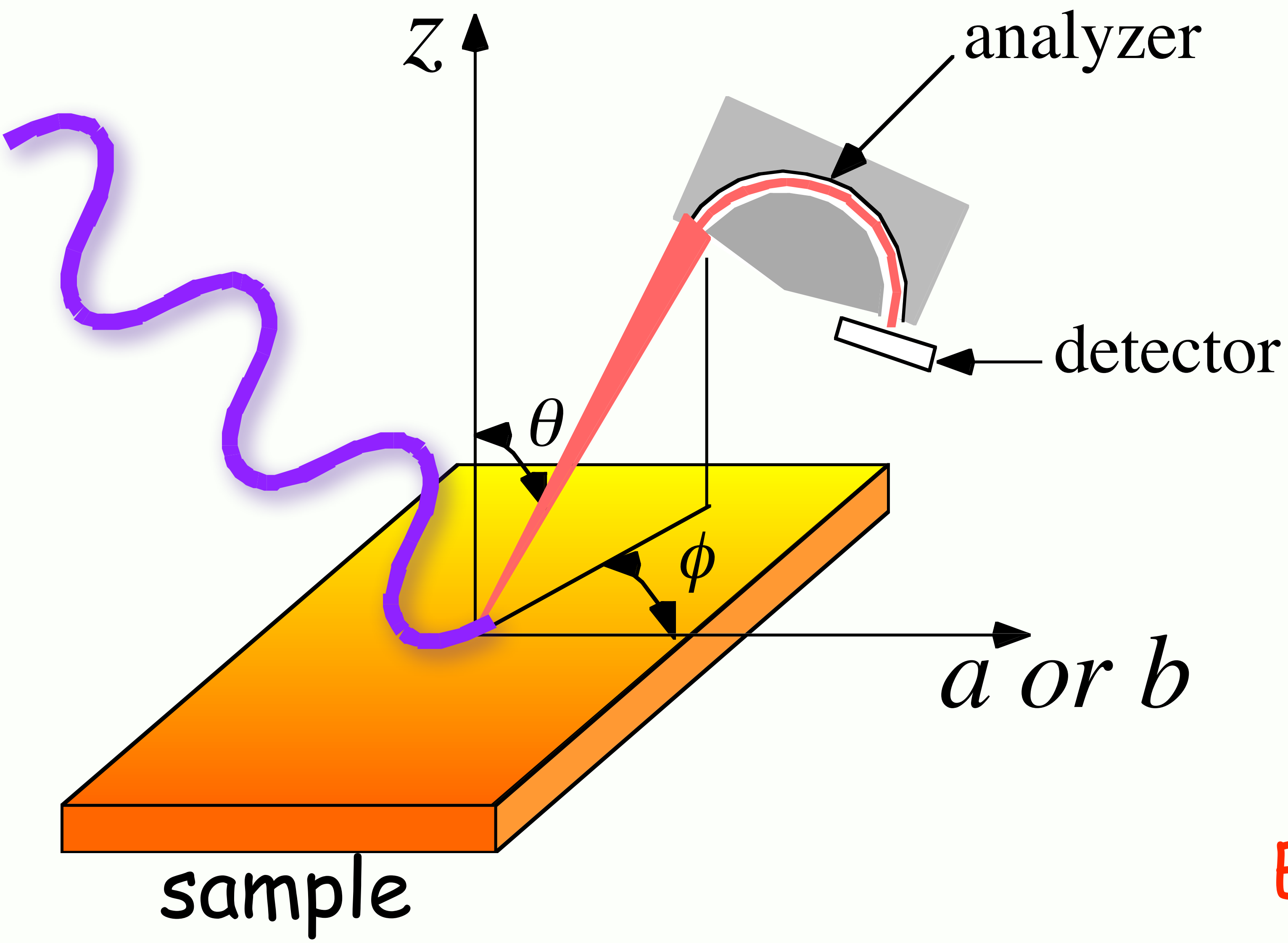


Kittel, Solid State Physics

$LaAgSb_2$



ARPES experiment



binding energy - E_b

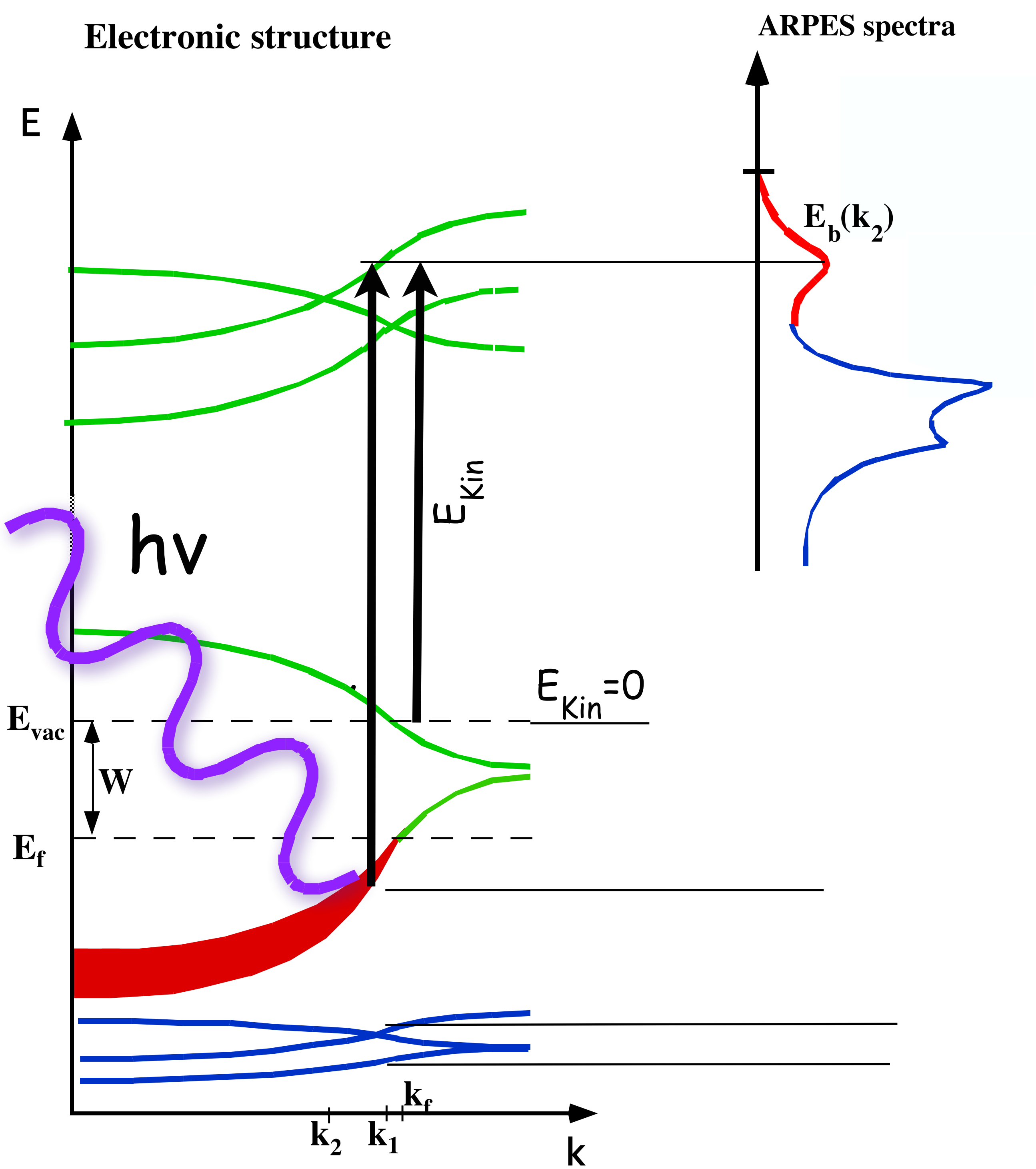
initial momentum - k_i

$$E_b = E - h\nu + W$$

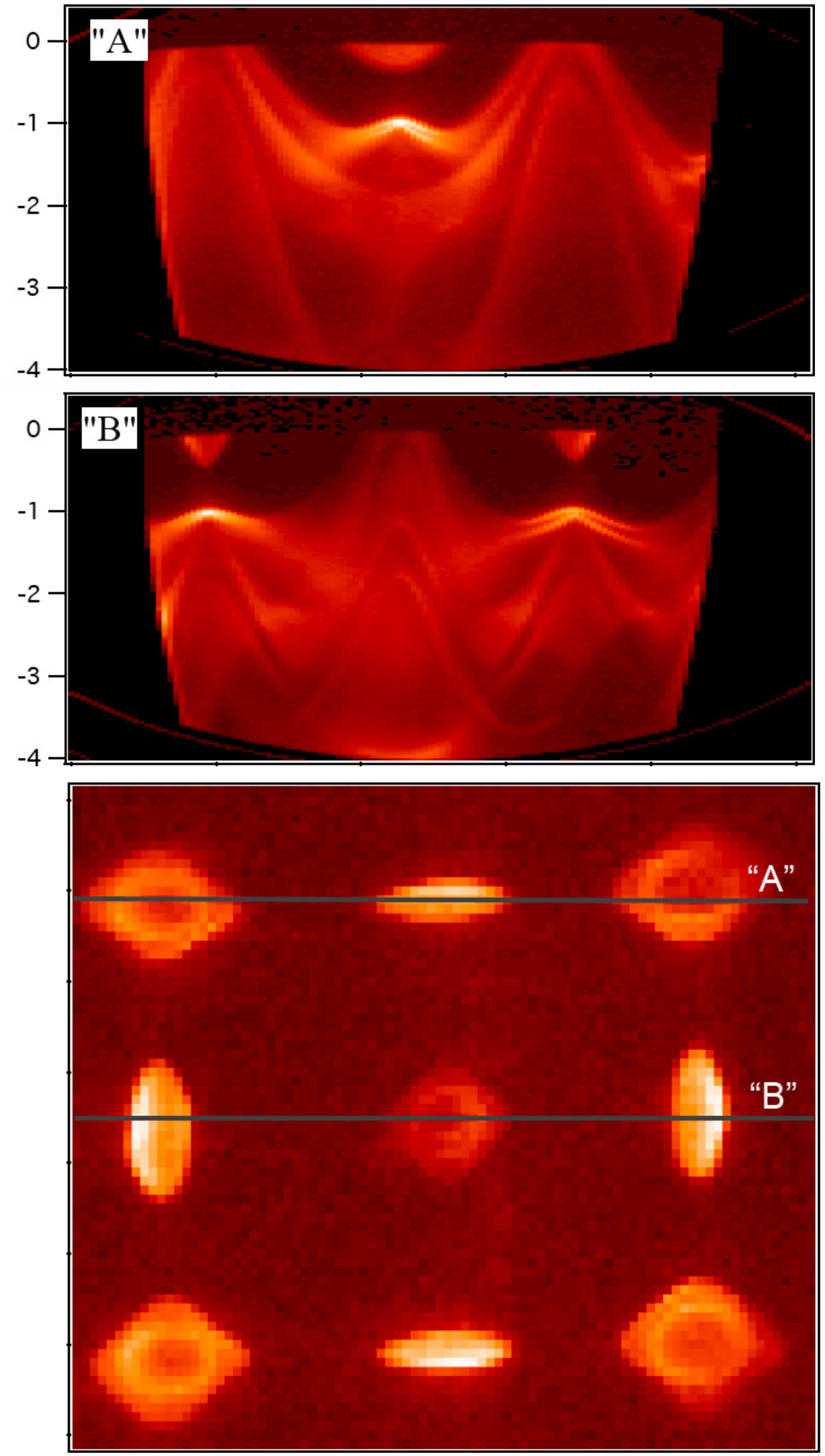
$$k^i_{\parallel} = k^f_{\parallel} = \sqrt{2mE/\hbar^2}\,\sin\theta$$

$$k^i_{\perp} = k^f_{\perp} - G = \sqrt{2mE/\hbar^2}\,\cos\theta - G$$

LuSb

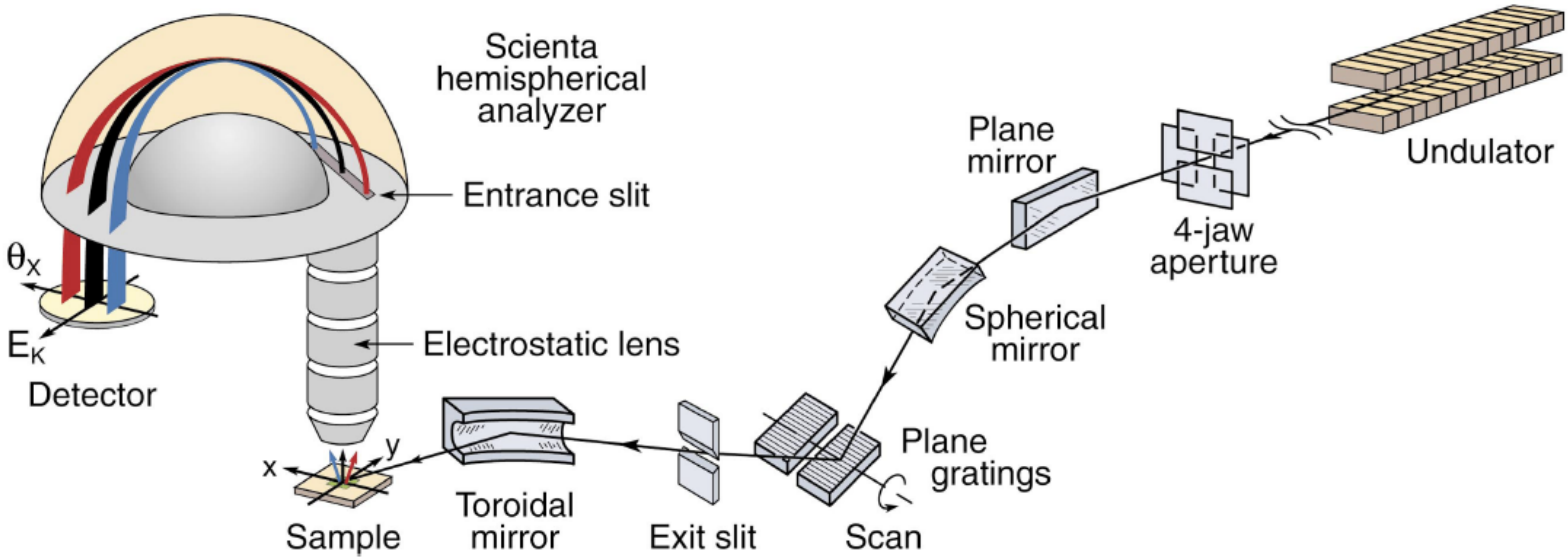


Electronic structure
ARPES spectra
E
hν
E_Kin
E_Kin=0
E_vac
W
E_f
E_b(k_2)
k_2
k_1
k_f
k



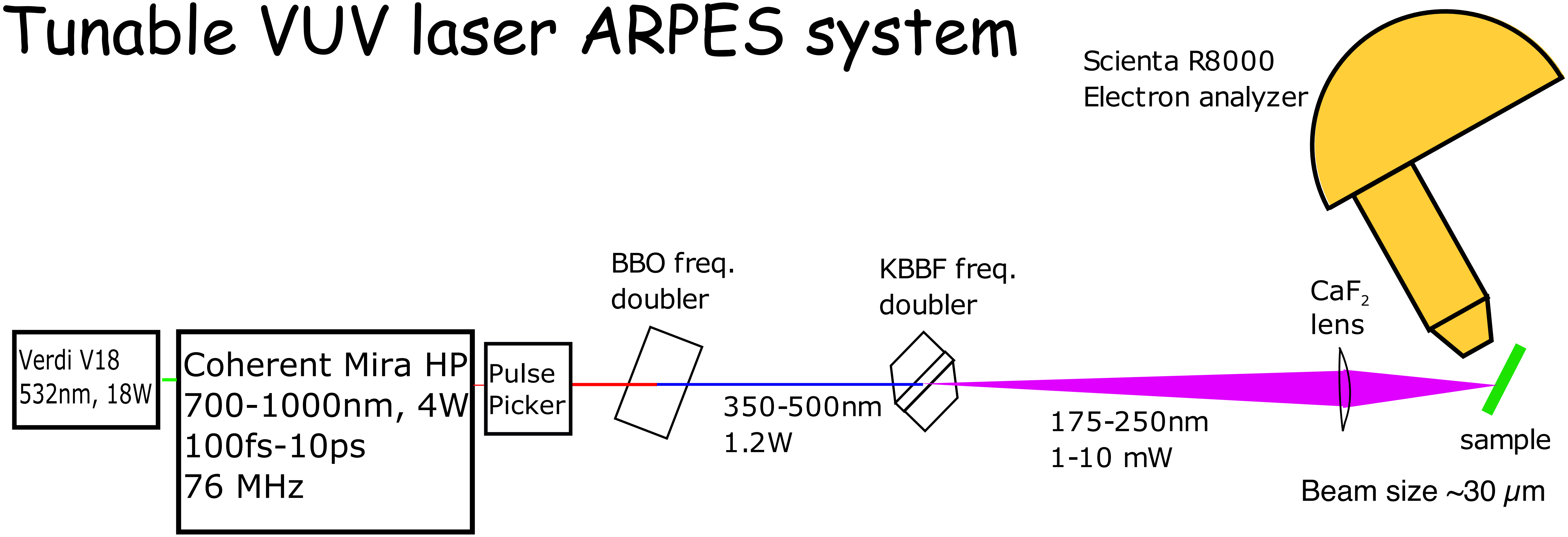
"A"
"B"
0
-1
-2
-3
-4
"A"
"B"

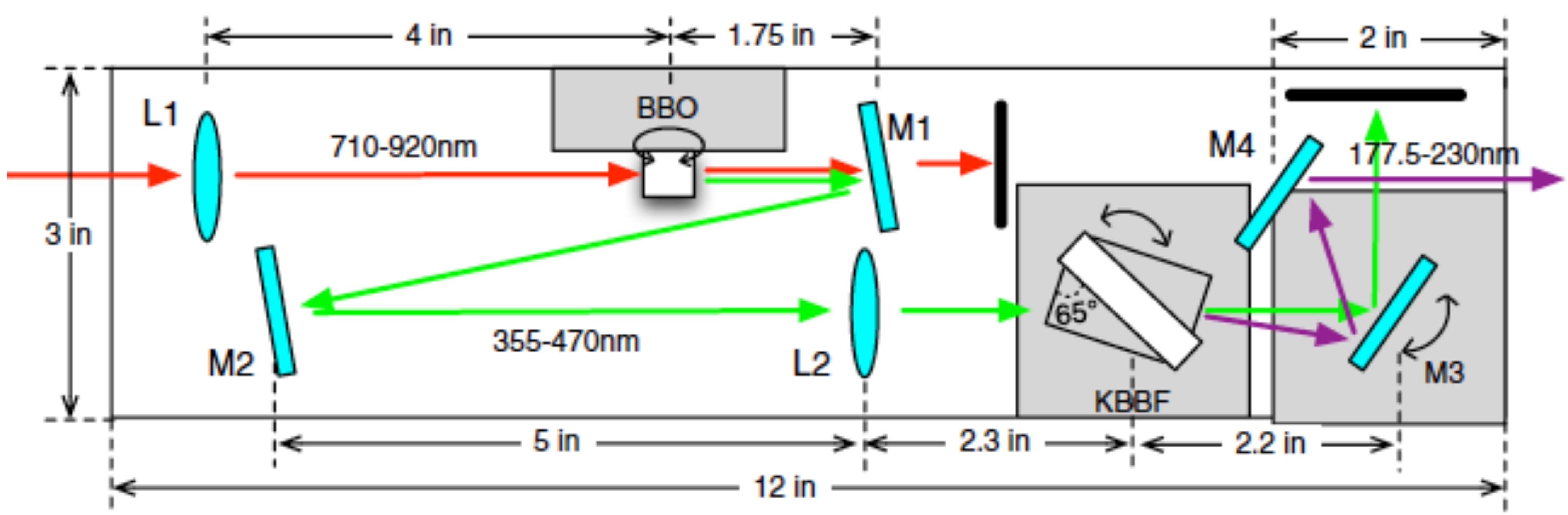
Synchrotron based ARPES measurements



A. Damascelli *et al*.

Tunable VUV laser ARPES system





R. Jiang et al., Rev. Sci. Instrum. 85, (2014).

Brief introduction to topology

Gauss-Bonnet theorem $$\int_M \kappa \, dA = 2\pi\chi = 2\pi(2-2g)$$

≠

=

g=0 g=1 g=1

Manuel Asorey

Analogy in solid state physics:

Wave function in periodic potential $\Psi_{m\mathbf{k}} = e^{i\mathbf{kr}} u_{m\mathbf{k}}(\mathbf{r})$

Schroedinger equation: $\hat{H}(\mathbf{k})|u_m(\mathbf{k})\rangle = E_m(\mathbf{k})|u_m(\mathbf{k})\rangle$

Berry connection: $\mathbf{A}^{(m)}(\mathbf{k}) = i\langle u_m(\mathbf{k})|\nabla_{\mathbf{k}} u_m(\mathbf{k})\rangle$ $\mathbf{k} = (k_x, k_y).$

Berry curvature: $\Omega^{(m)}(\mathbf{k}) = \nabla_{\mathbf{k}} \times i\langle u_m(\mathbf{k})|\nabla_{\mathbf{k}} u_m(\mathbf{k})\rangle$

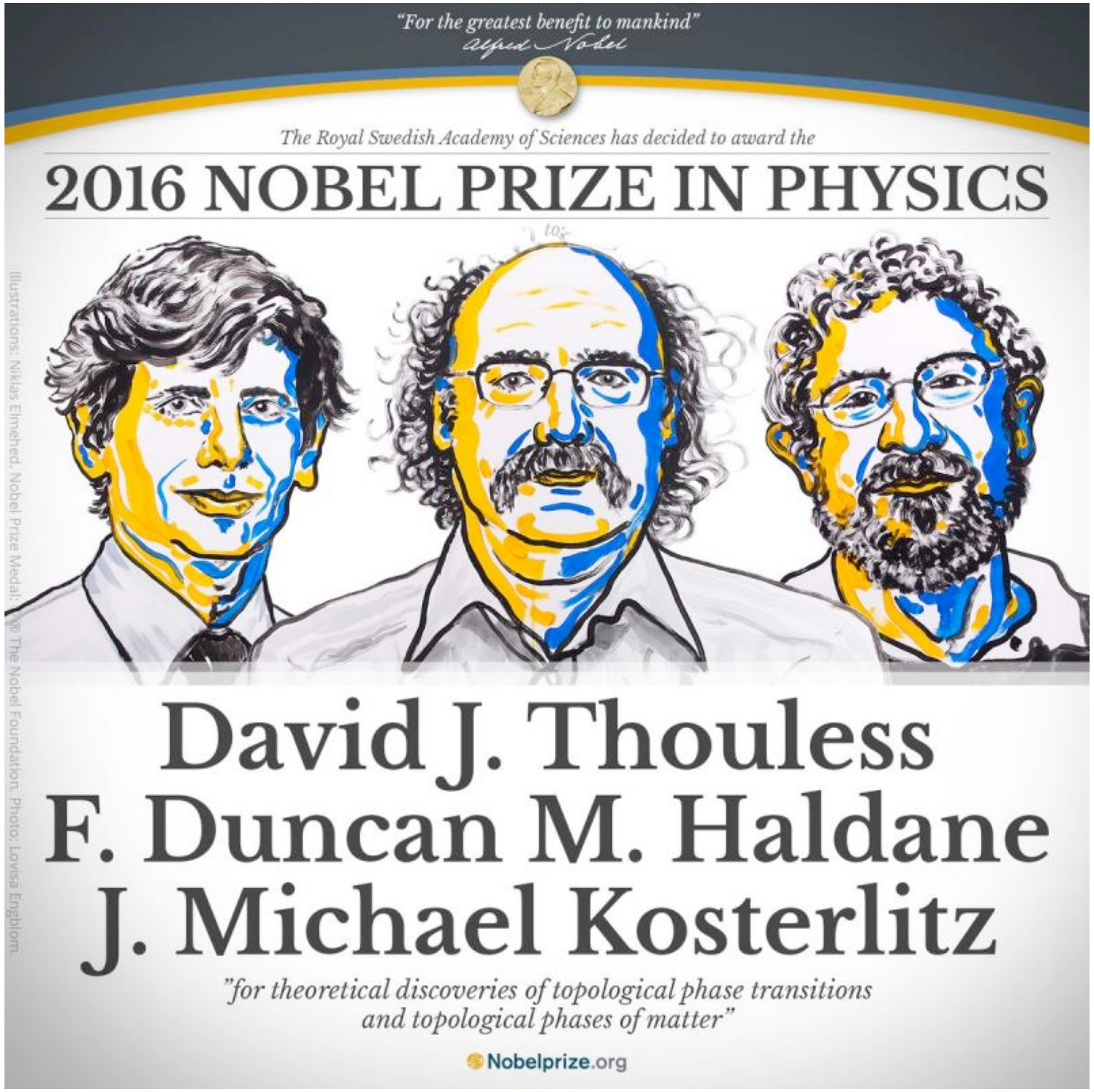
Chern number: $Q^{(m)} = -\frac{1}{2\pi}\int_{BZ} \Omega^{(m)}(\mathbf{k}) d\mathbf{k}$

J. K. Asbóth, L. Oroszlány, and A. Pályi, arXiv:1509.02295

D. Xiao, M-Ch Chang, and Q. Niu, Rev. Mod. Phys. **82**, 1959.

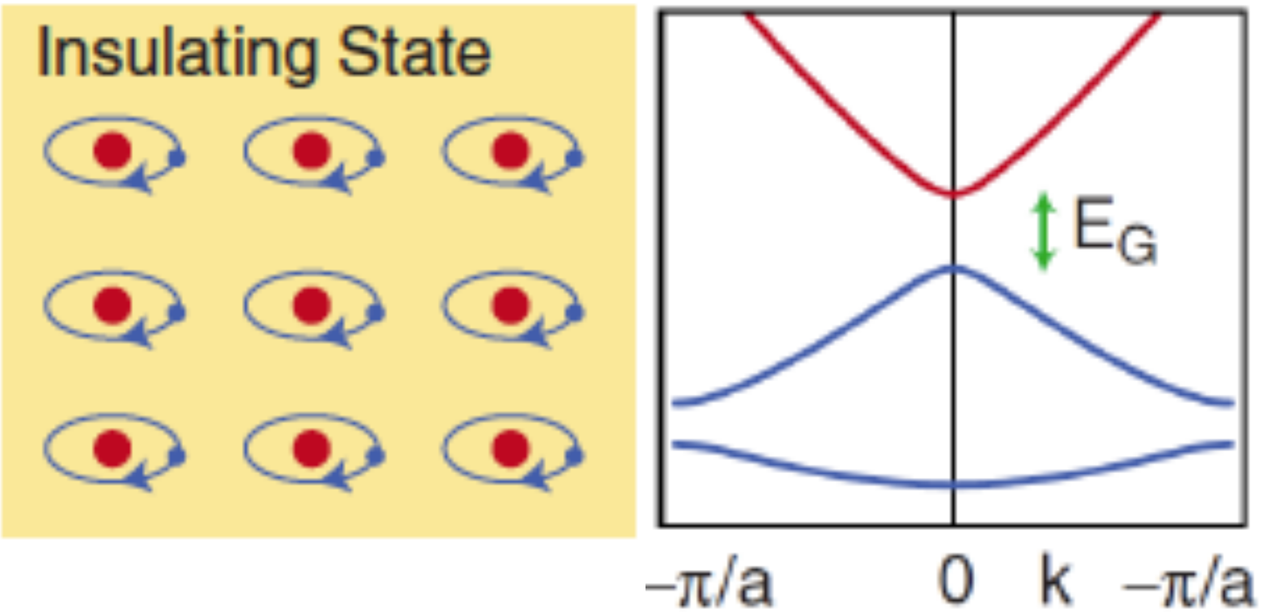
Nobel Prize in Physics 2016

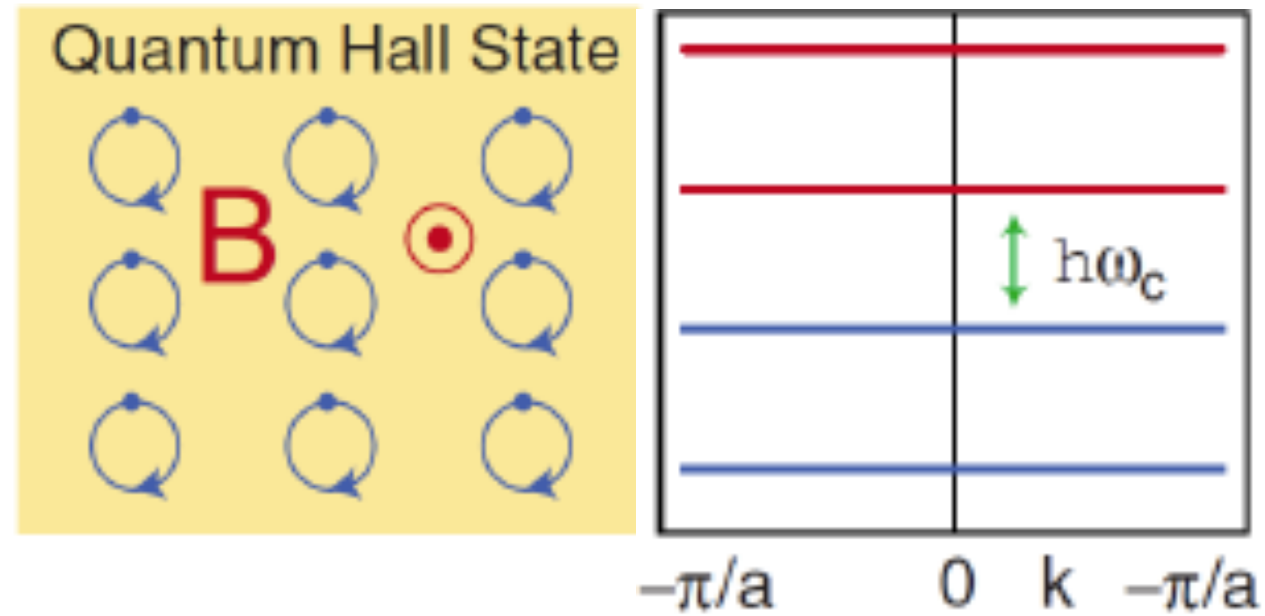
”for theoretical discoveries of topological phase transitions and topological phases of matter”



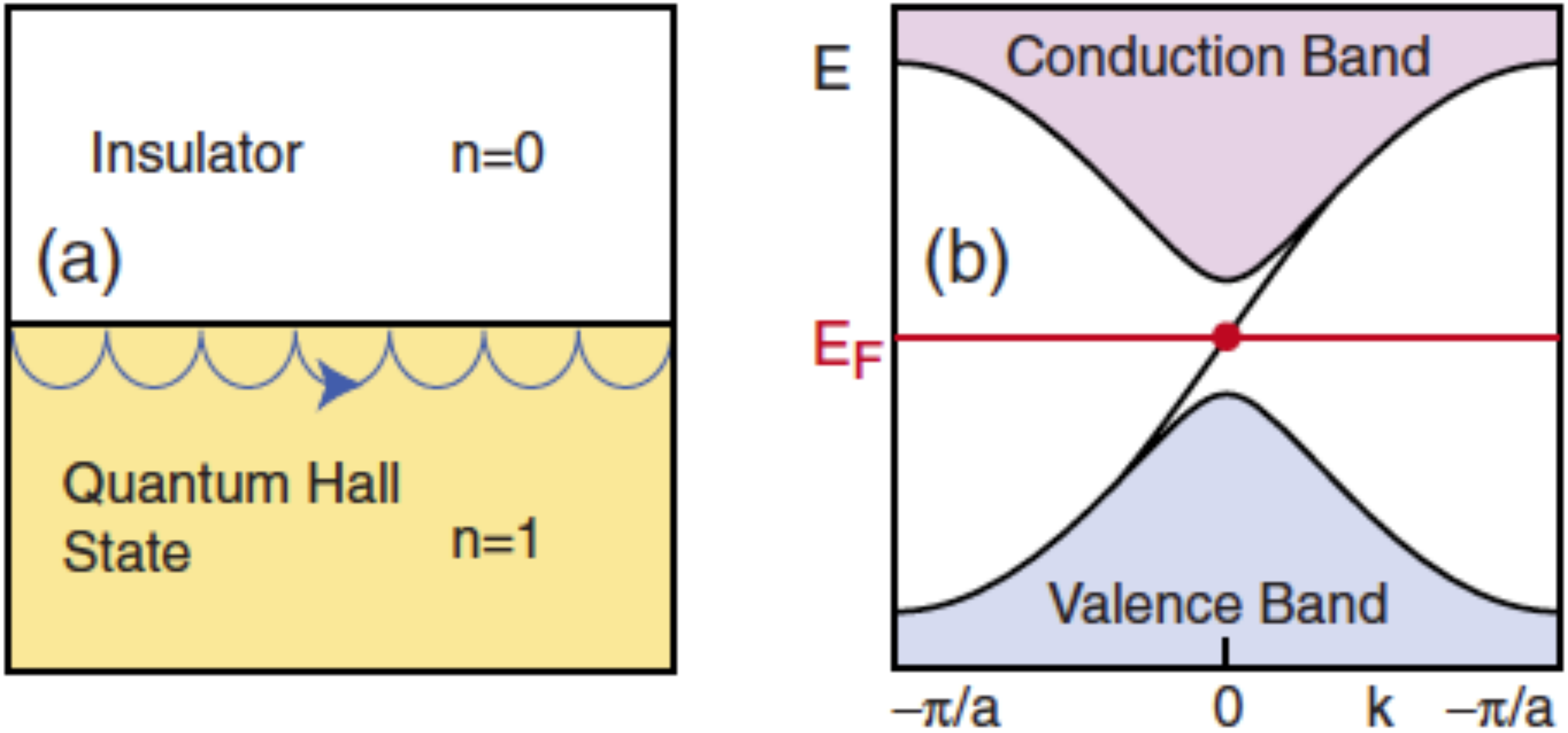
trivial state

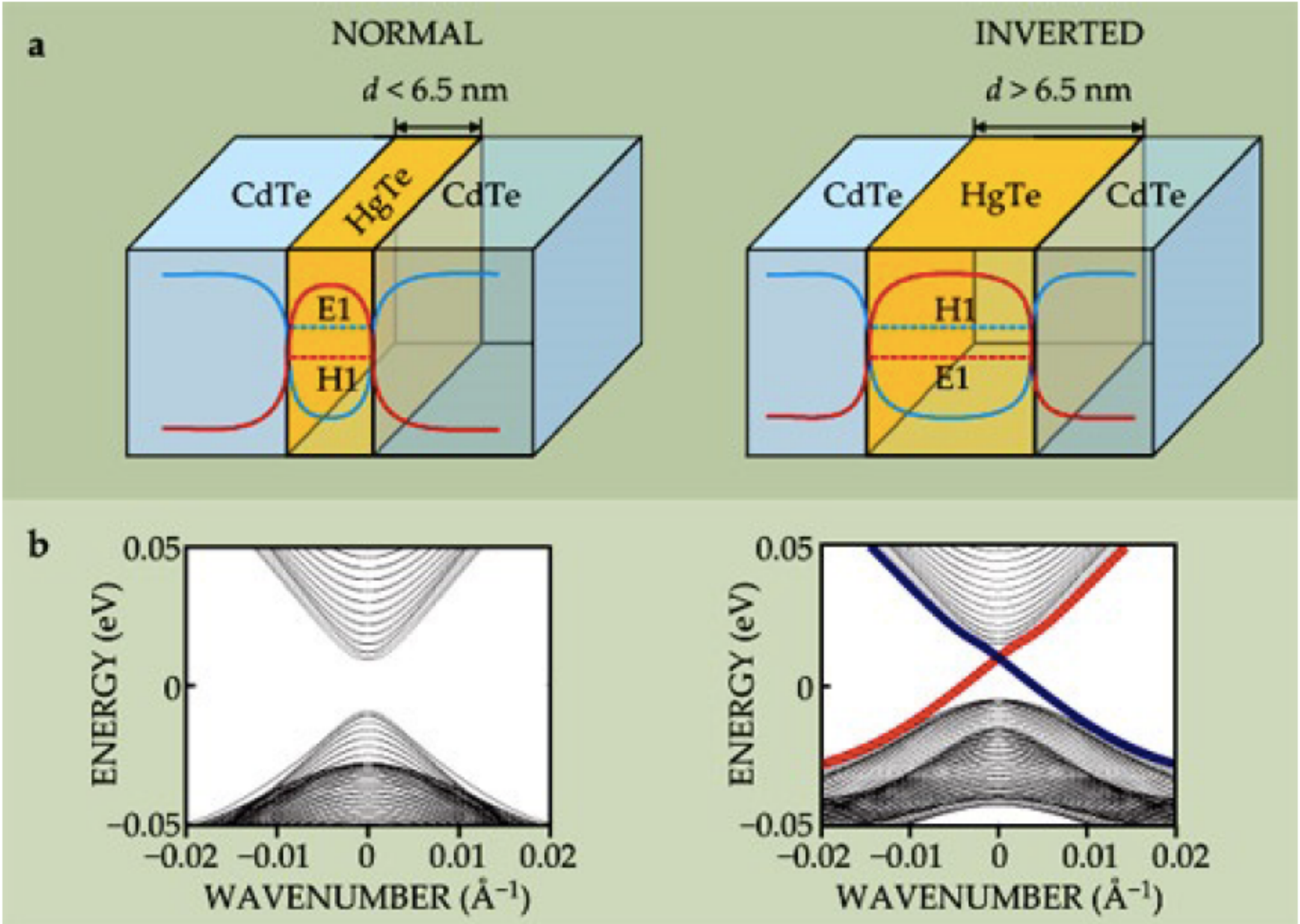
topological state





M. Z. Hasan and C. L. Kane, Rev. Mod. Phys., Vol. 82, No. 4, October–December 2010


Insulator
n=0
(a)
Quantum Hall
State
n=1
E
Conduction Band
(b)
E_F
Valence Band
–π/a
0
k
–π/a

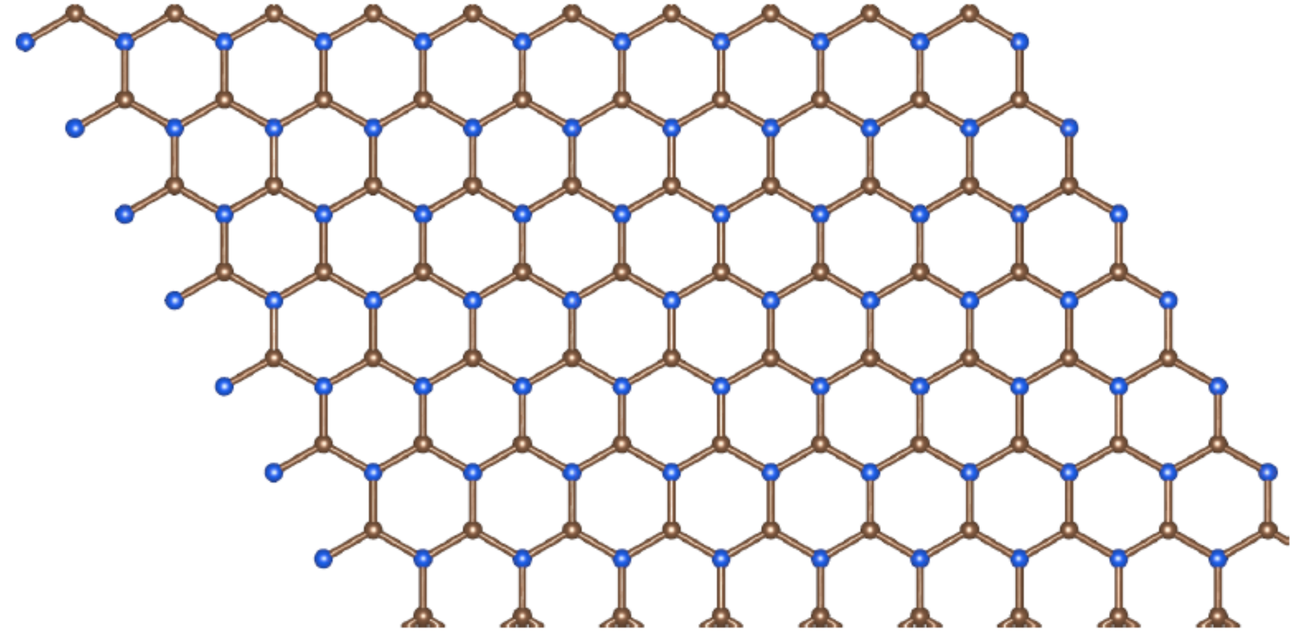


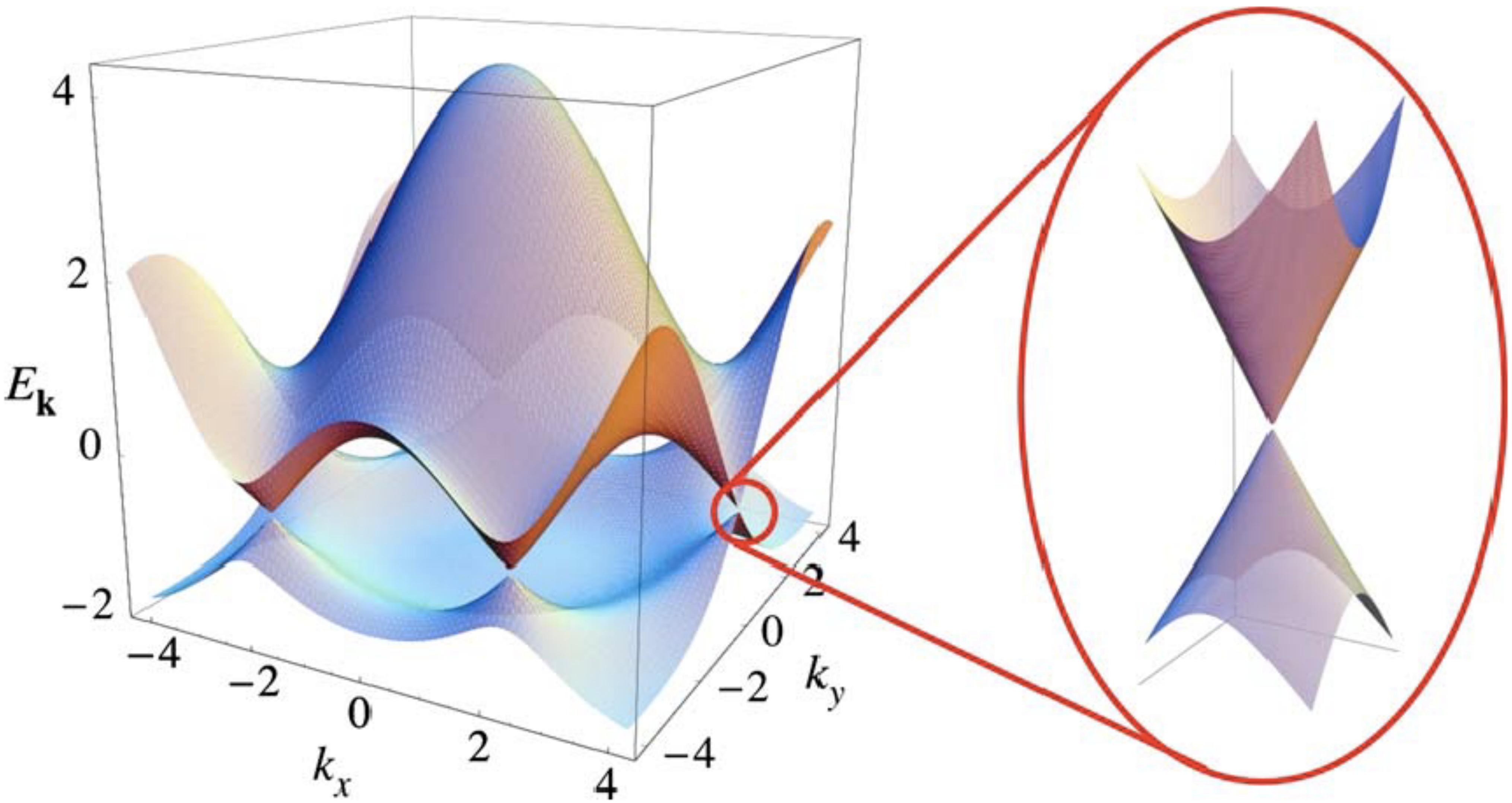
S. Zhang. Topological insulators. *Scholarpedia*, 10(7):30275, 2015. revision 151969.

Graphene

$$E = \pm\sqrt{m_0^2 c^4 + p^2 c^2}$$

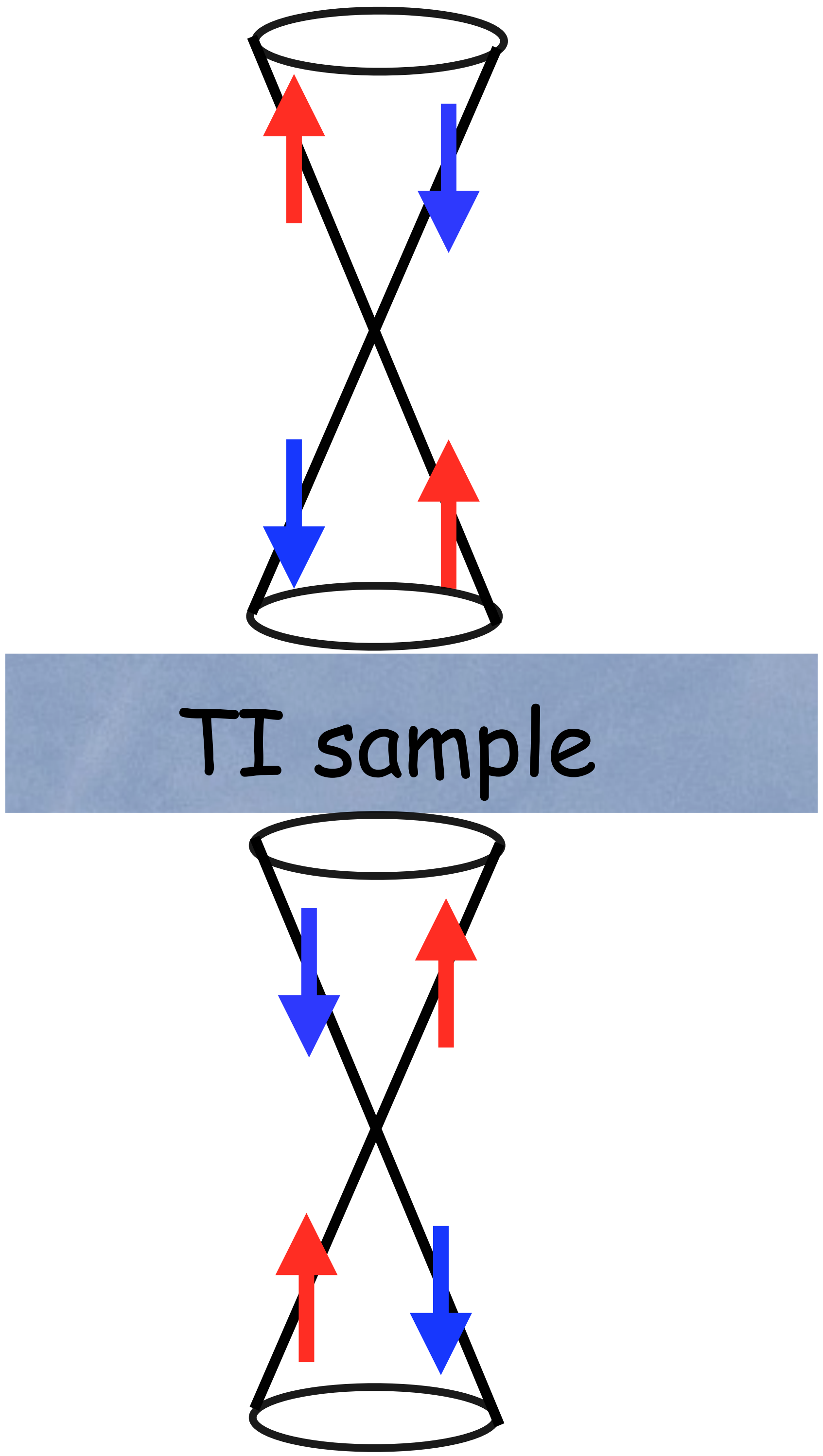
$$m_0 = 0 \Rightarrow E = pc$$





Topological insulators:

Highly unusual surface state



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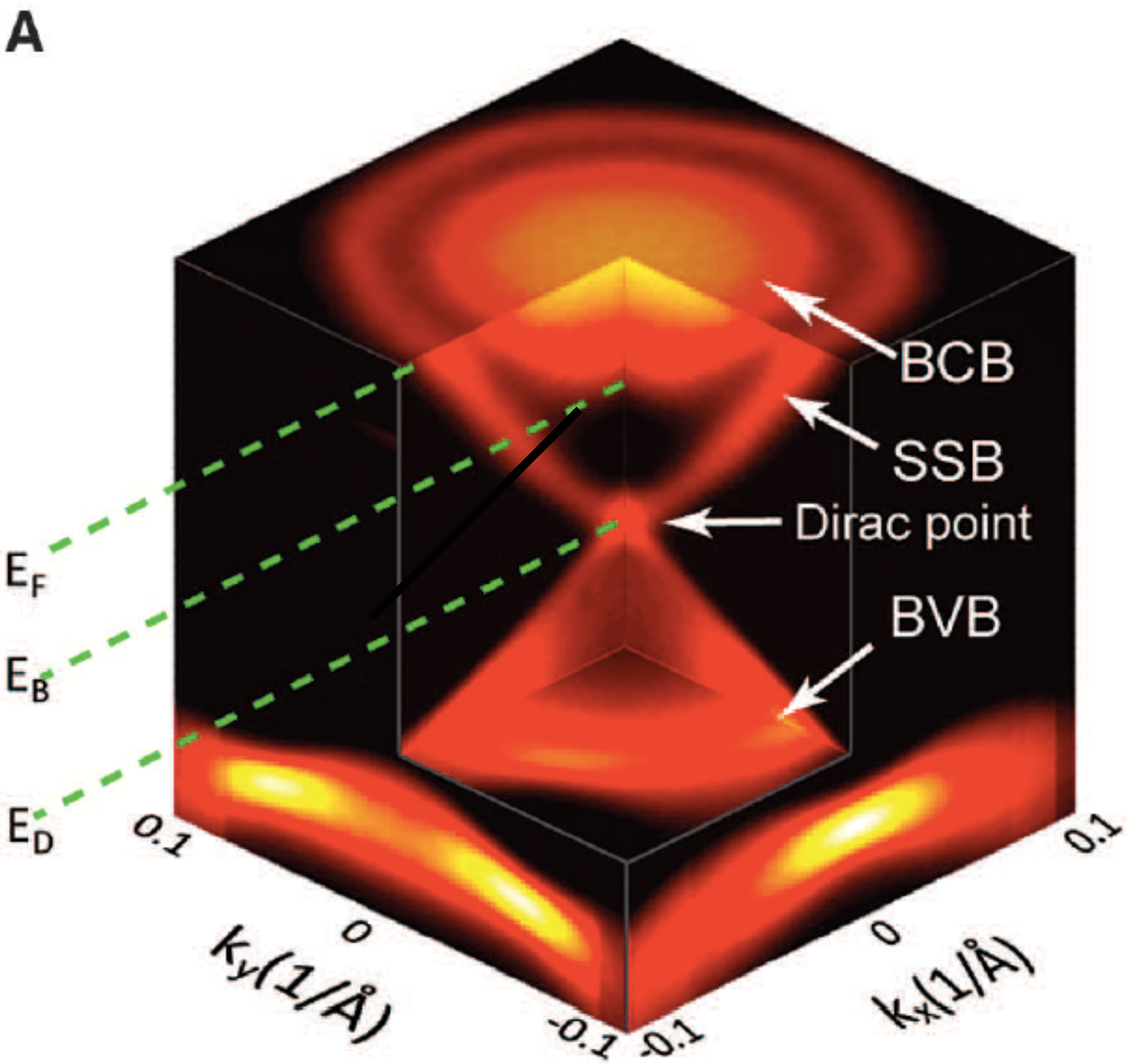
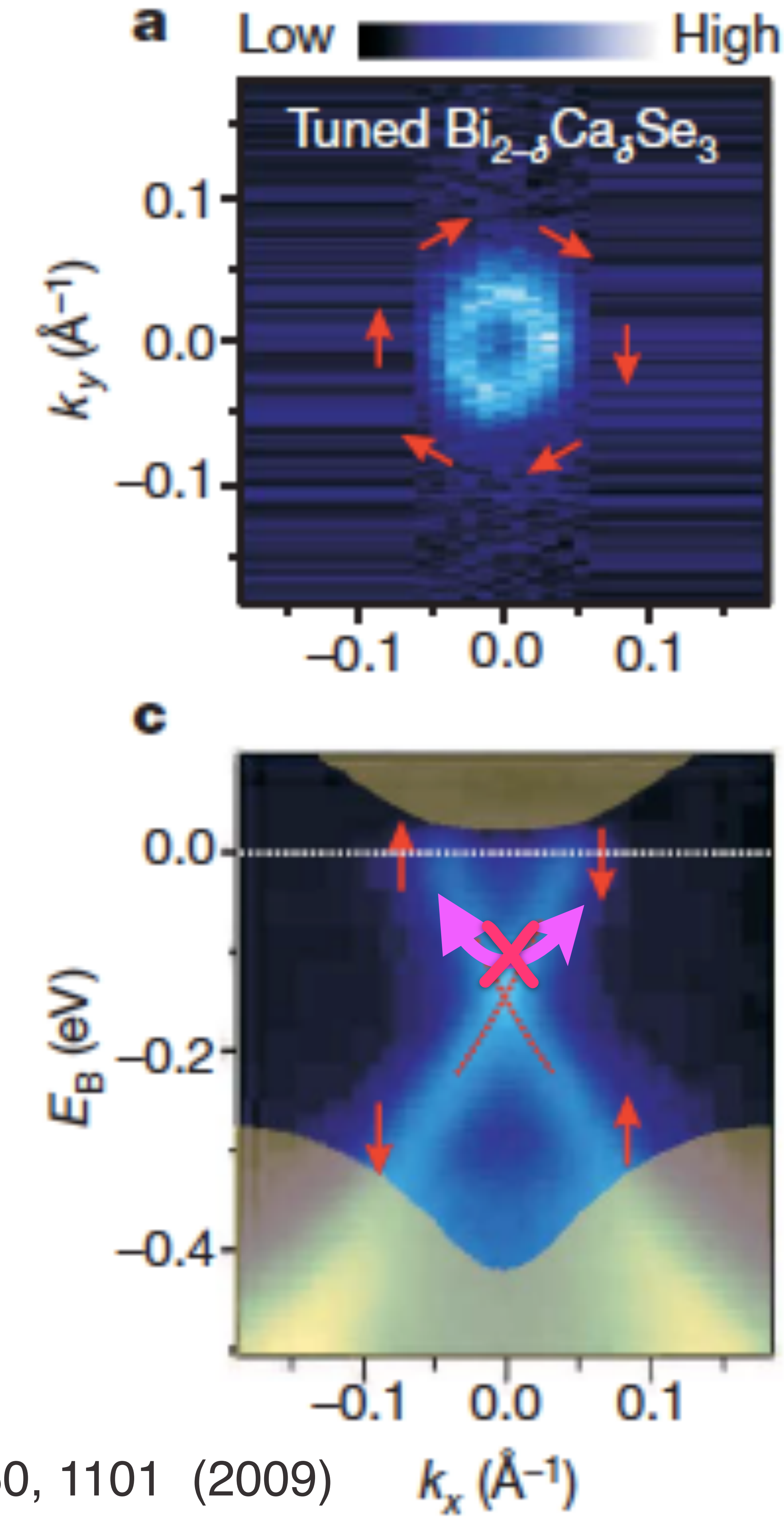
Liang Fu and C. L. Kane, Phys. Rev. B 76, 045302 (2007).

Topological insulators:

Highly unusual surface state

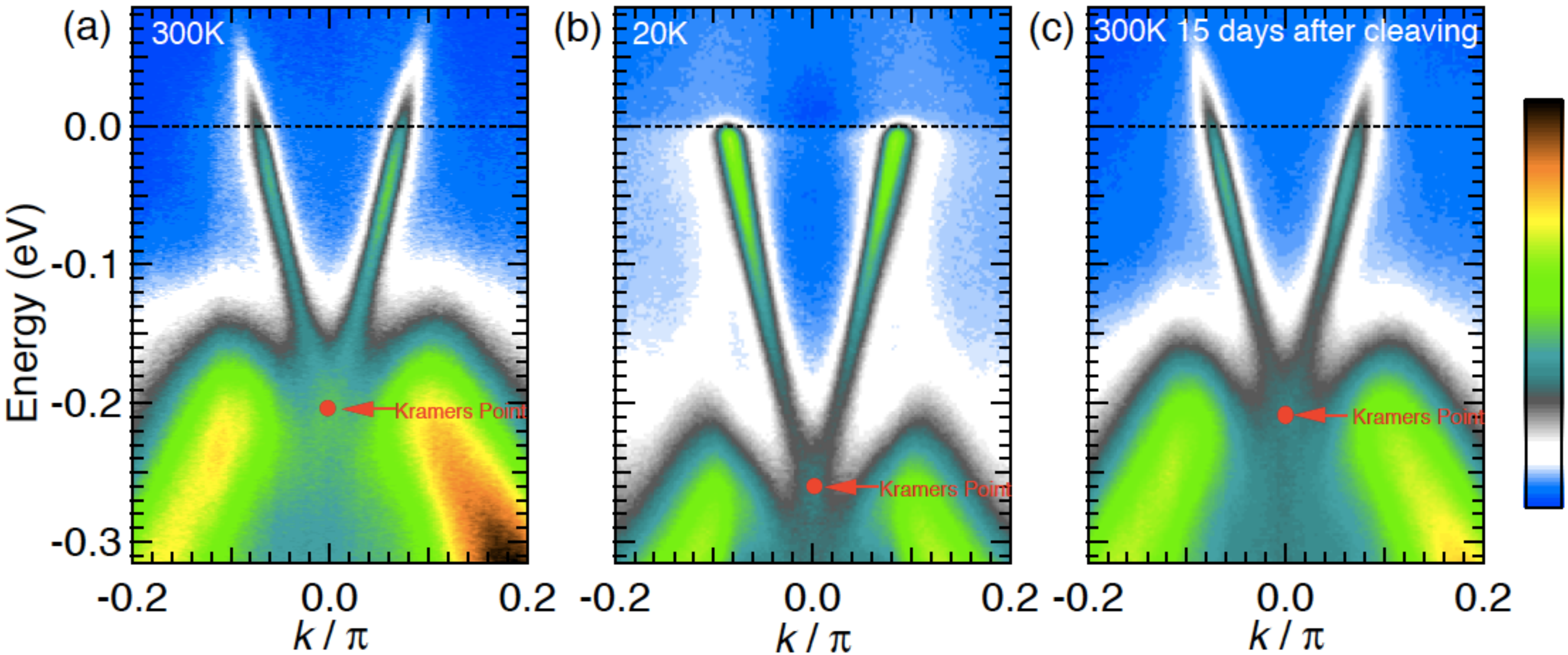


Y. Chen et al., Science 329, 659 (2010).



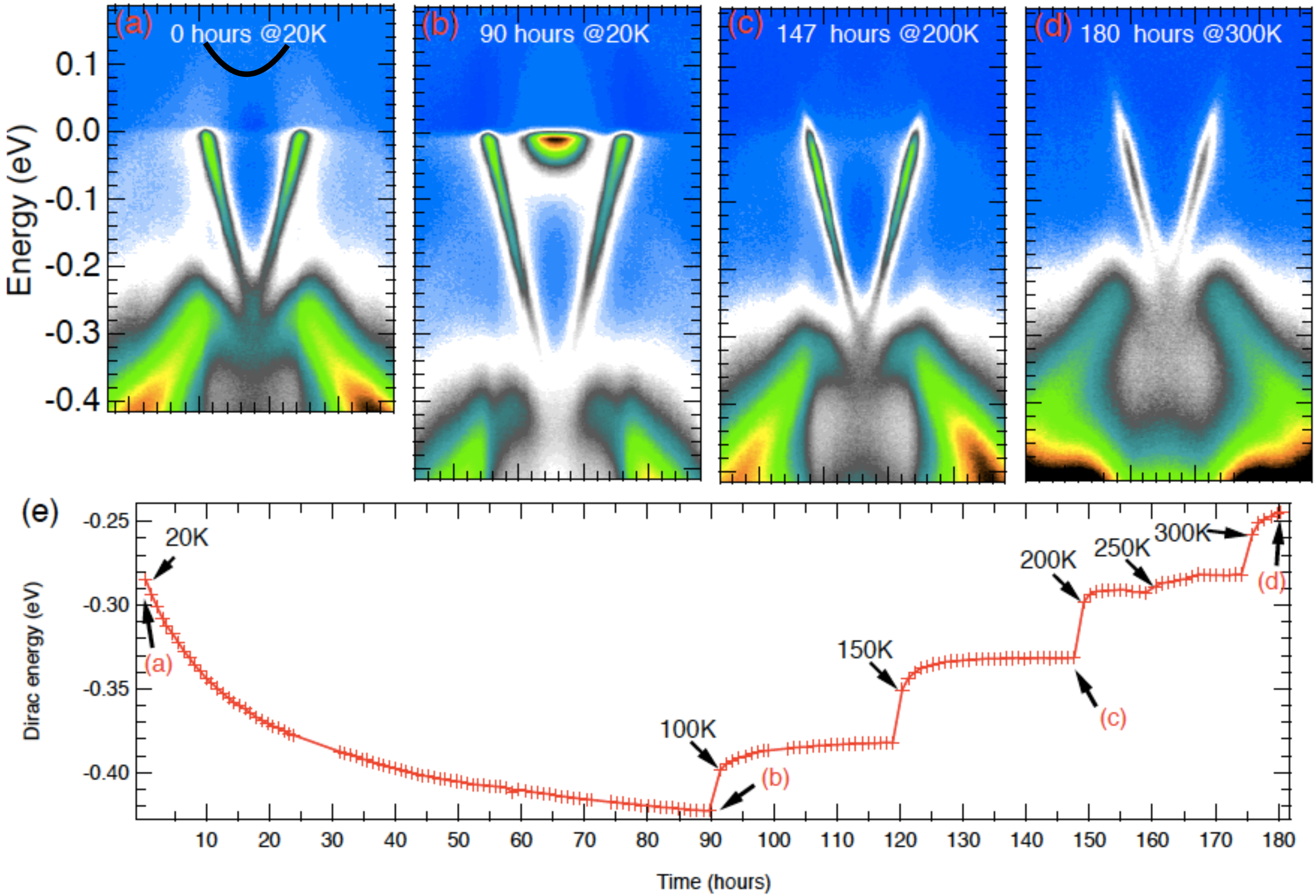
D. Hsieh et al., Nature 460, 1101 (2009)

Tuning properties of topological insulators: $Bi_2Te_{2.8}Se_{0.2}$ - a true topological insulator



Rui Jiang *et al.*, Phys. Rev. B. **86,** 085112 (2012

Tuning properties of $Bi_2Te_{2.8}Se_{0.2}$



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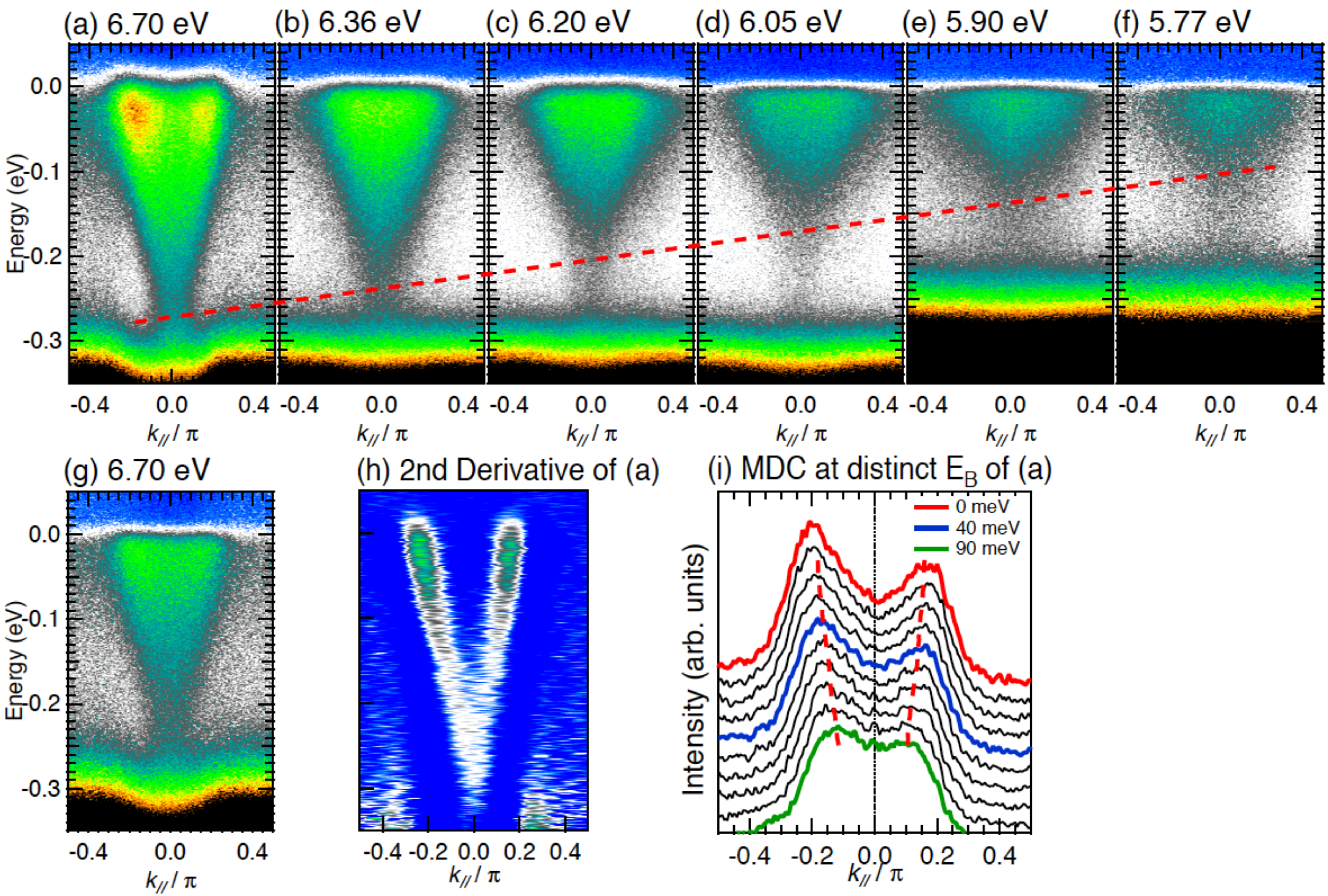
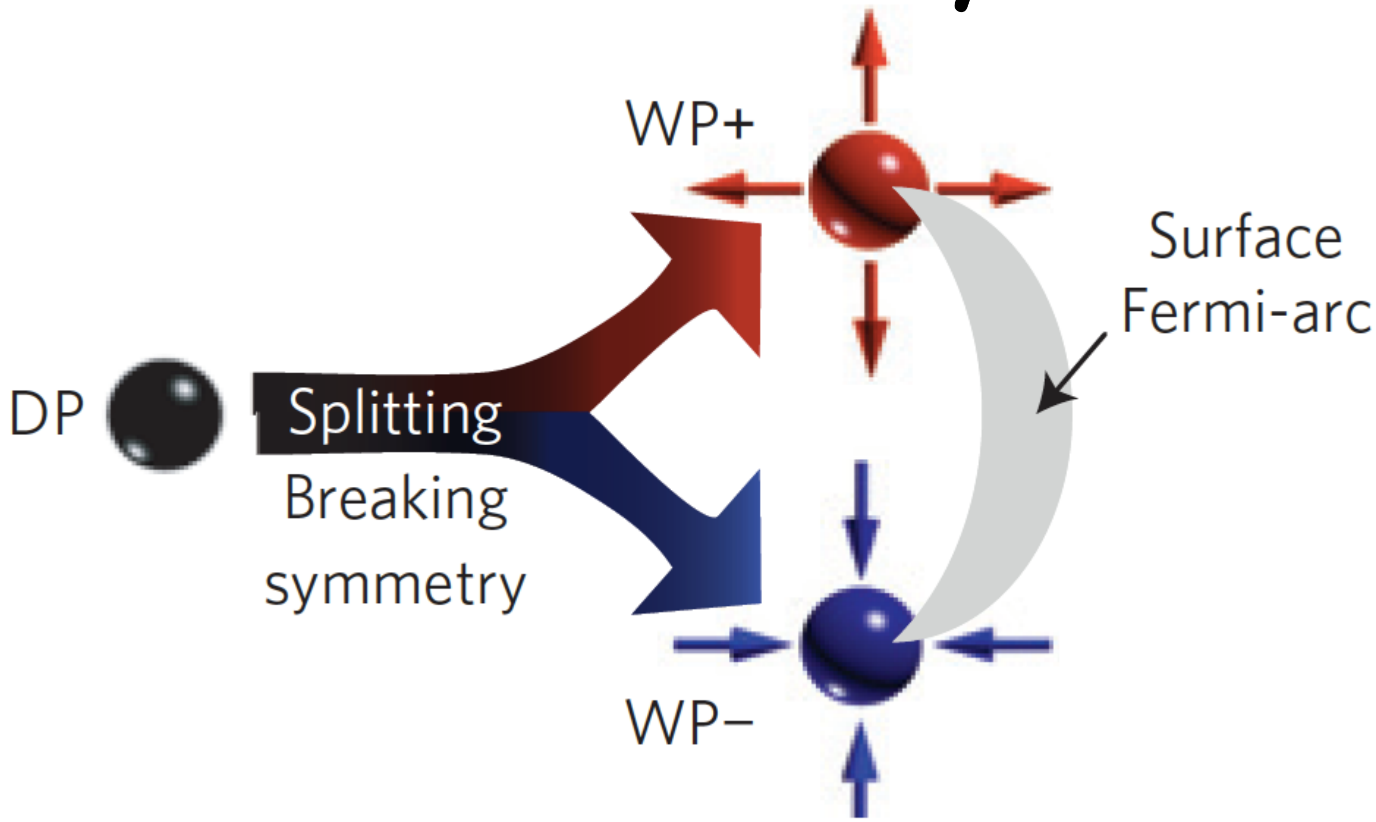
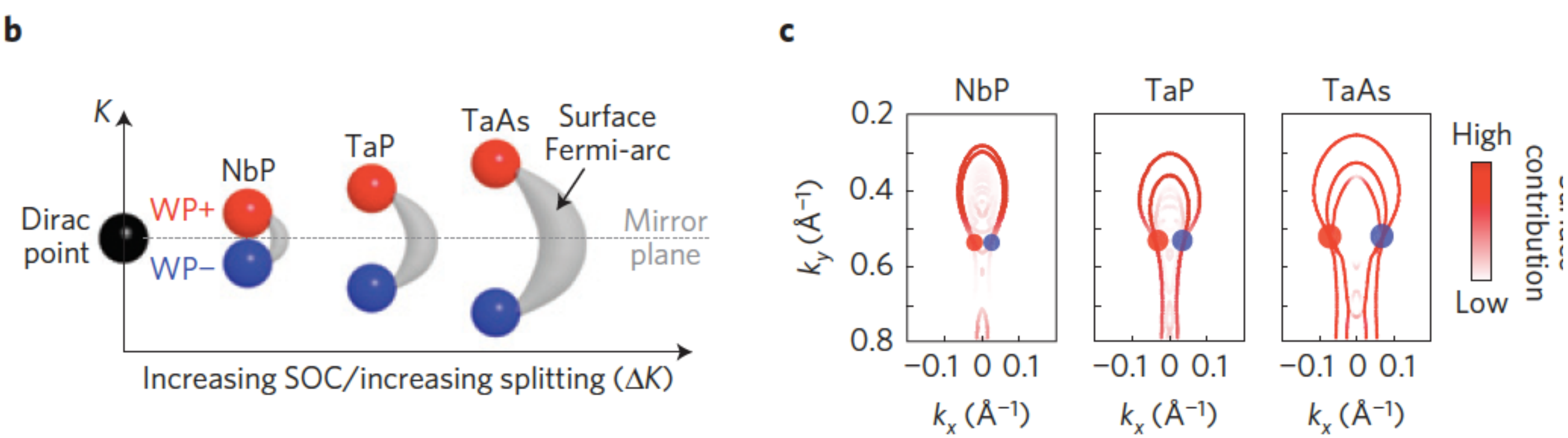
Rui Jiang *et al.*, Phys. Rev. B. **86,** 085112 (2012)

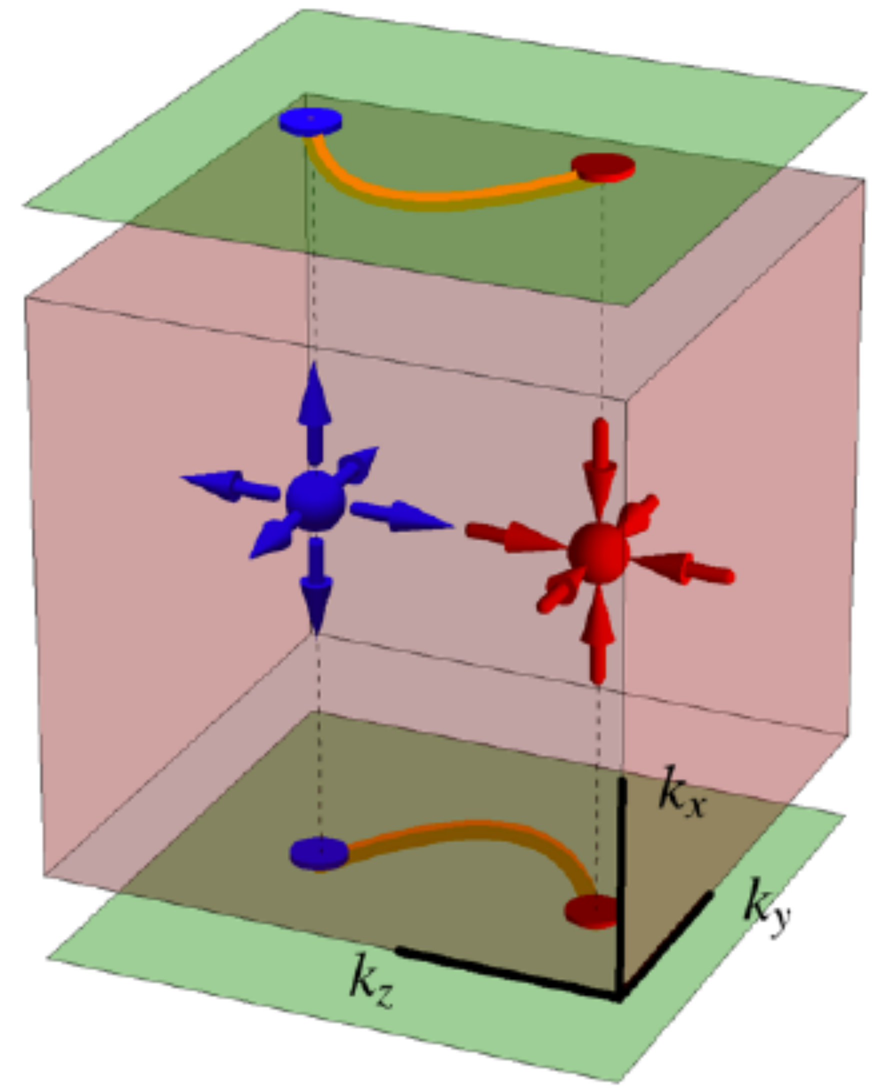
3D Dirac semimetal - Cd_3As_2



Weyl semimetals







Z. K. Liu et al., Nat Mater 15, 27 (2016).

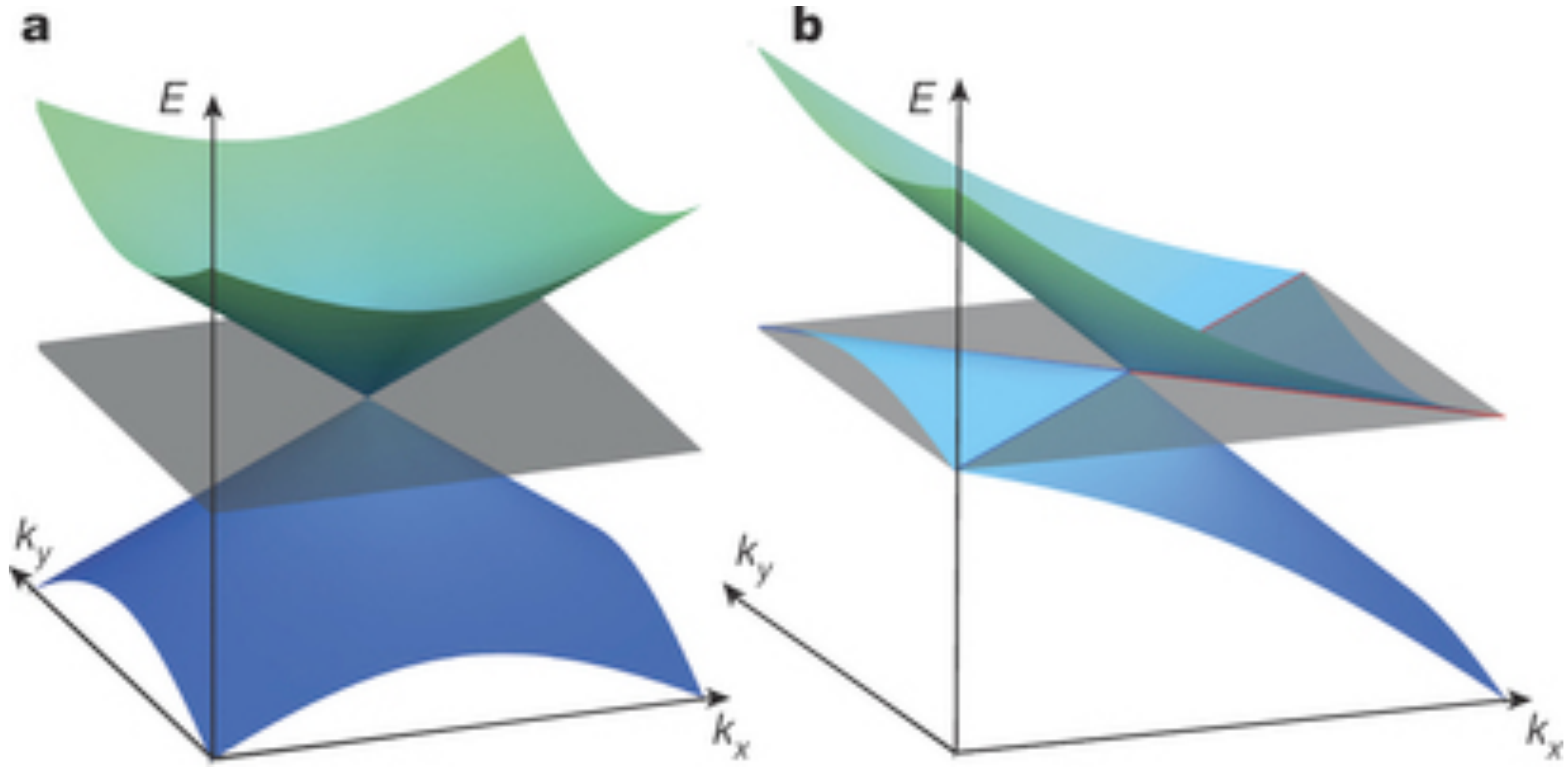
H. Weyl, Electron and Gravitation. I, Z. Phys. 56, 330 (1929).

X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011).

L. Balents, Weyl Electrons Kiss, Physics 4, 36 (2011).

G. Xu, H. Weng, Z. Wang, X. Dai, and Z. Fang, Phys. Rev. Lett. 107, 186806 (2011).

Weyl semimetals



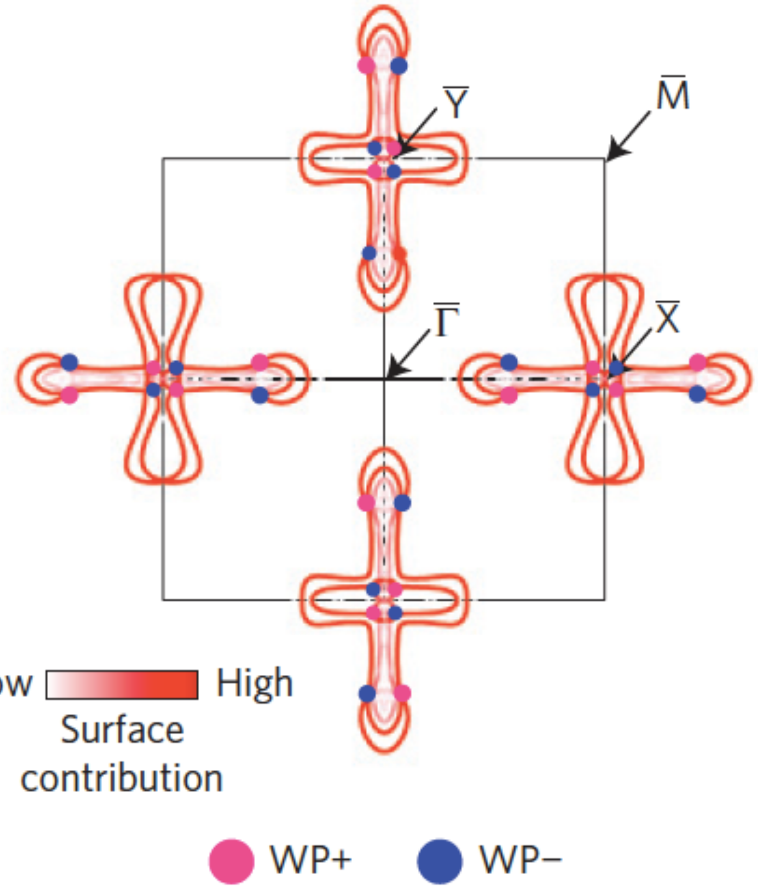
Type I: TaAs, NbAs
TaP, NbP

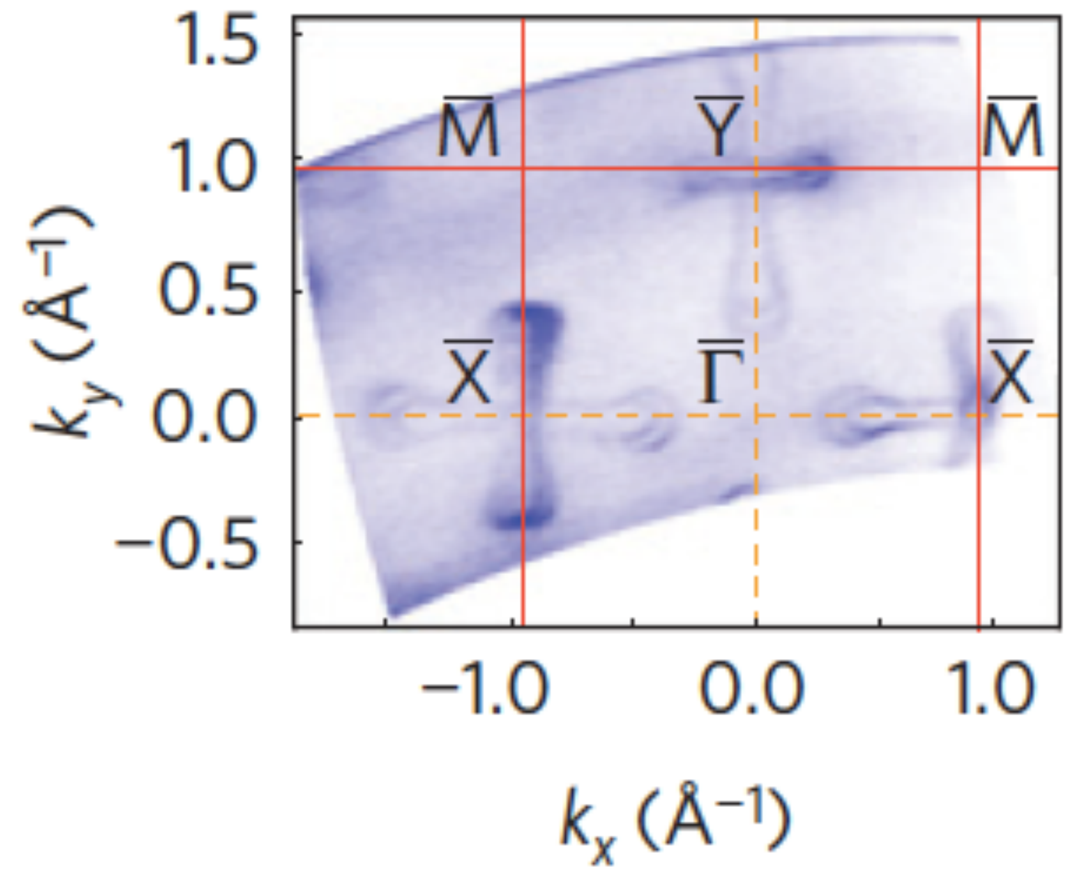
Type II: WTe_2, $MoTe_2$

S.-Y. Xu et al., Science 349, 613 (2015).
S.-Y. Xu et al., Nat Phys 11, 748 (2015).
L. X. Yang et al., Nat Phys 11, (2015).

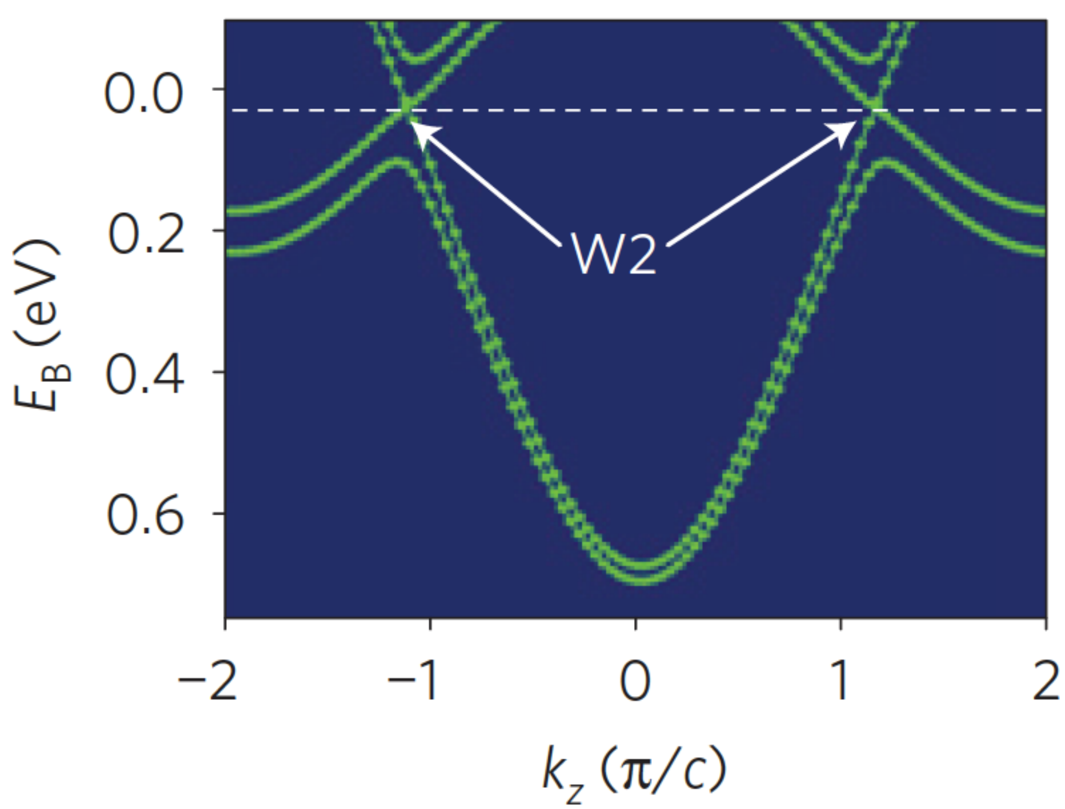
Alexey A. Soluyanov, Nature 527, 495–498 (2015)
Lunan Huang et al., arXiv:1603.06482
Yun Wu et al., arXiv:1604.05176

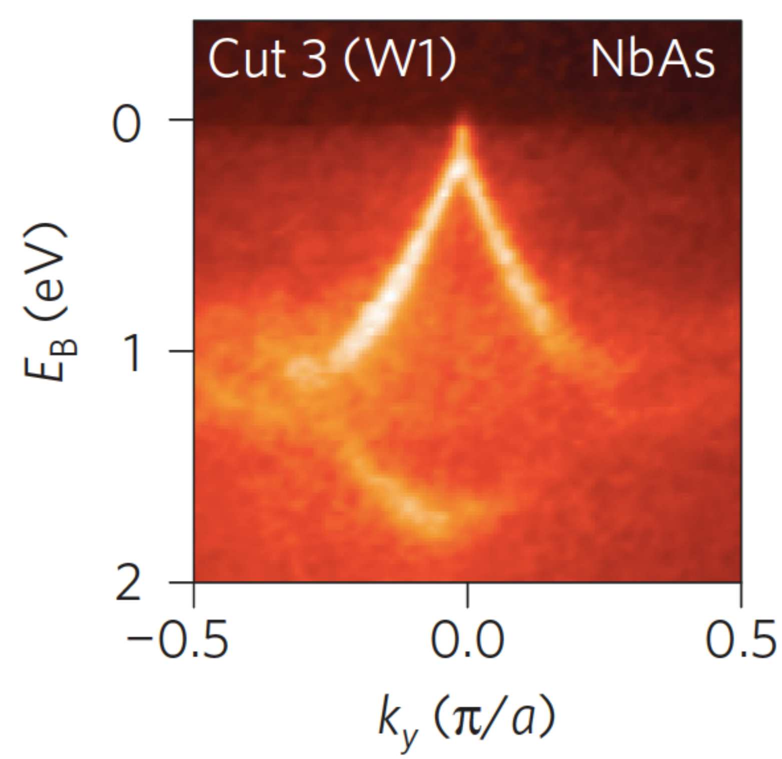
Type I: TaAs NbAs





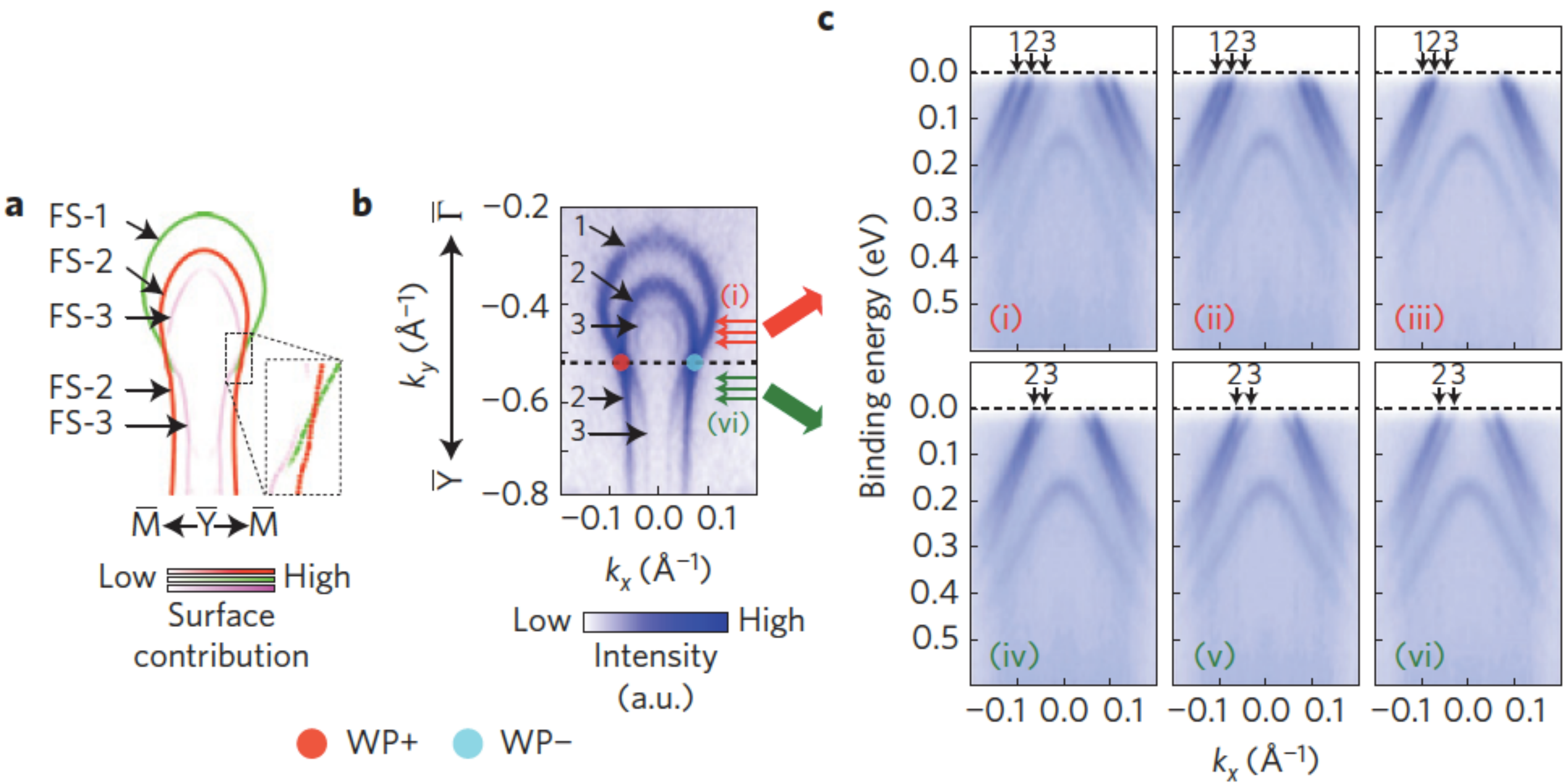
L. X. Yang et al., Nat Phys 11, 728 (2015).





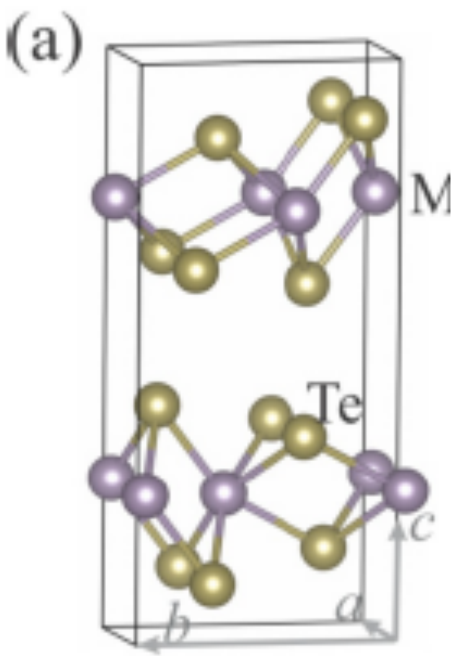
S.-Y. Xu et al., Nature Physics 11, 748 (2015).

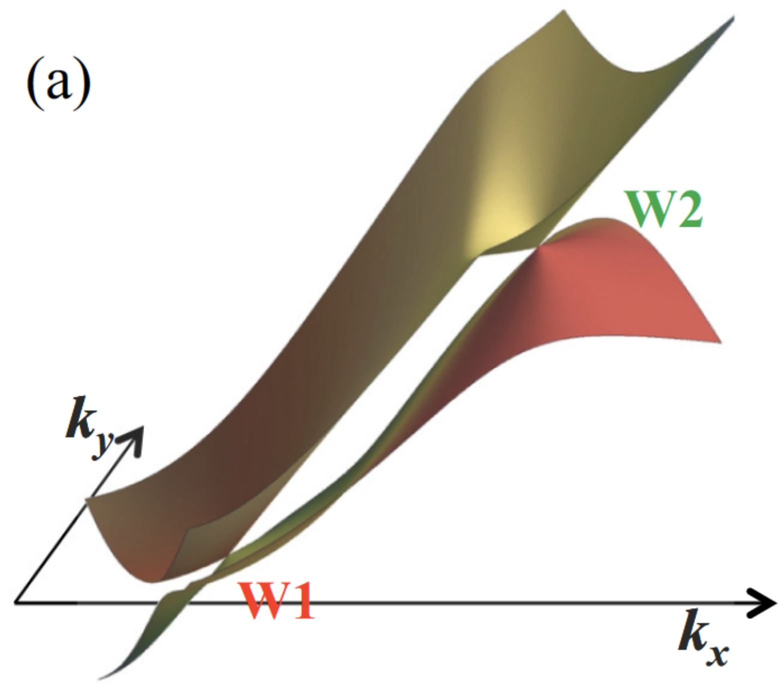
Type I: TaAs, NbAs

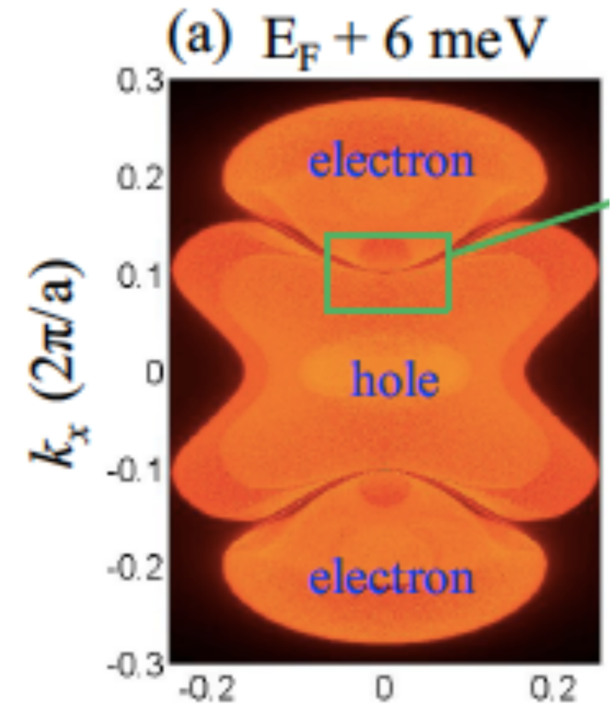


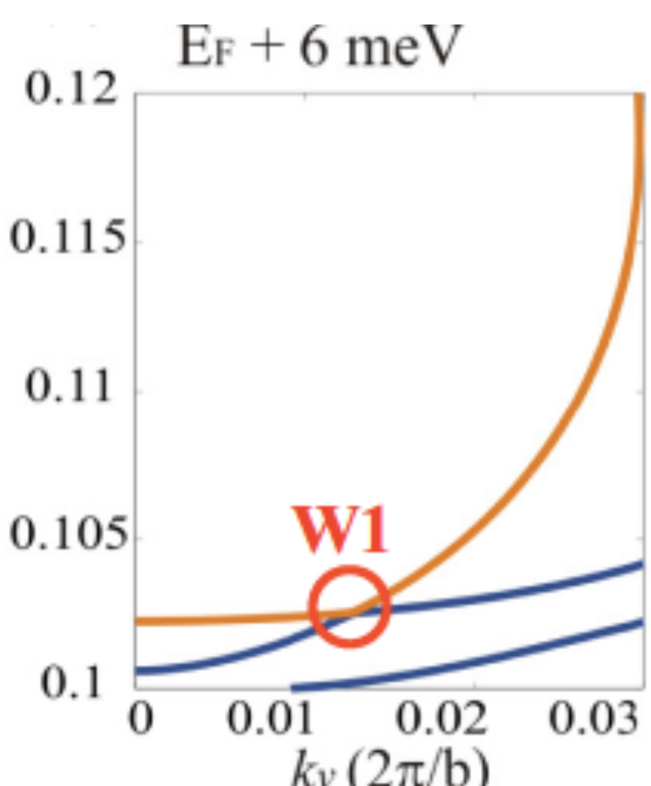
L. X. Yang et al., Nat Phys 11, 728 (2015).

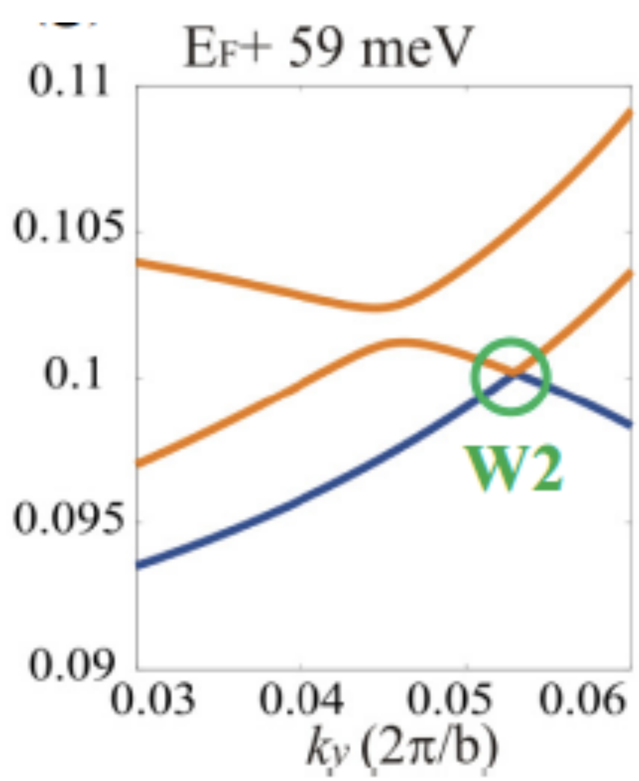
Prediction of Weyl II semimetallic state in $MoTe_2$

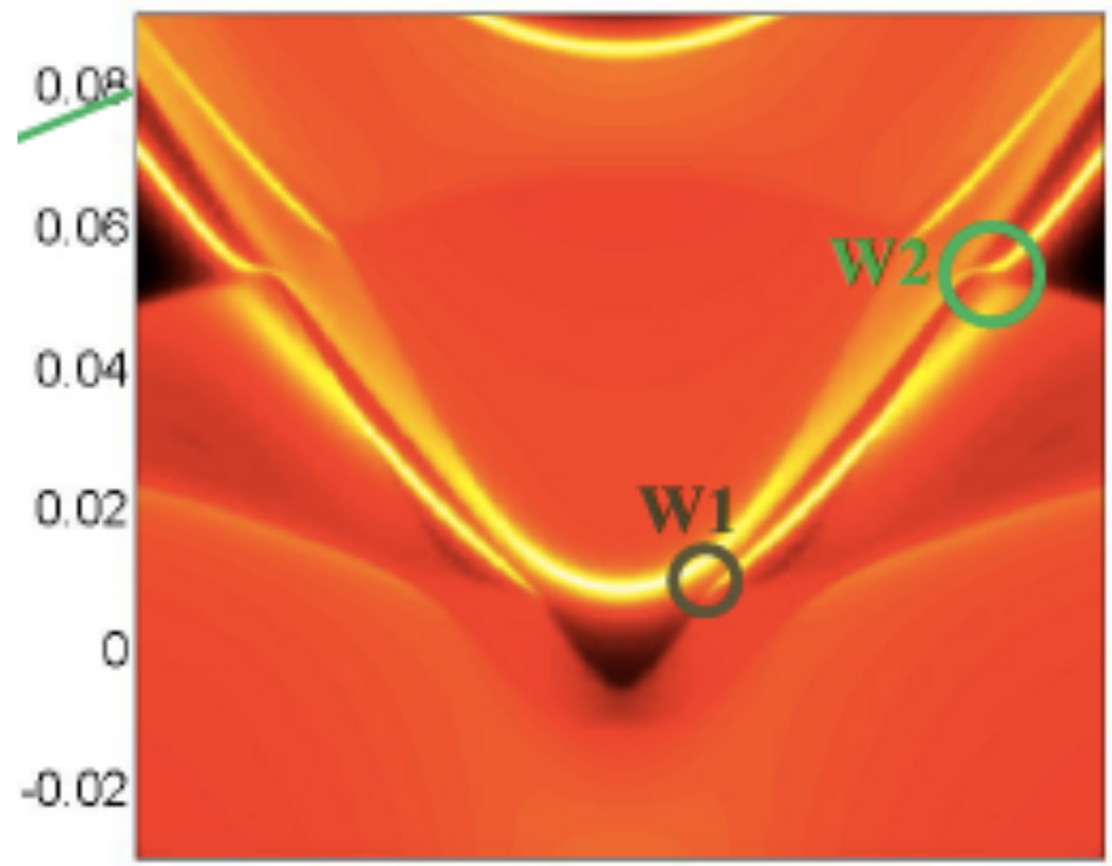










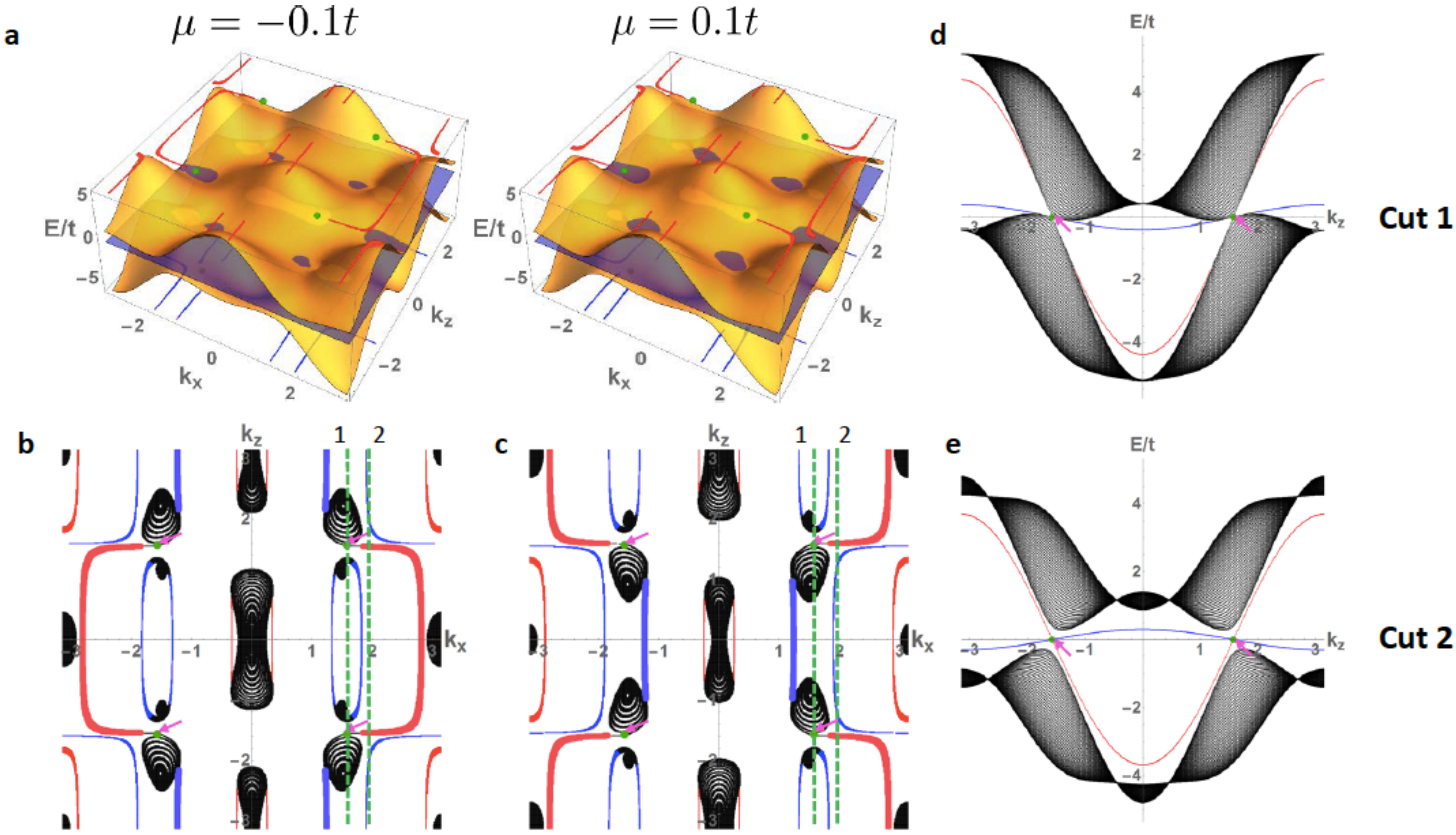


Qian et al, Science 346, 1344 (2014)

Alexey A. Soluyanov, Nature 527, 495–498 (2015)

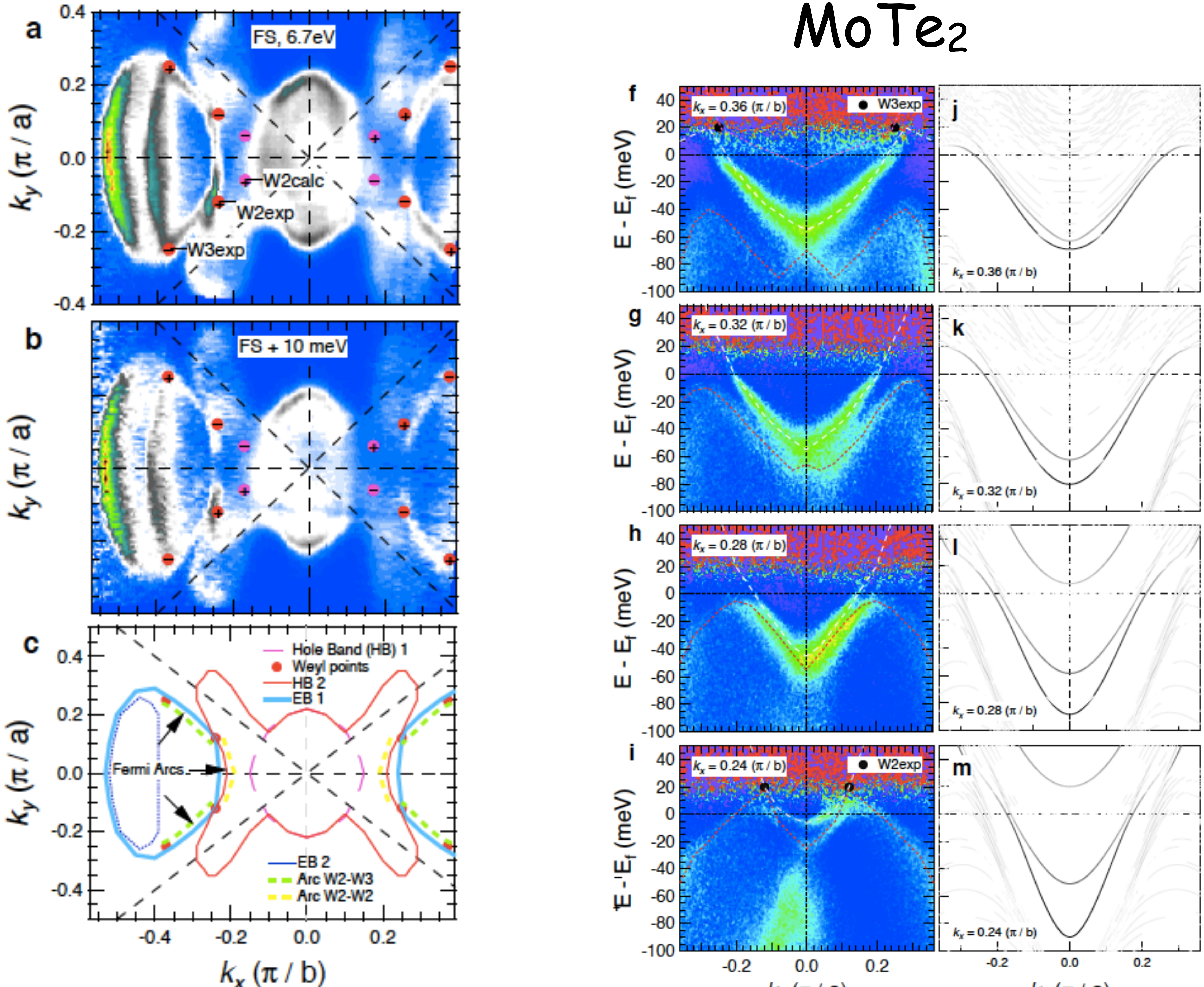
Yan Sun et al., Phys. Rev. B 92, 161107(R) (2015)

"Simplified" model of Weyl II semimetal



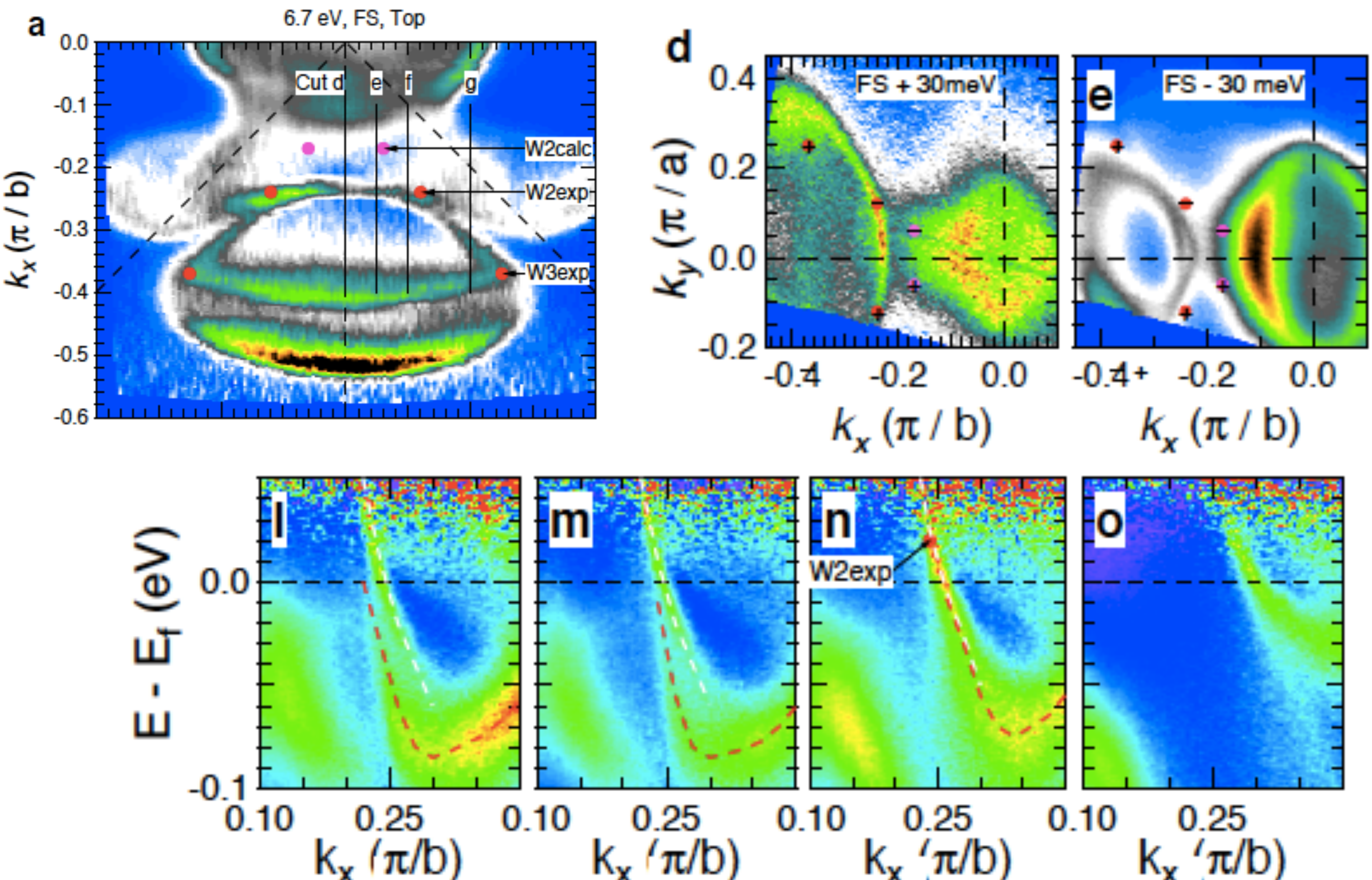
Lunan Huang et al., Nature Materials 15, 1155–1160 (2016)

MoTe$_2$



Lunan Huang et al., Nature Materials 15, 1155–1160 (2016)

Signatures of type II Weyl semimetal in $MoTe_2$



Lunan Huang et al., Nature Materials 15, 1155–1160 (2016)

Electronic properties of WTe_2

~500,000%

LETTER

doi:10.1038/nature13763

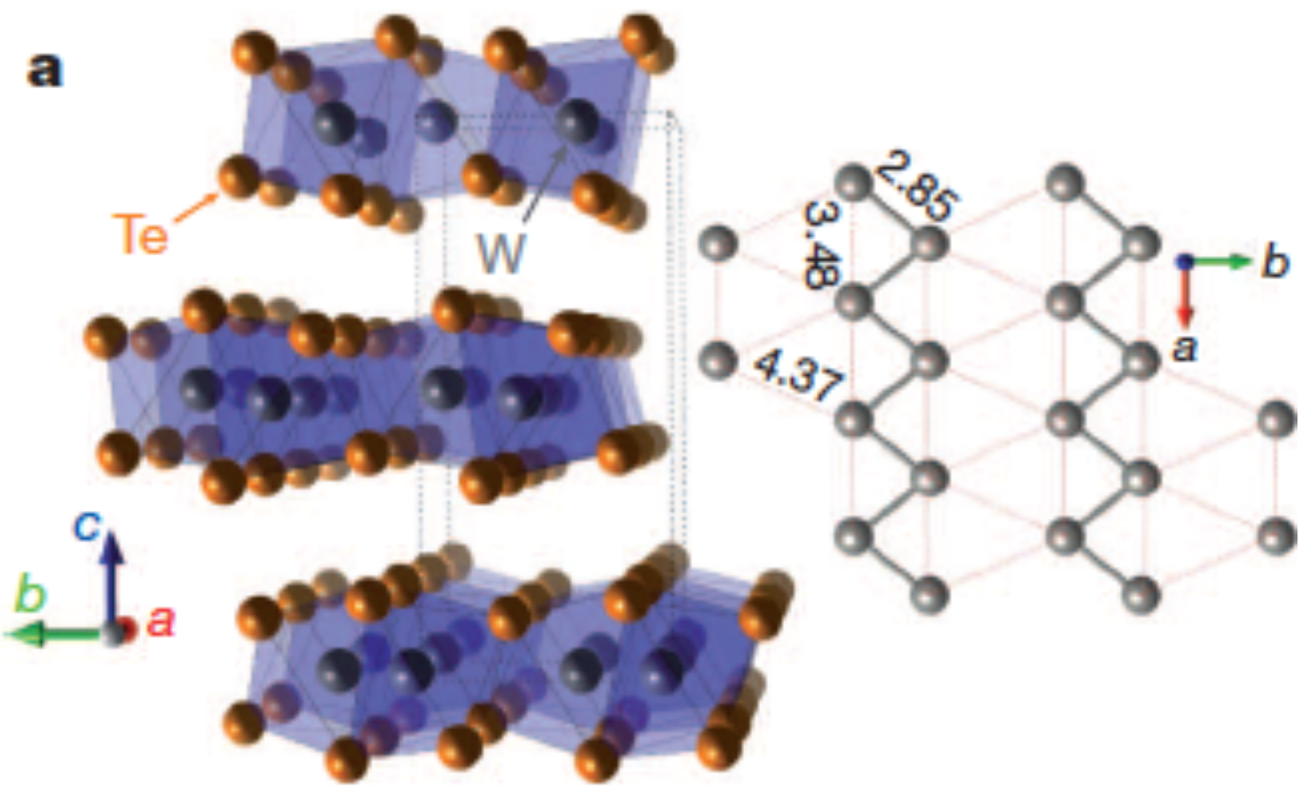
titanic

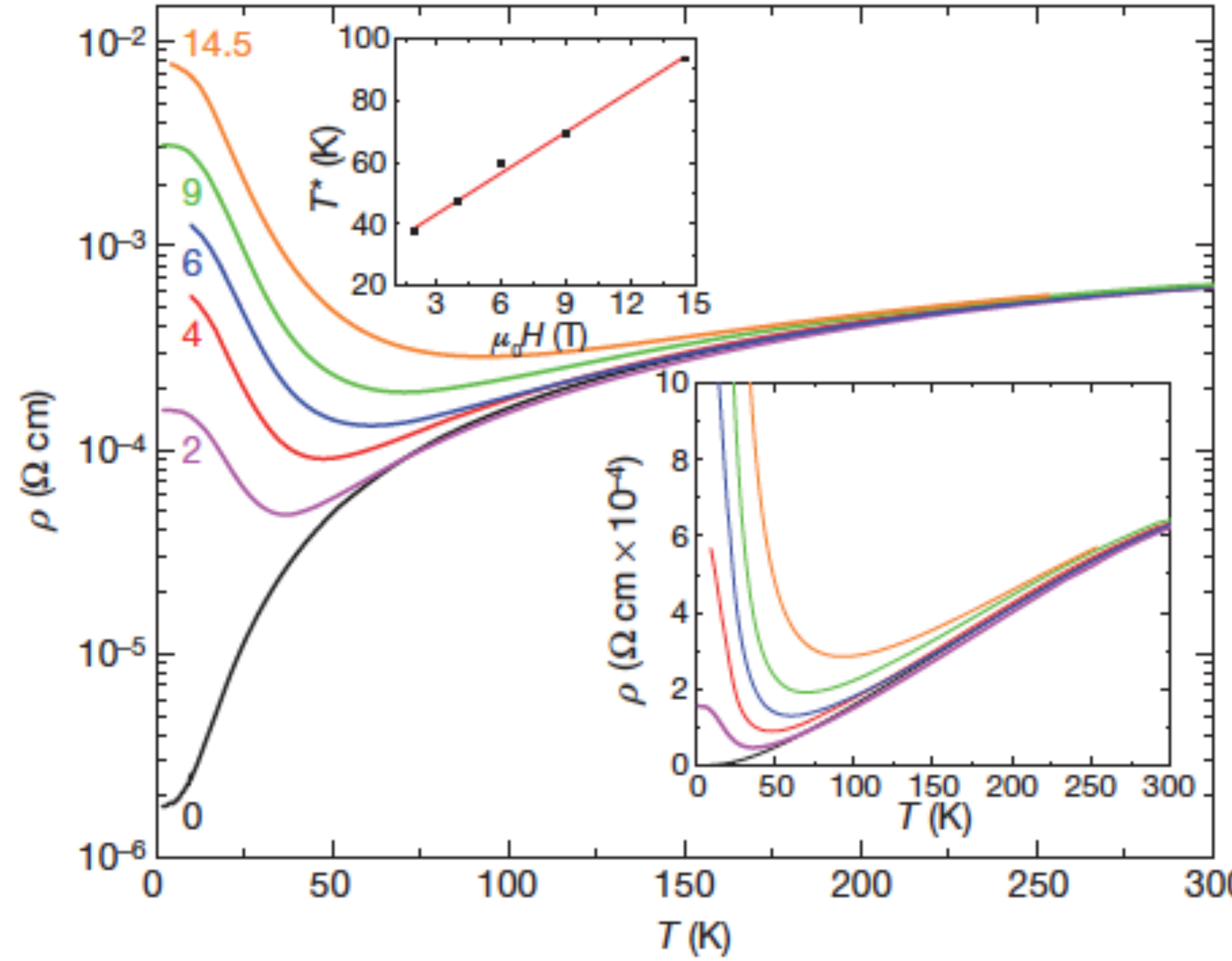
Large, non-saturating magnetoresistance in WTe_2

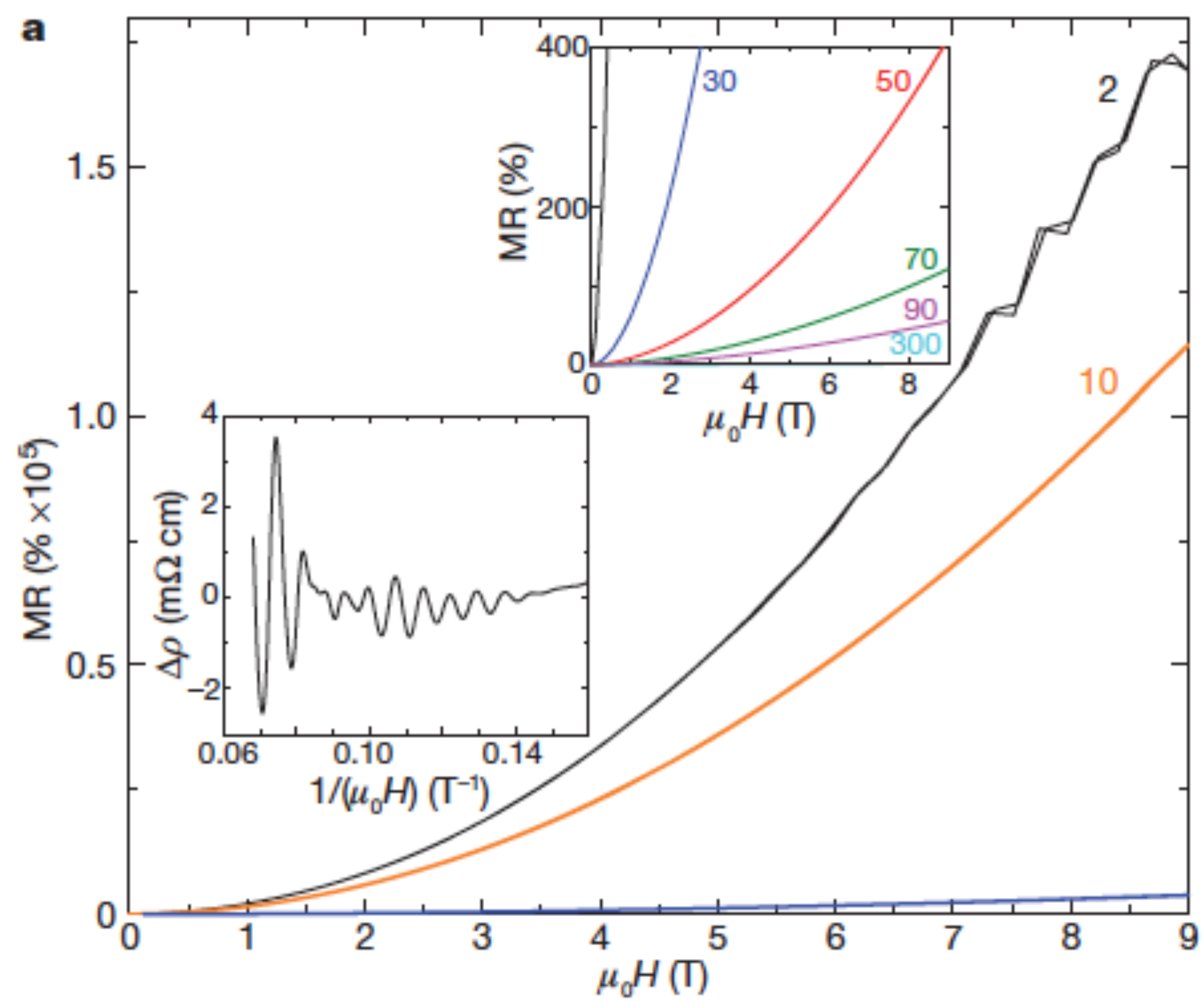
Mazhar N. Ali[1], Jun Xiong[2], Steven Flynn[1], Jing Tao[3], Quinn D. Gibson[1], Leslie M. Schoop[1], Tian Liang[2], Neel Haldolaarachchige[1], Max Hirschberger[2], N. P. Ong[2] & R. J. Cava[1]

M. N. Ali et al., Nature 514, 205 (2014).

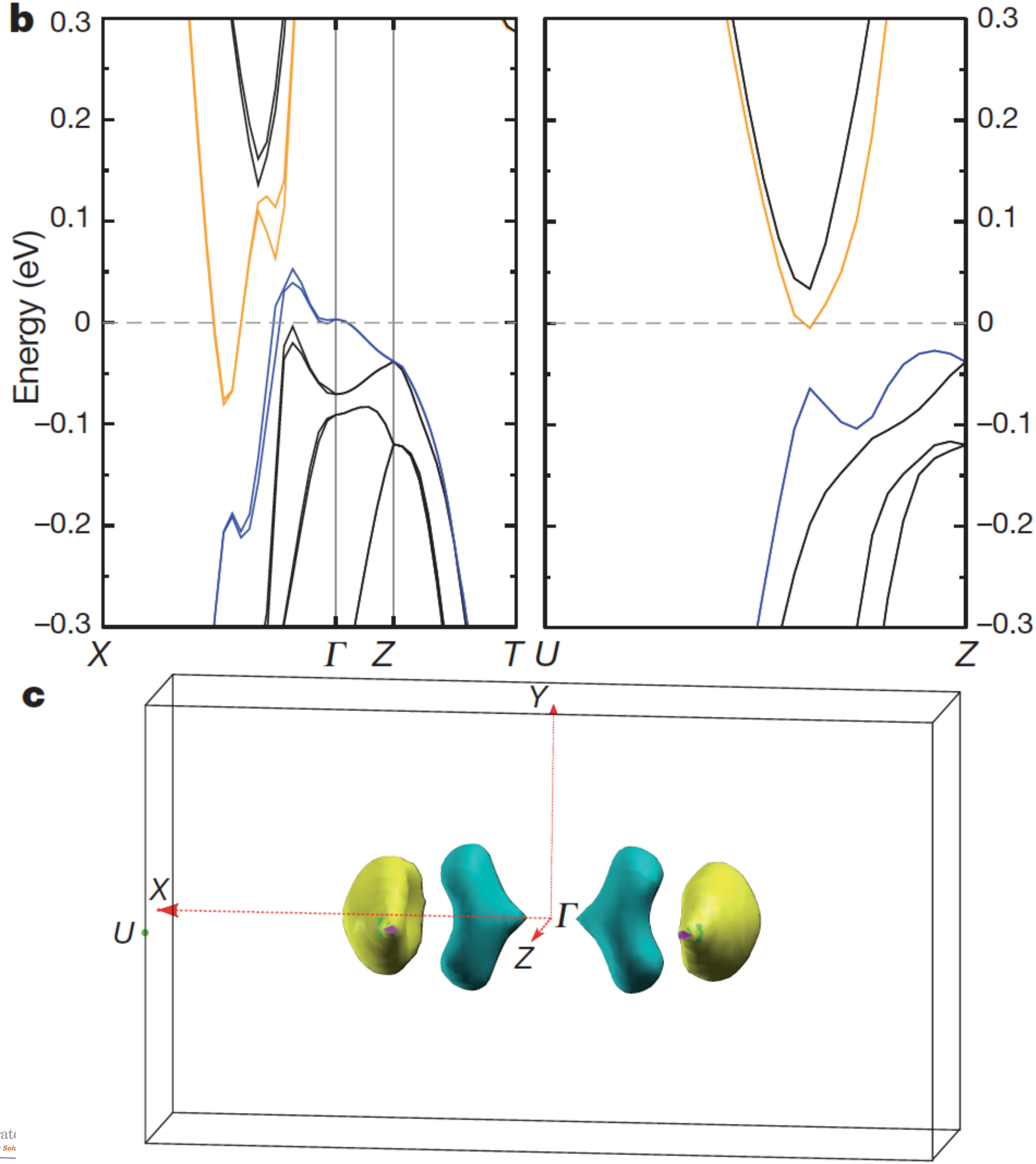
WTe_2





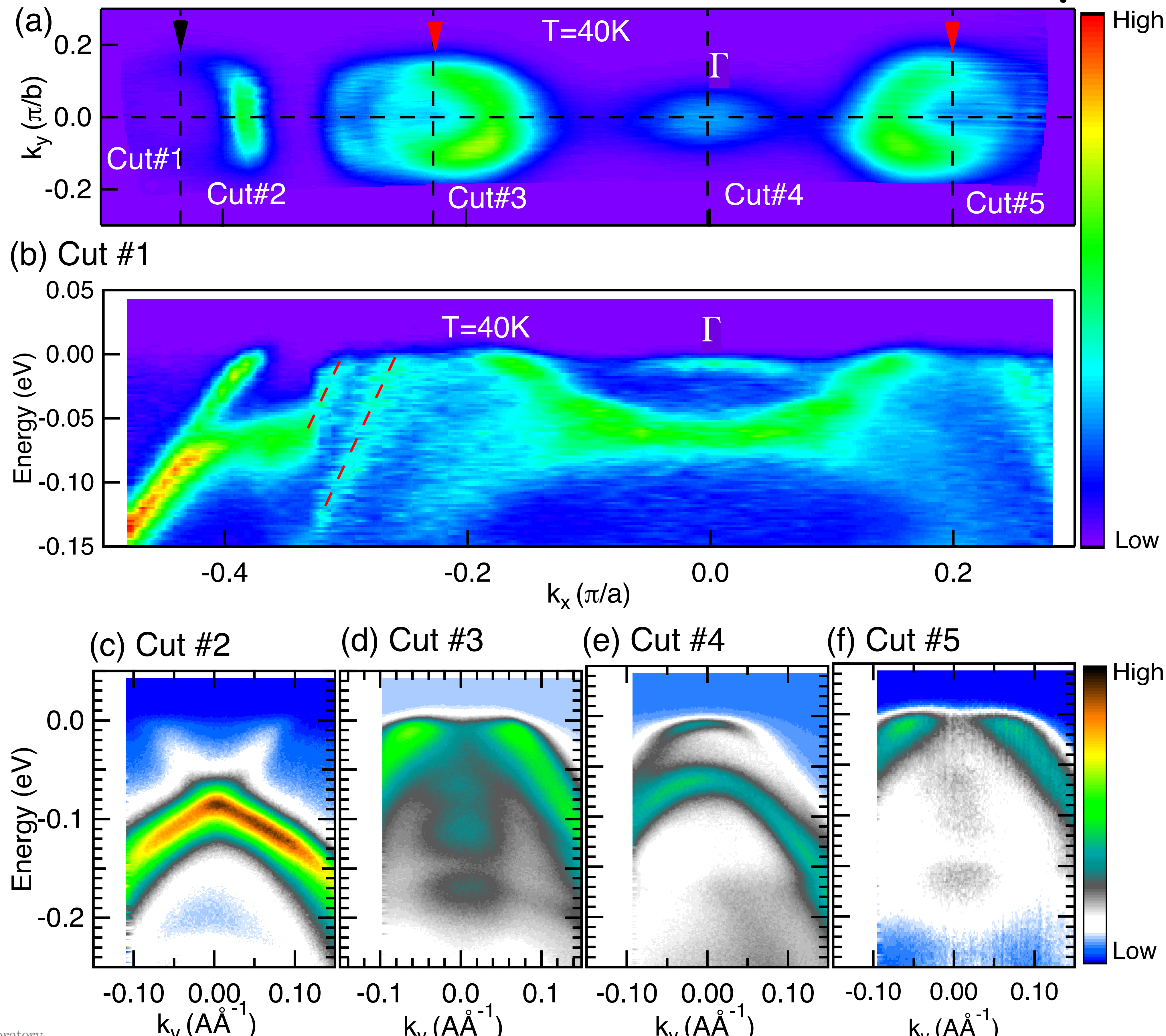


M. N. Ali et al., Nature 514, 205 (2014).



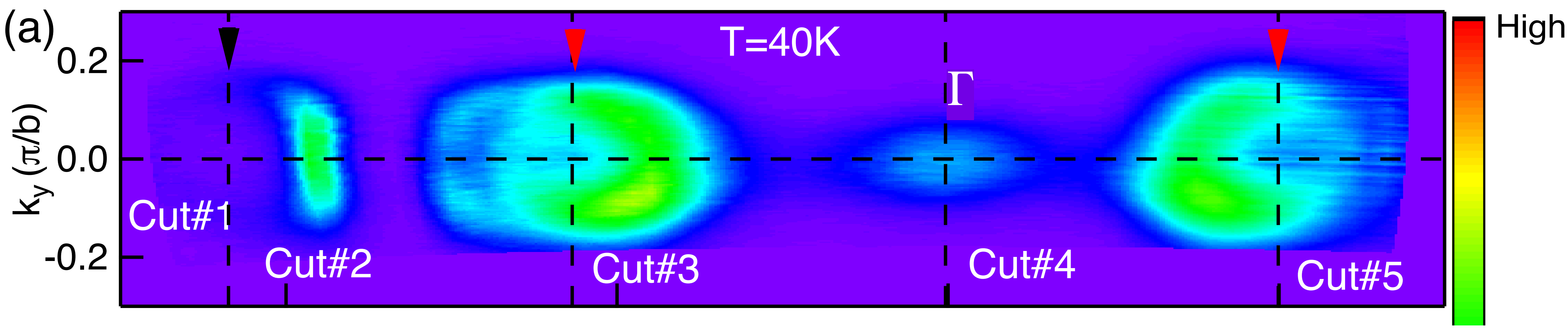
M. N. Ali et al.,
Nature 514, 205 (2014).

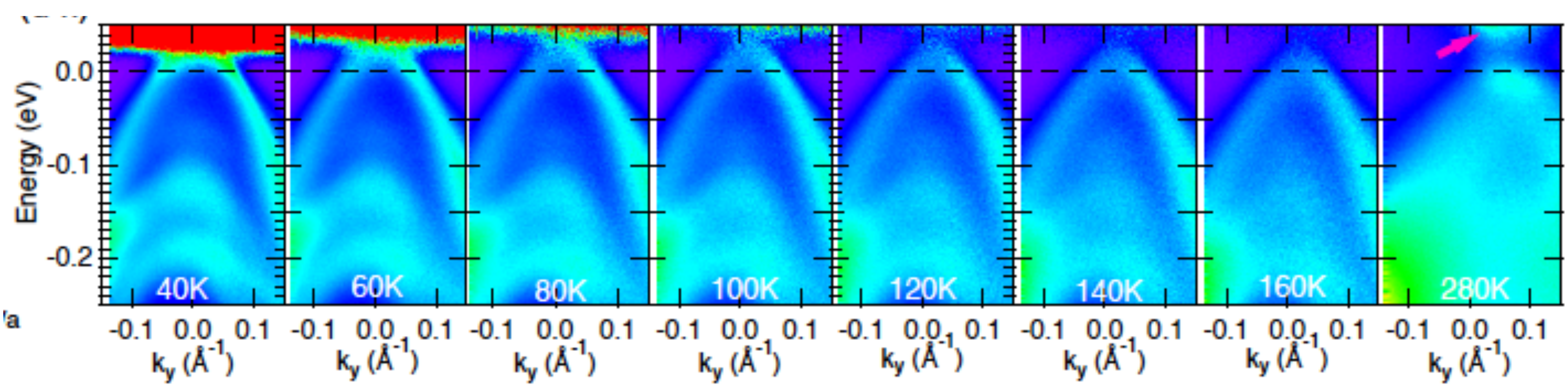
WTe_2 Fermi surface and band dispersion



Yun Wu *et al*., Phys. Rev. Lett. **115**, 166602 (2015).

WTe_2: temperature induced Lifshitz transition





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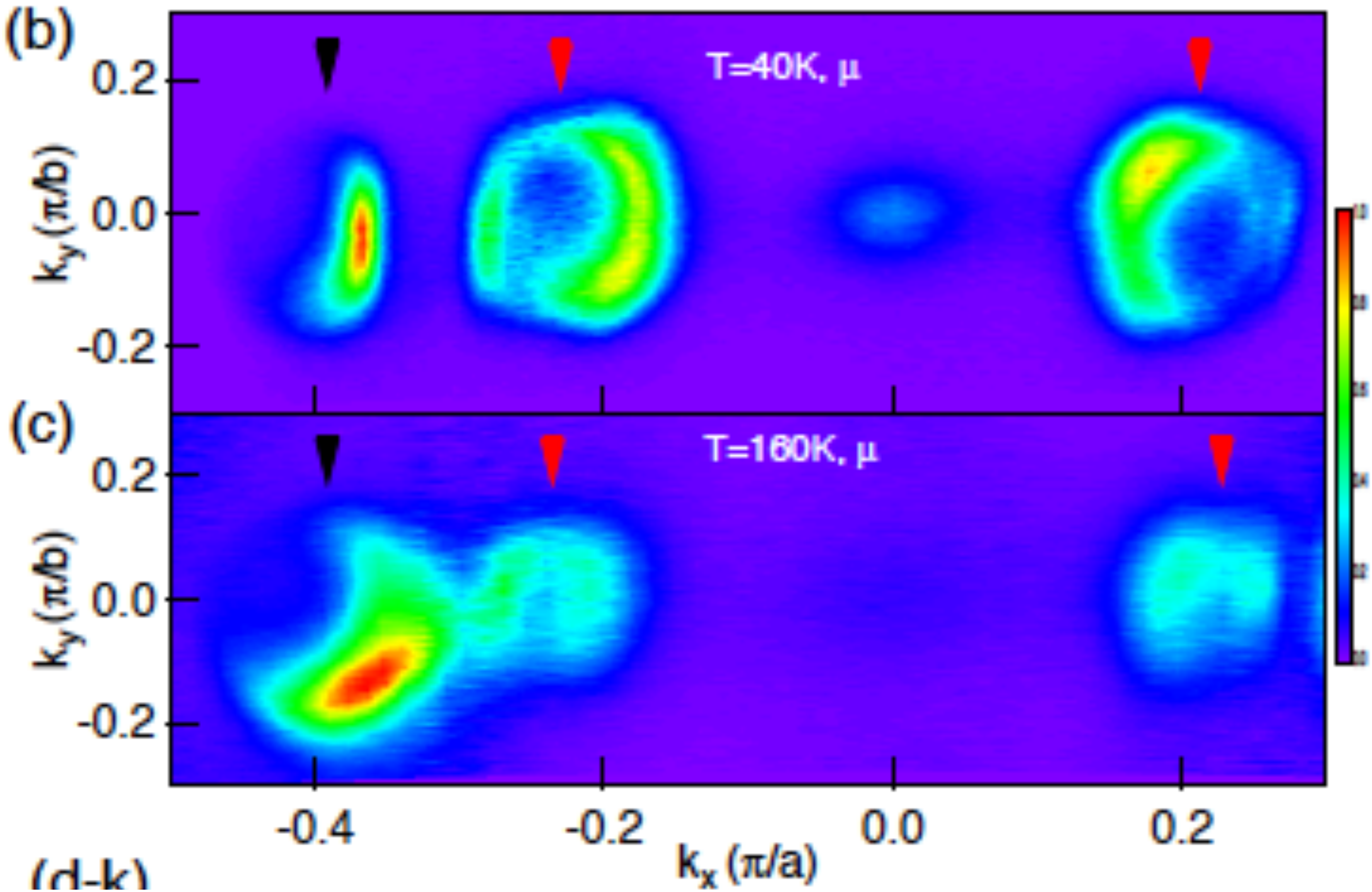

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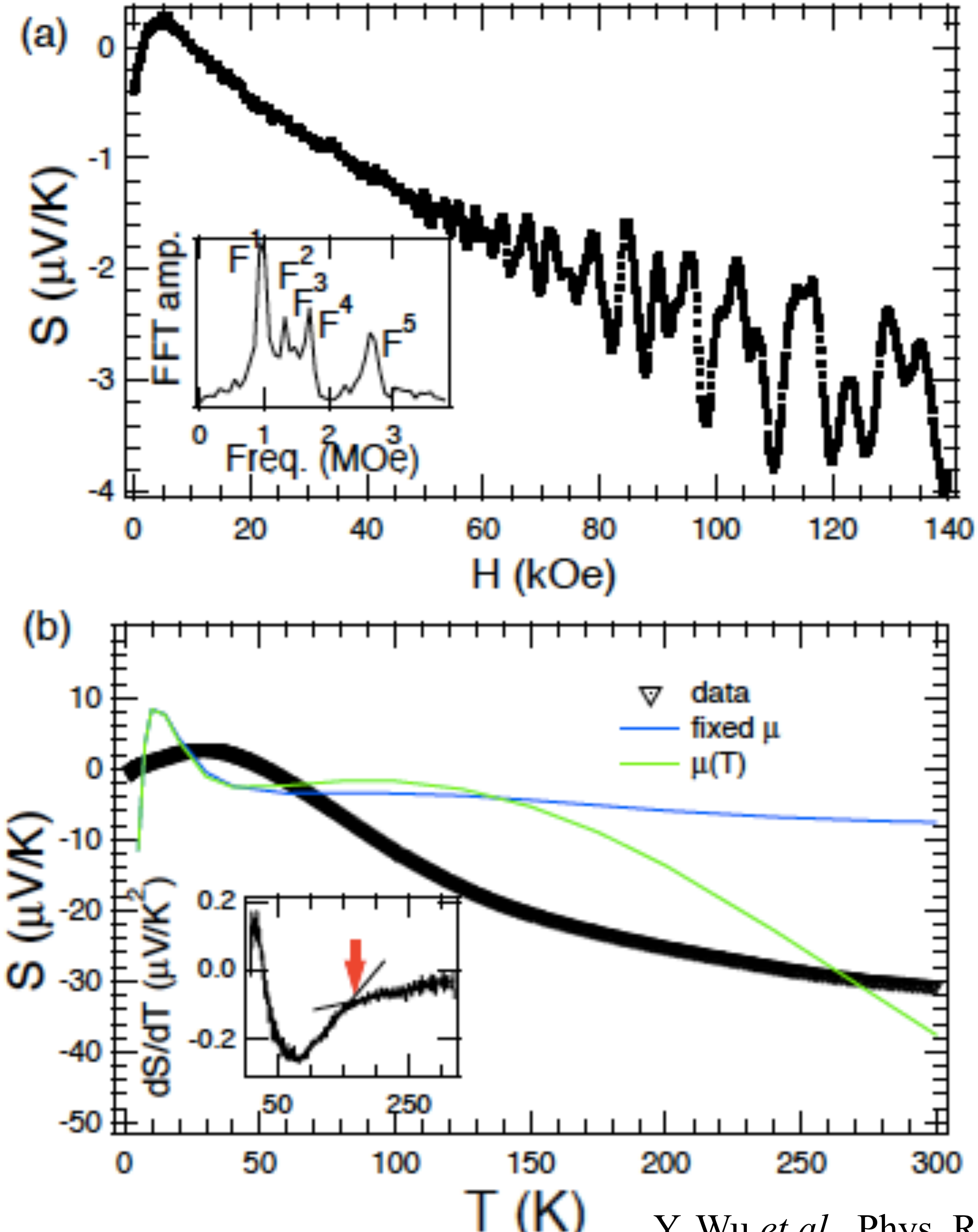
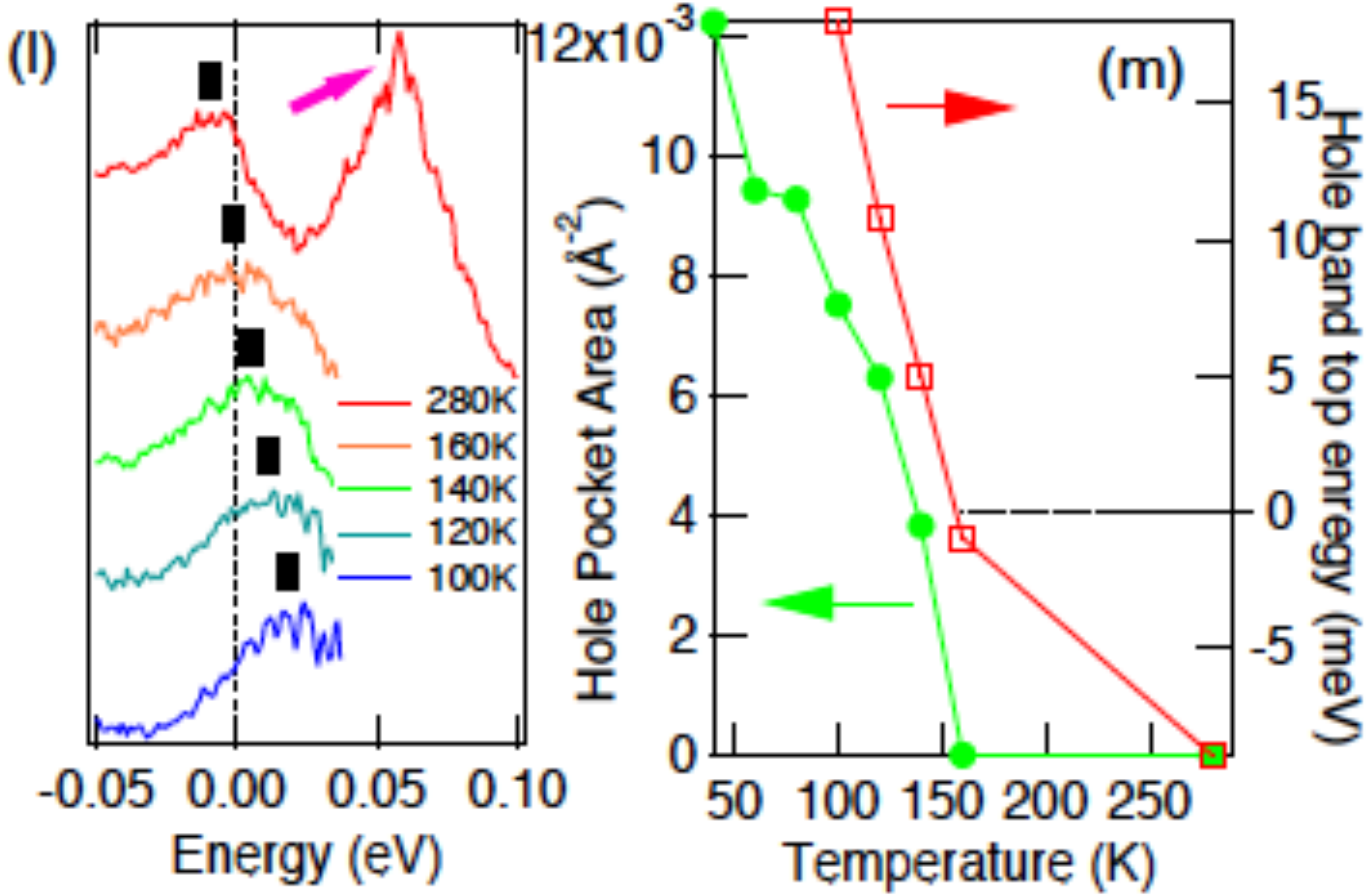
Yun Wu *et al*., Phys. Rev. Lett. **115**, 166602 (2015).

Temperature and magnetic field dependence



Y, Wu *et al*., Phys. Rev. Lett. **115**, 166602 (2015).



(l)
280K
160K
140K
120K
100K
-0.05 0.00 0.05 0.10
Energy (eV)
(m)
12x10^-3
10
8
6
4
2
0
Hole Pocket Area (Å^-2)
50 100 150 200 250
Temperature (K)
15
10
5
0
-5
Hole band top enregy (meV)

$f(\varepsilon) = \frac{1}{\ldots}$

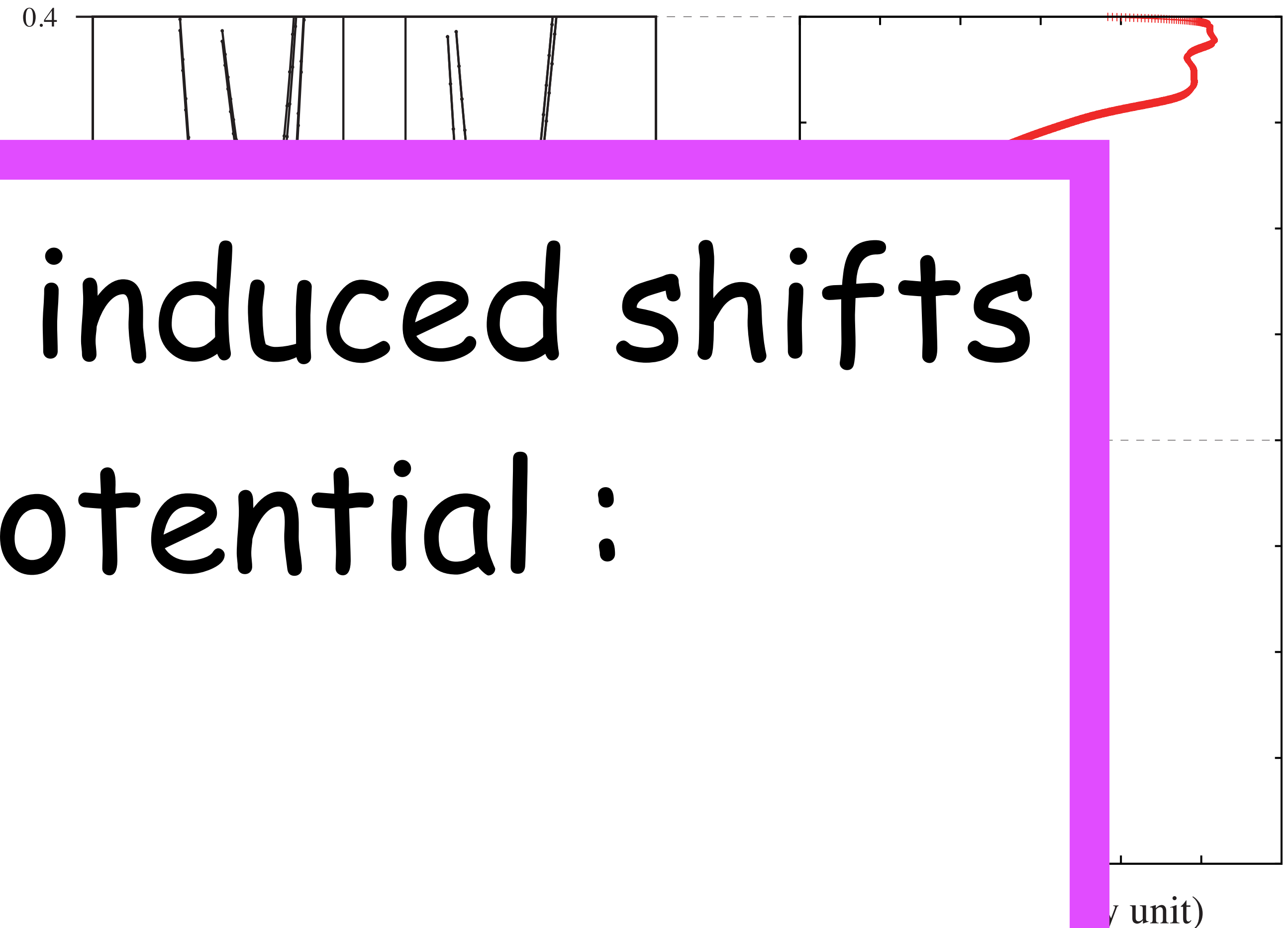
$N = \int_0^{\varepsilon_F} D(\varepsilon \ldots$

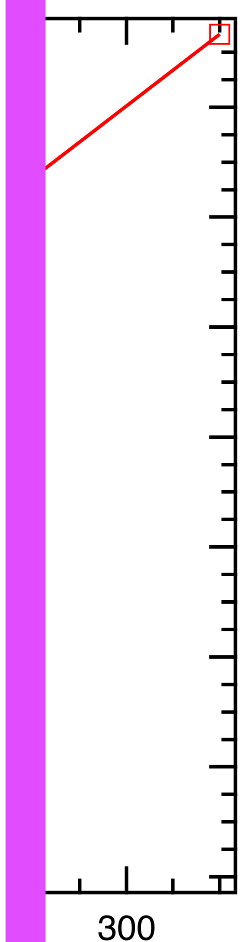
$N = \int_0^{\infty} f(\varepsilon \ldots$

$\approx \int_0^{\mu} D(\varepsilon')d\varepsilon' \ldots$

$= \frac{2a}{3}\mu^{3/2} + \ldots$

$\mu = \varepsilon_F[\ldots$





Temperature induced shifts of chemical potential :

- pnictides
- Topological insulators
- 3D Dirac SM
- Weyl Semimetals
- <u>thermoelectrics</u>

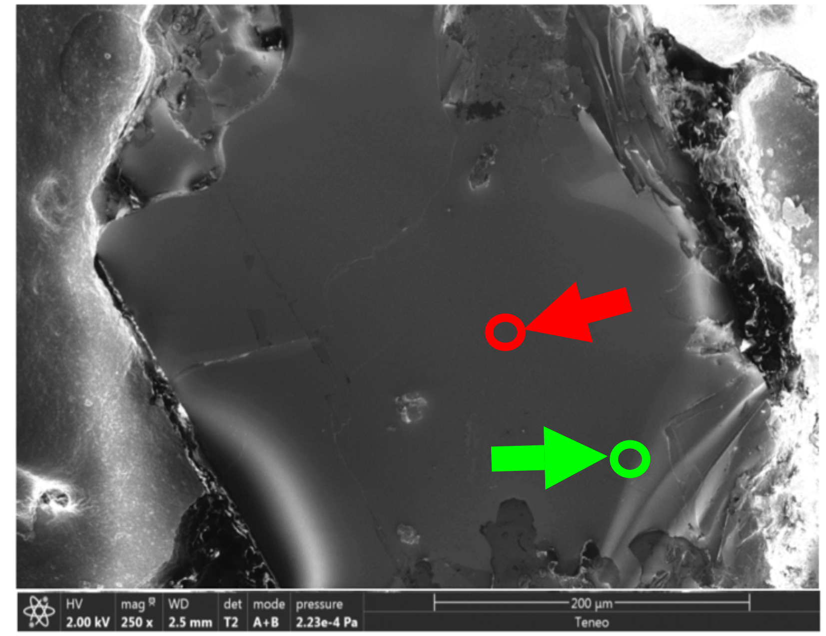
Yun Wu *et al.*, Phys. Rev. Lett. **115**, 166602 (2015).

WTe_2

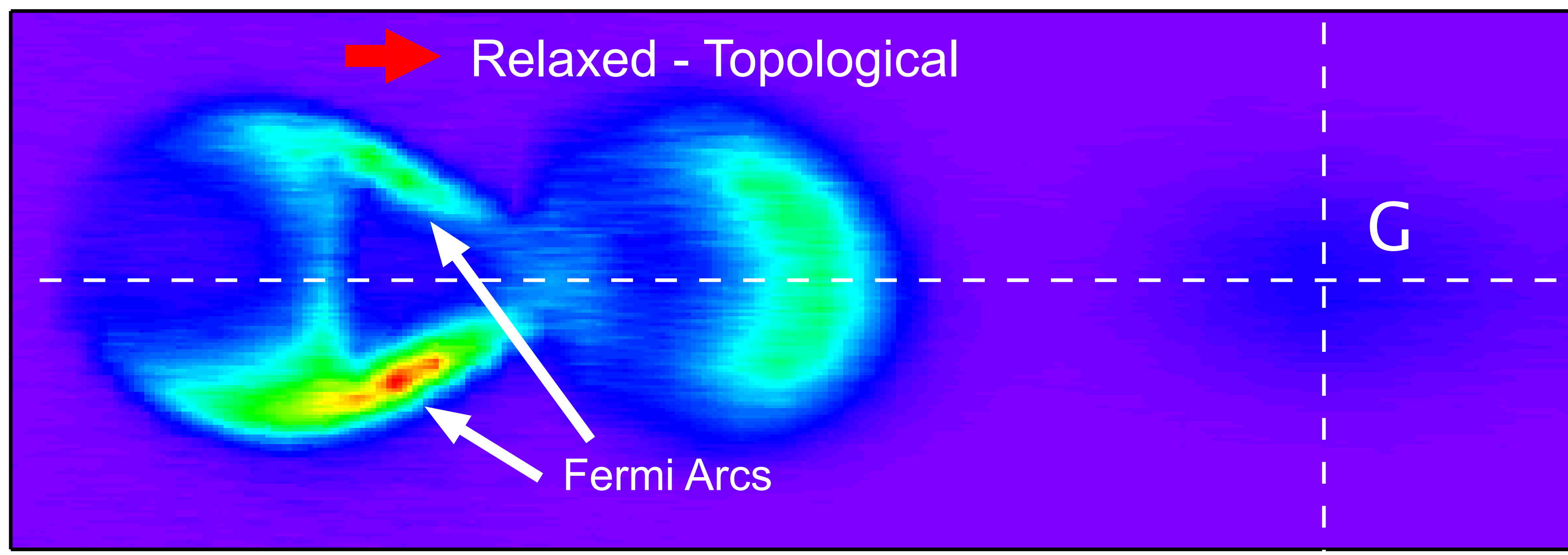
M. N. Ali et al., Nature 514, 205 (2014).

two types of surface terminations:

a)



b)

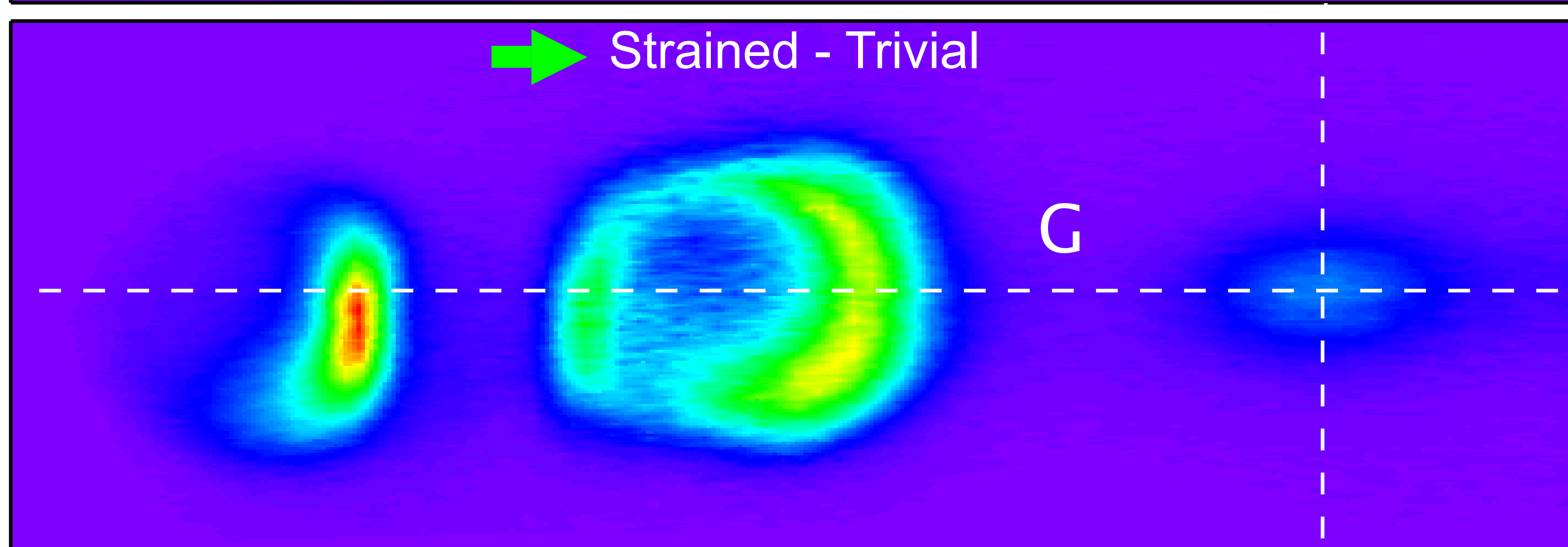


N- Normal

Yun Wu et al.,
Phys. Rev. Lett. 115, 166602 (2015).

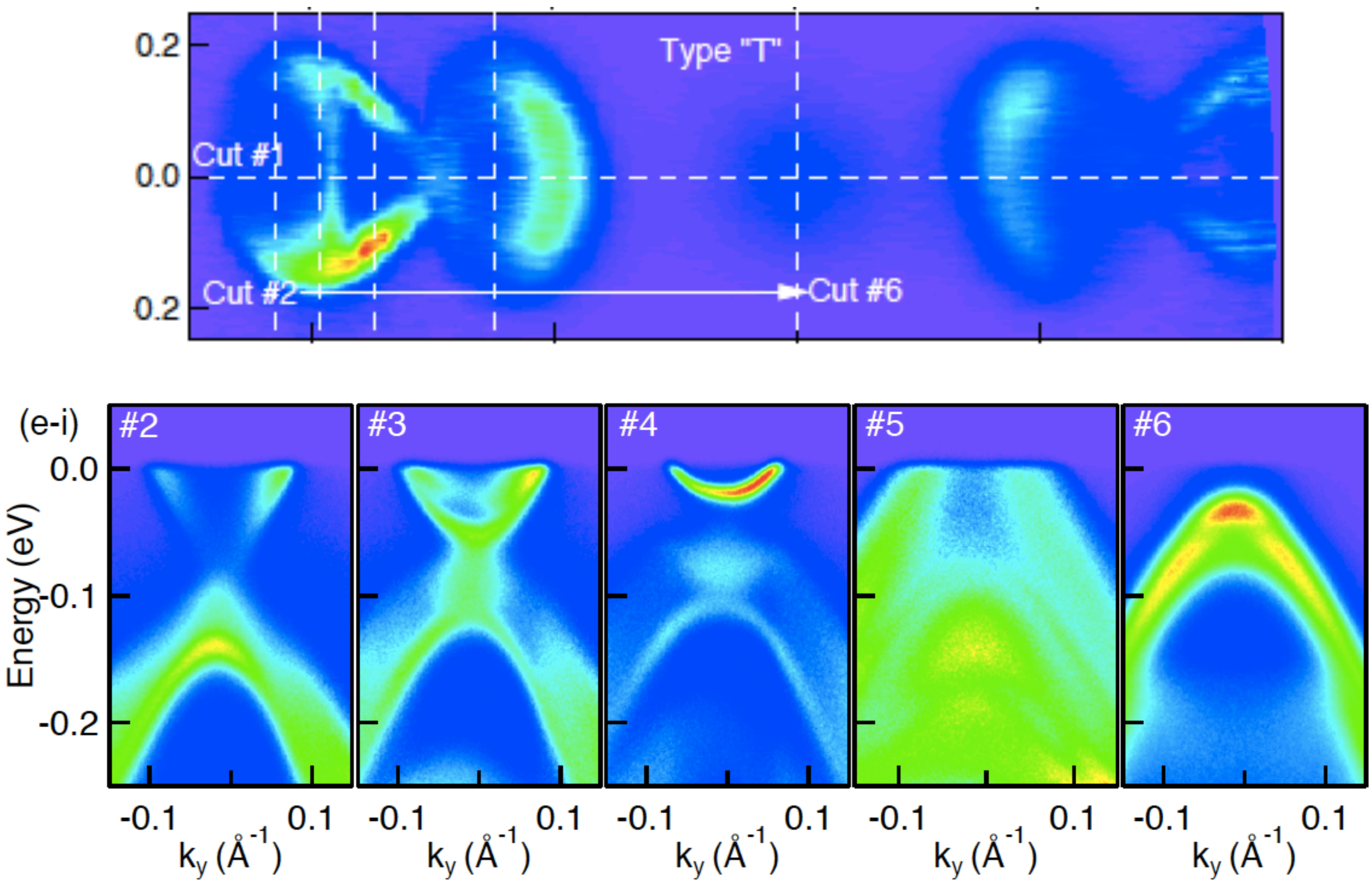
T- Topological

c)



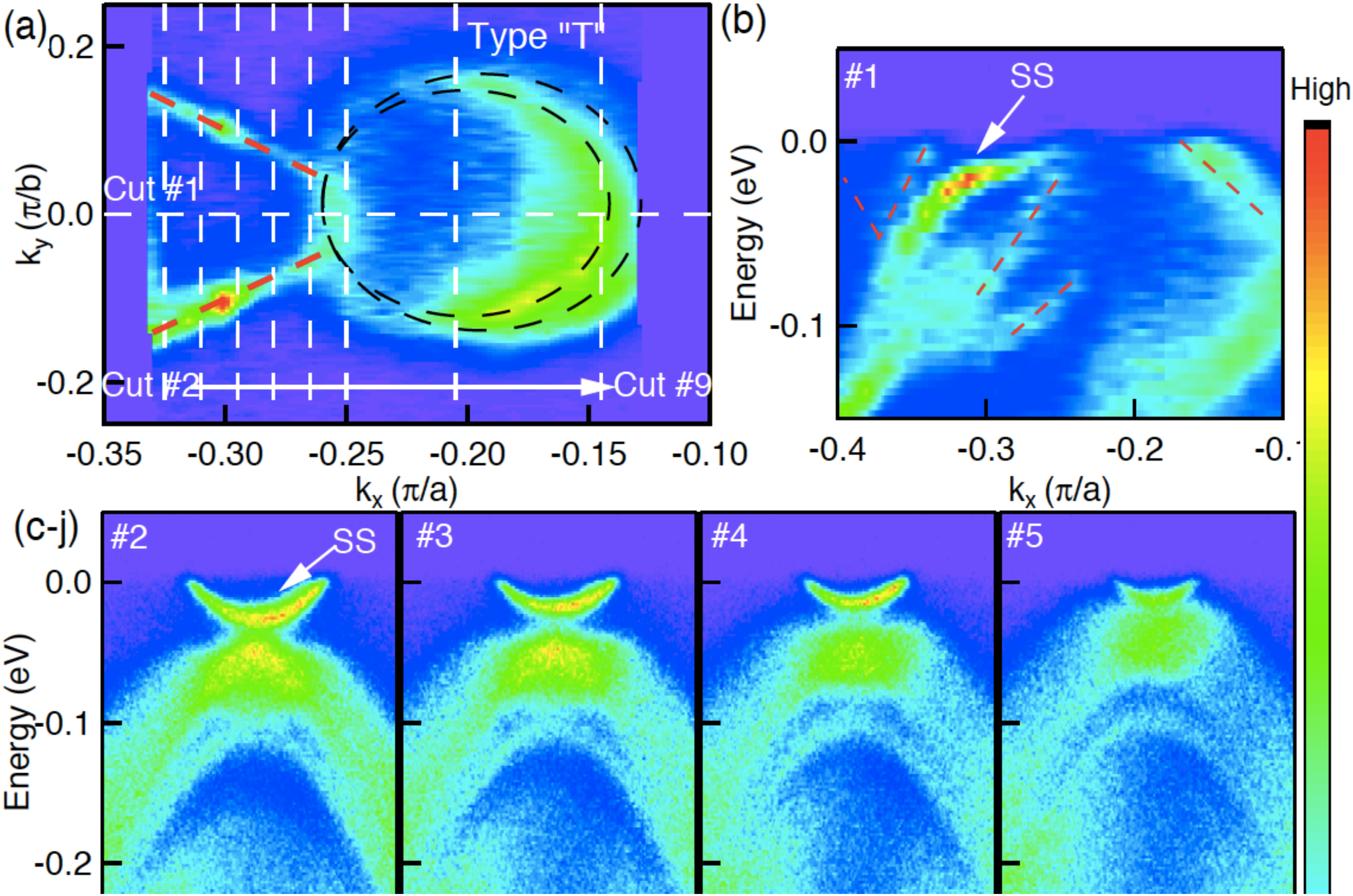
Yun Wu et al.,
Phys. Rev. B **94**, 121113(R) (2016)

Fermi arcs in WTe_2



Yun Wu et al., Phys. Rev. B **94**, 121113(R) (2016)

Fermi arcs in WTe_2



Yun Wu et al., Phys. Rev. B **94**, 121113(R) (2016)

"plain" and "titanic" Magnetoresistance

~500,000%

PHYSICAL REVIEW B **85**, 035135 (2012)

Magnetic field effects on transport properties of $PtSn_4$

Eundeok Mun,[1] Hyunjin Ko,[2] Gordon J. Miller,[2] German D. Samolyuk,[1,*] Sergey L. Bud'ko,[1] and Paul. C. Canfield[1]
[1]*Ames Laboratory US Department of Energy and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*
[2]*Ames Laboratory US Department of Energy and Department of Chemistry, Iowa State University, Ames, Iowa 50011, USA*
(Received 6 October 2011; revised manuscript received 17 January 2012; published 31 January 2012)

E. Mun et al., Phys. Rev. B 85, 035135 (2012).

LETTER ~500,000%

doi:10.1038/nature13763

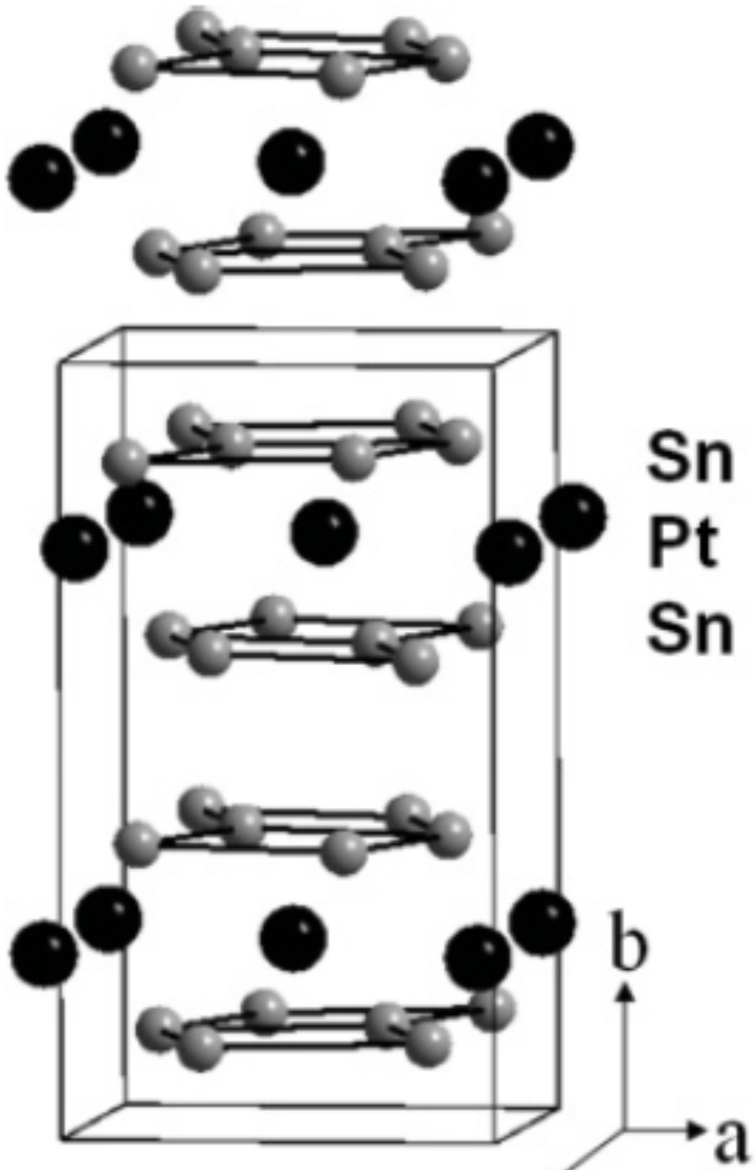
titanic

Large, non-saturating magnetoresistance in WTe_2

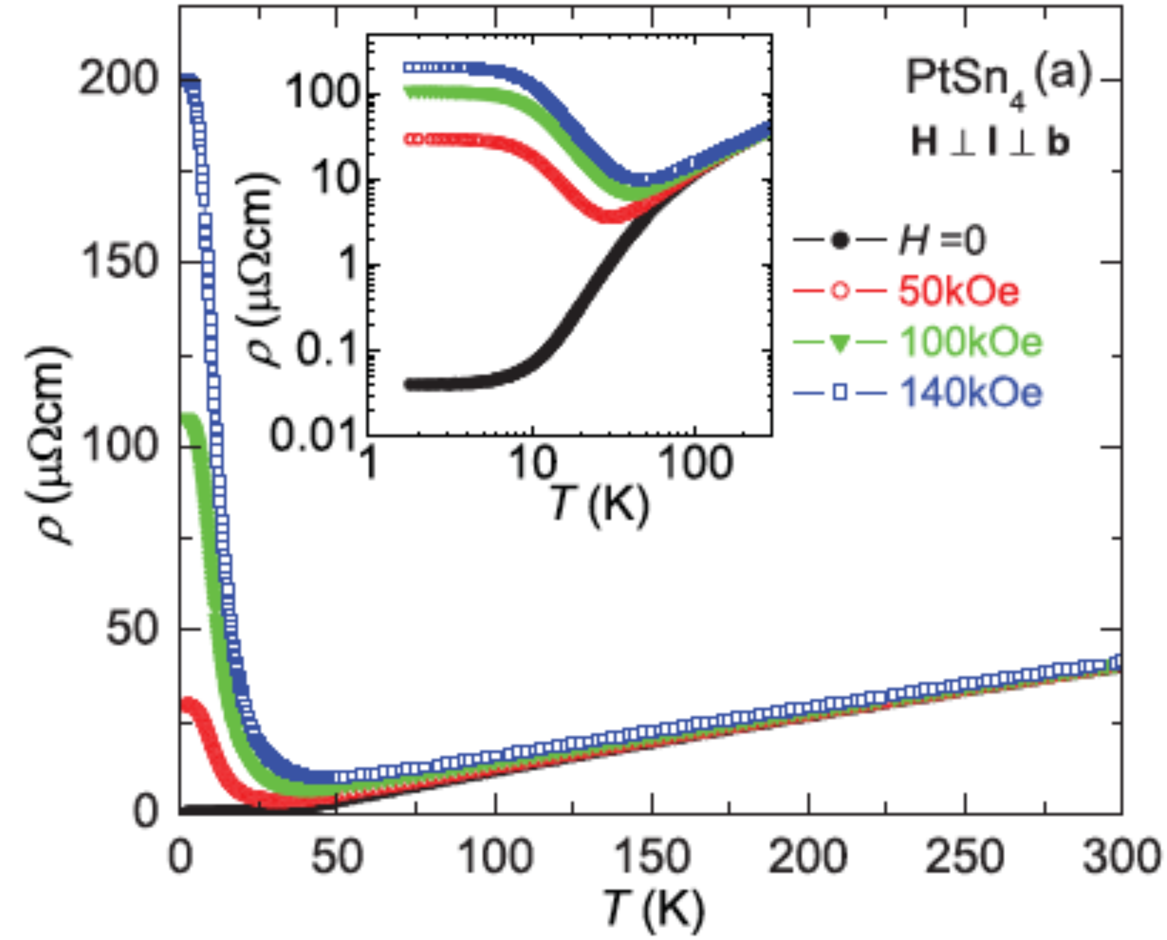
Mazhar N. Ali[1], Jun Xiong[2], Steven Flynn[1], Jing Tao[3], Quinn D. Gibson[1], Leslie M. Schoop[1], Tian Liang[2], Neel Haldolaarachchige[1], Max Hirschberger[2], N. P. Ong[2] & R. J. Cava[1]

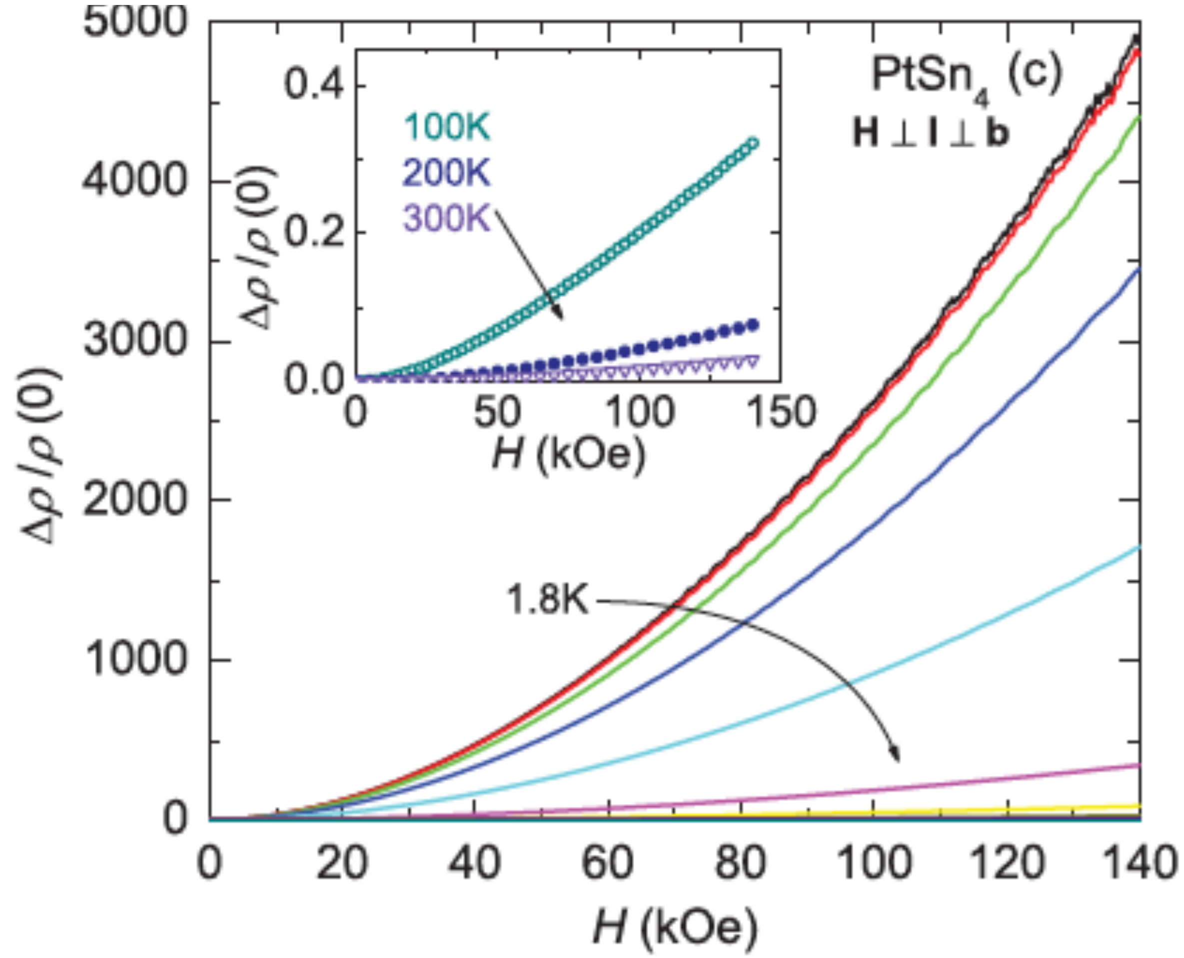
M. N. Ali et al., Nature 514, 205 (2014).

$PtSn_4$



(a)





E. Mun et al., Phys. Rev. B 85, 035135 (2012).

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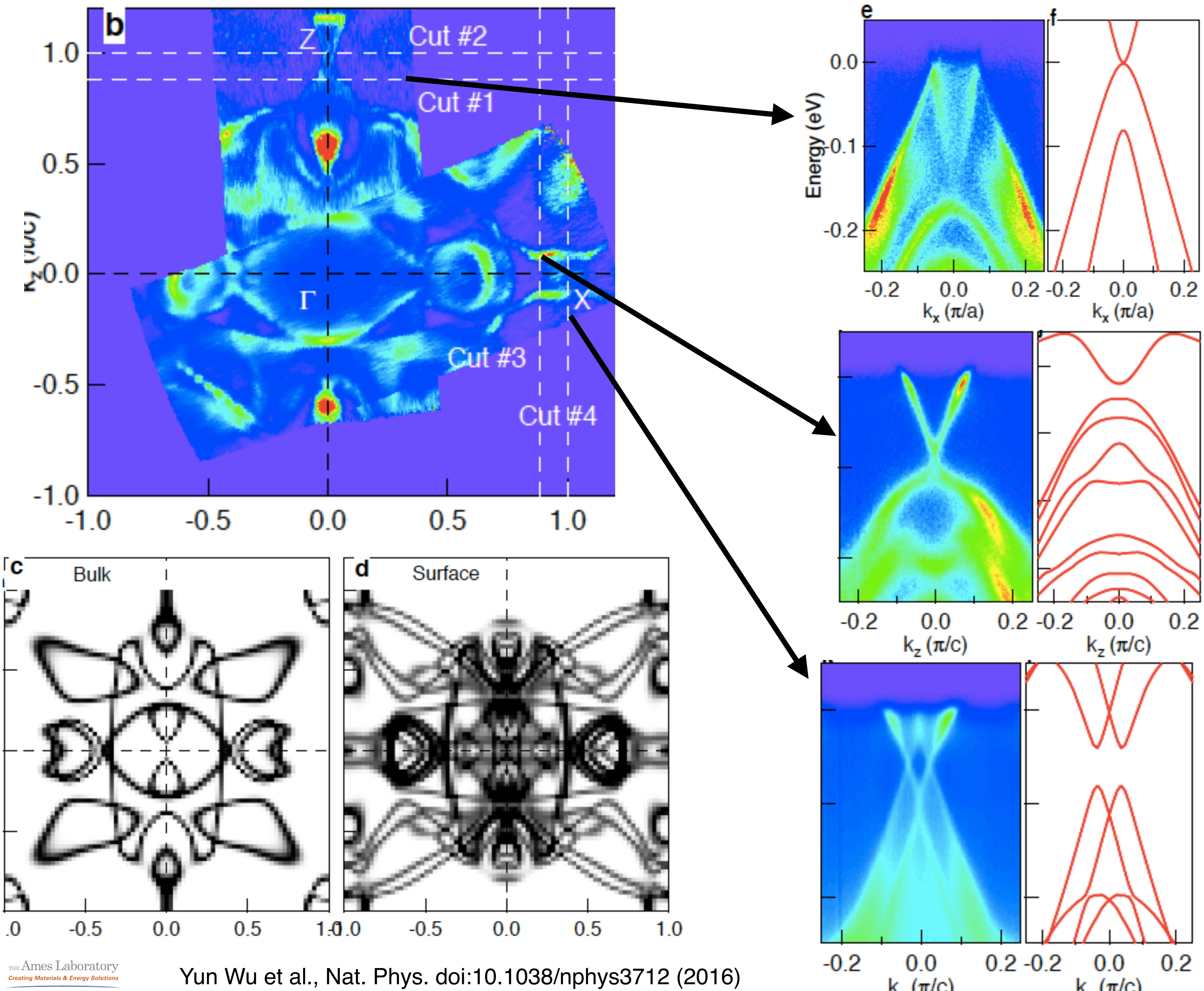
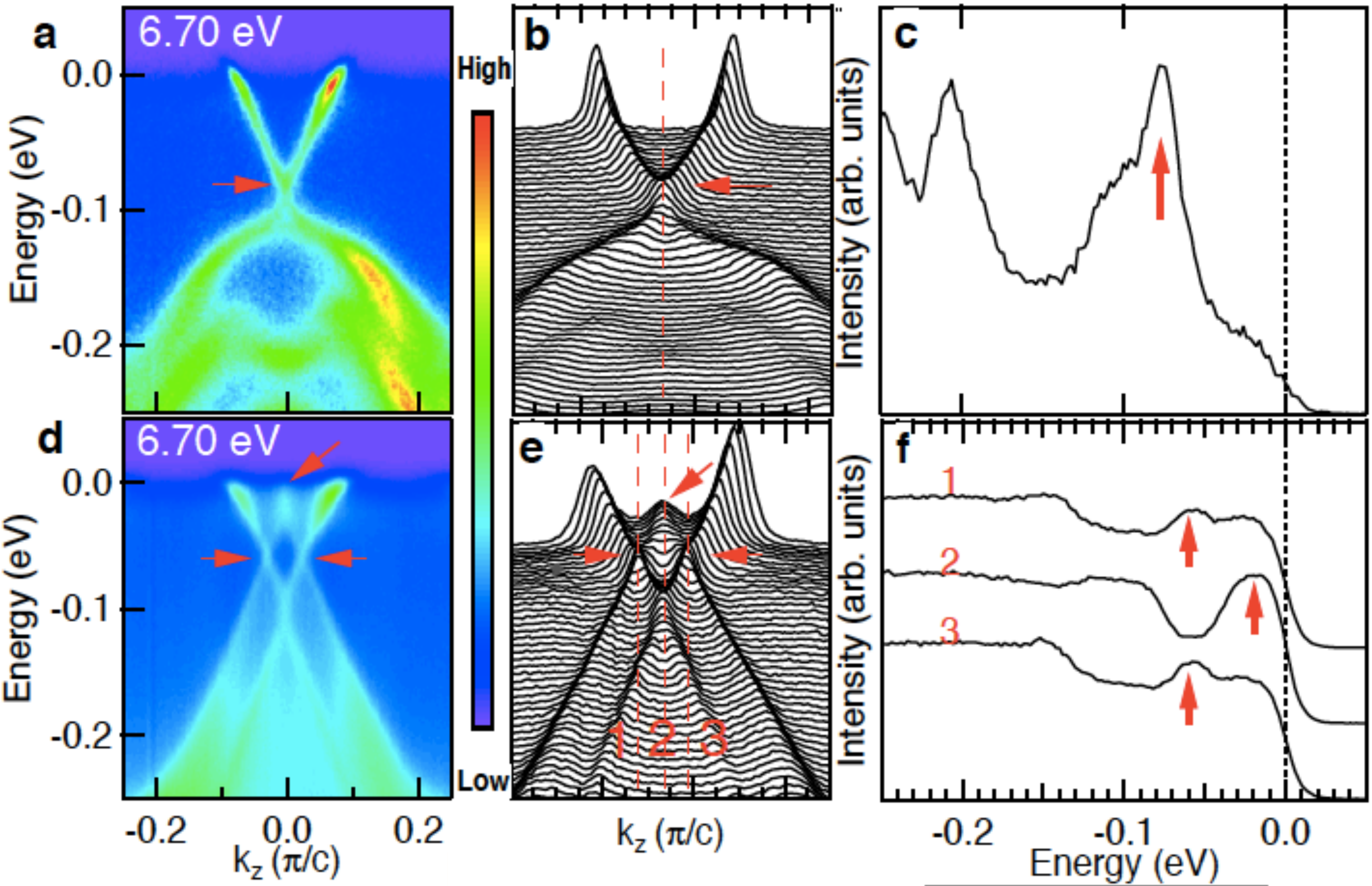
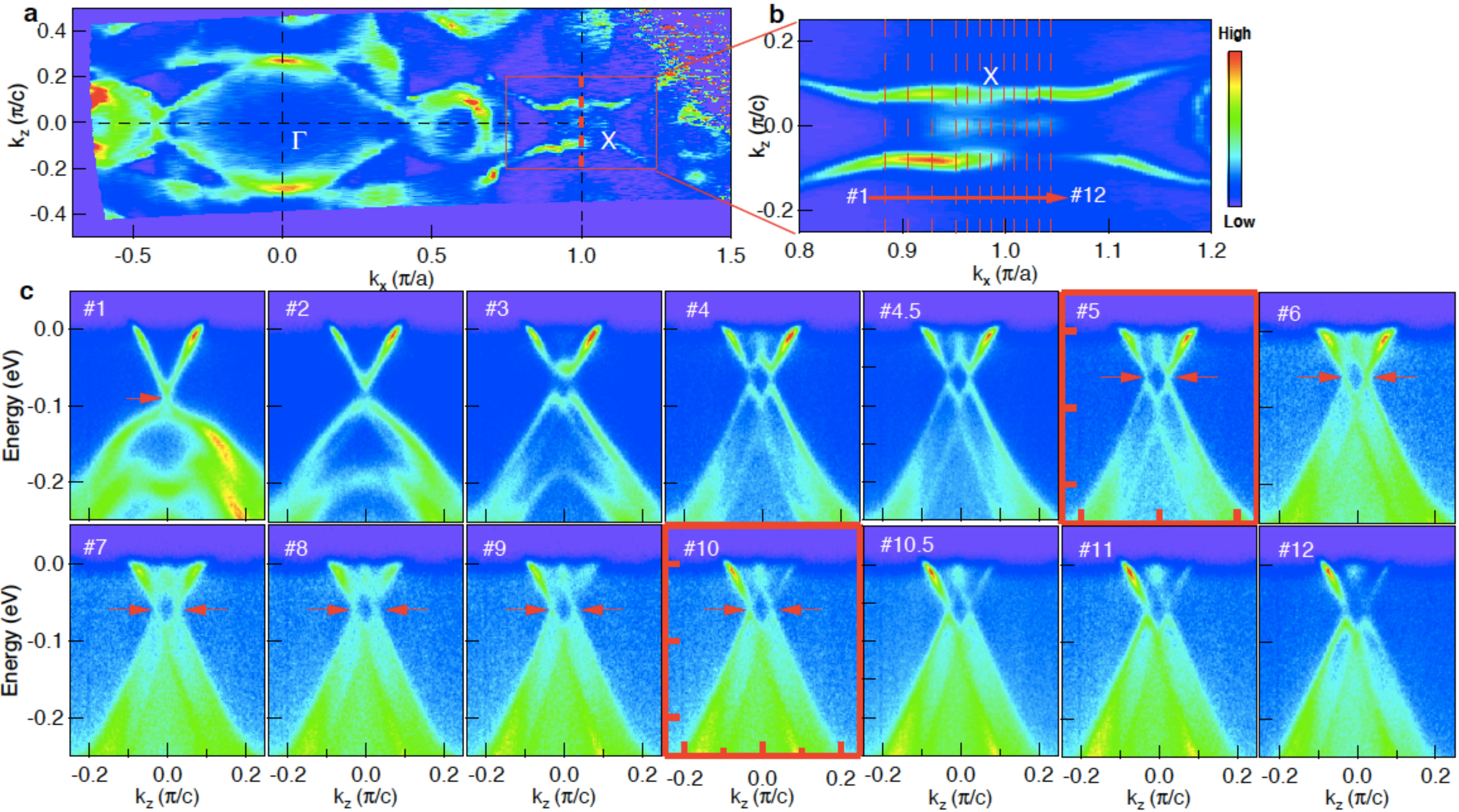


Yun Wu et al., Nat. Phys. doi:10.1038/nphys3712 (2016)



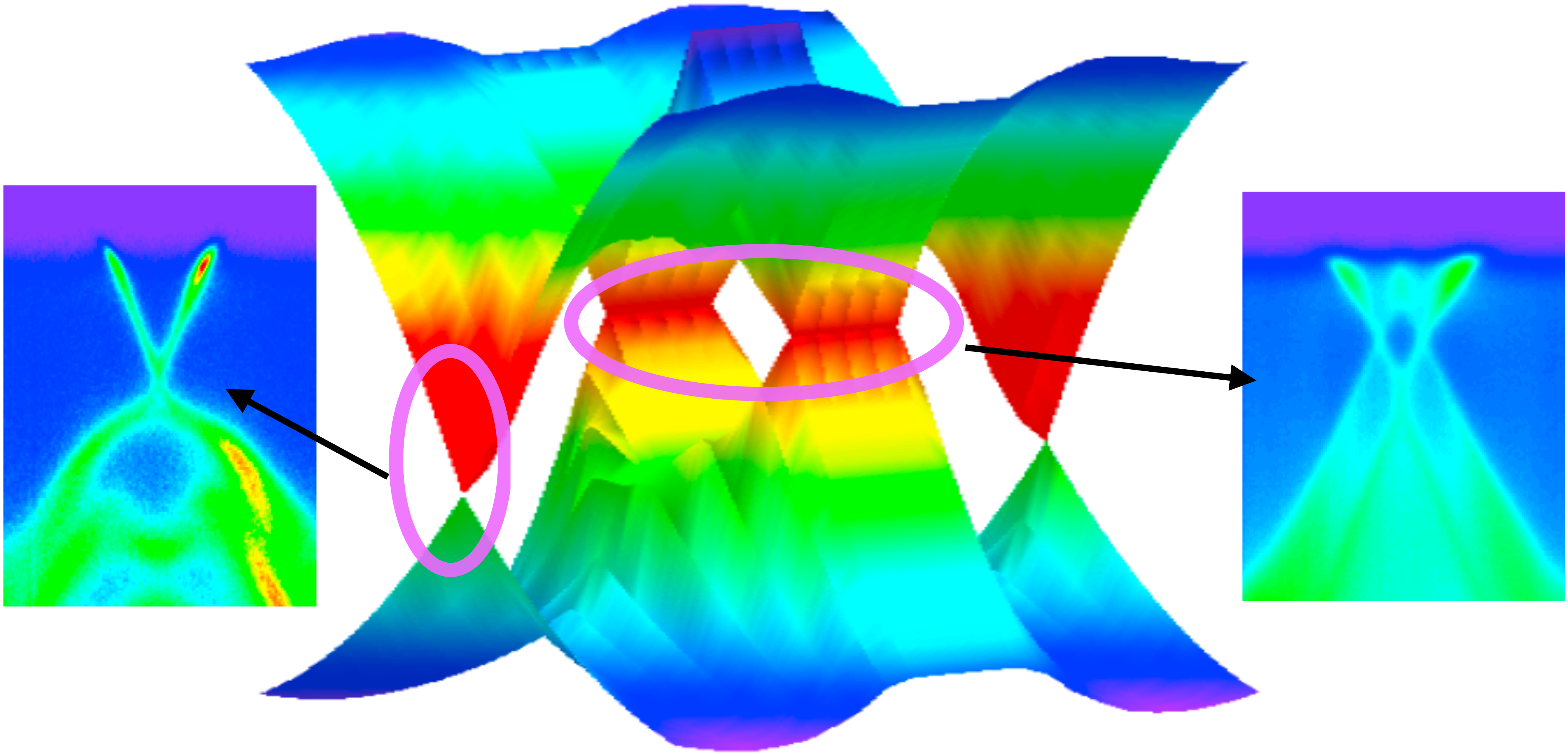
a
6.70 eV
0.0
-0.1
-0.2
Energy (eV)
High
Low
b
c
Intensity (arb. units)
d
6.70 eV
0.0
-0.1
-0.2
Energy (eV)
-0.2
0.0
0.2
kz (π/c)
e
1 2 3
kz (π/c)
f
1
2
3
Intensity (arb. units)
-0.2
-0.1
0.0
Energy (eV)

Dirac arc nodes in $PtSn_4$



Yun Wu et al., Nat. Phys. doi:10.1038/nphys3712 (2016)

Dirac arc nodes in $PtSn_4$



Yun Wu et al., Nat. Phys. doi:10.1038/nphys3712 (2016)

Conclusions:

- $Bi_2Te_{2.8}Se_{0.2}$ is a "true" topological insulator with Fermi energy located inside of the bulk band gap

- TI properties can be reversibly tuned at the surface by hydrogen absorption

- We discovered spectroscopic evidence that both WTe2 and MoTe2 are type II Weyl semimetals

- $PtSn_4$ is a novel topological material hosting Dirac node arcs (DNA) that yet have to be understood by theory