ARPES studies of Dirac materials

Inna Vishik

Physics 250 (Special topics: spectroscopies of quantum materials)

UC Davis, Fall 2016

Topics

- Graphene
- Topological crystalline insulators
- Weyl Semimetals
- Dirac Semimetals

Dirac equation

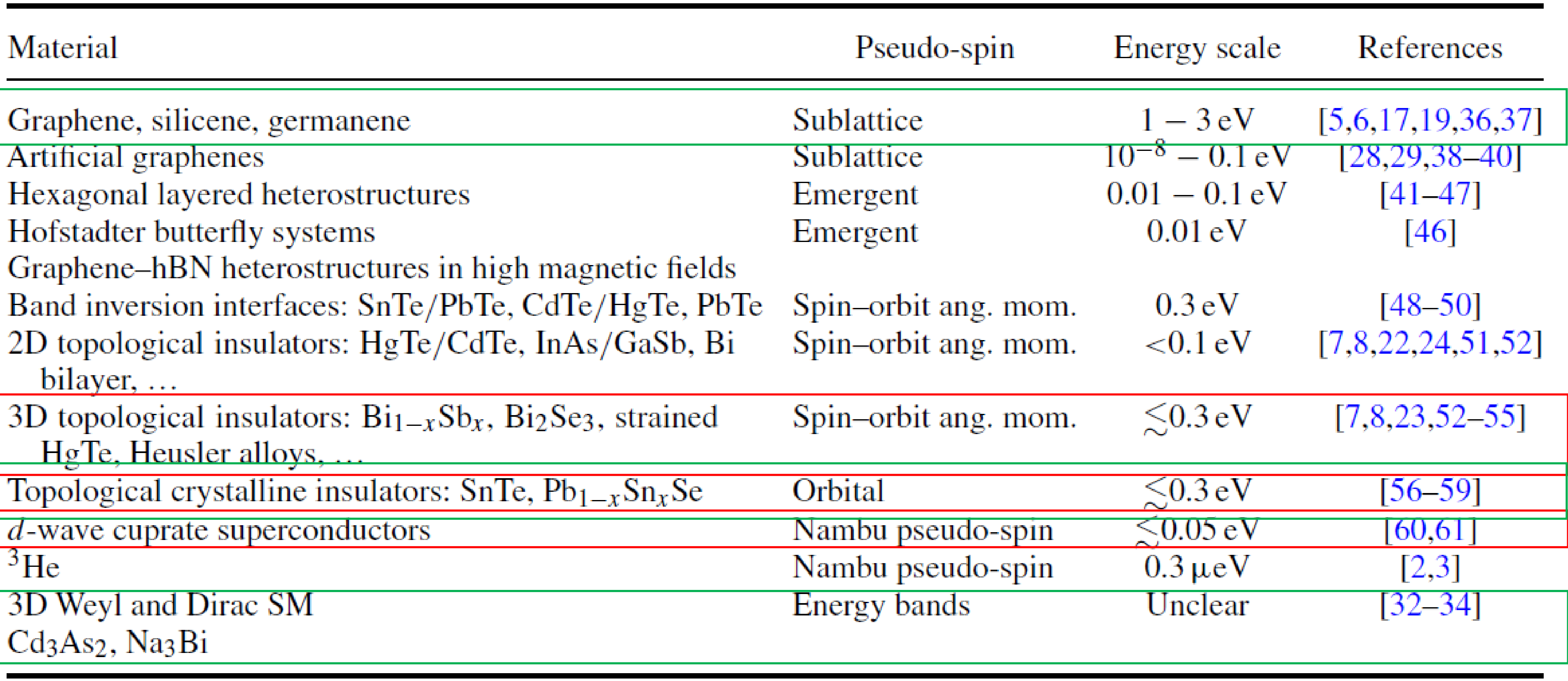
- Dirac equation in 2 dimensions:

$$H_D = c\boldsymbol{\sigma}\cdot\boldsymbol{p} + mc^2\sigma_z$$
$$\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$$

- In condensed matter context, *c* is replaced by v_F
- Massless version: linear quasiparticle dispersion
- Massive version: electrons and holes have same mass

Many examples of Dirac materials

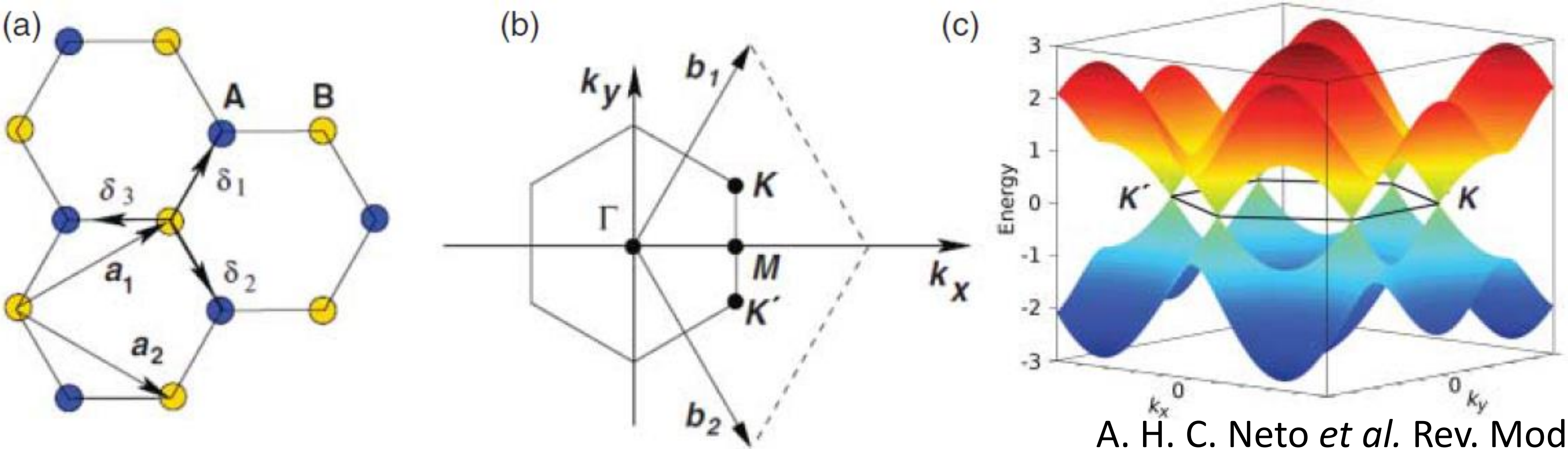
$$H_D = c\boldsymbol{\sigma}\cdot\boldsymbol{p} + mc^2\sigma_z$$



Material	Pseudo-spin	Energy scale	References
Graphene, silicene, germanene	Sublattice	$1-3$ eV	[5,6,17,19,36,37]
Artificial graphenes	Sublattice	$10^{-8}-0.1$ eV	[28,29,38–40]
Hexagonal layered heterostructures	Emergent	$0.01-0.1$ eV	[41–47]
Hofstadter butterfly systems Graphene–hBN heterostructures in high magnetic fields	Emergent	0.01 eV	[46]
Band inversion interfaces: SnTe/PbTe, CdTe/HgTe, PbTe	Spin–orbit ang. mom.	0.3 eV	[48–50]
2D topological insulators: HgTe/CdTe, InAs/GaSb, Bi bilayer, …	Spin–orbit ang. mom.	$<$0.1 eV	[7,8,22,24,51,52]
3D topological insulators: $Bi_{1-x}Sb_x$, Bi_2Se_3, strained HgTe, Heusler alloys, …	Spin–orbit ang. mom.	$\lesssim$0.3 eV	[7,8,23,52–55]
Topological crystalline insulators: SnTe, $Pb_{1-x}Sn_xSe$	Orbital	$\lesssim$0.3 eV	[56–59]
d-wave cuprate superconductors	Nambu pseudo-spin	$\lesssim$0.05 eV	[60,61]
^{3}He	Nambu pseudo-spin	0.3 μeV	[2,3]
3D Weyl and Dirac SM Cd_3As_2, Na_3Bi	Energy bands	Unclear	[32–34]

T. O. Wehling *et al.* Adv. Phys. **63** 1-76 (2014)

Graphene



A. H. C. Neto *et al.* Rev. Mod. Phys. **81** 109 (2009)

Tight binding Hamiltonian with only NN hopping:

$$\widehat{H} = -t \sum_{<i,j>} a_i^\dagger b_j + a_j^\dagger b_i$$

2x2 matrix in momentum space representation:

$$H(\boldsymbol{k}) = \begin{pmatrix} 0 & \xi(\boldsymbol{q}) \\ \xi^*(\boldsymbol{q}) & 0 \end{pmatrix}$$

Energy bands: $\epsilon(\boldsymbol{k}) = \pm|\xi(\boldsymbol{k})|$ where $\xi(\boldsymbol{k}) = -t\left(e^{i\boldsymbol{\delta_1}\cdot\boldsymbol{k}} + e^{i\boldsymbol{\delta_2}\cdot\boldsymbol{k}} + e^{i\boldsymbol{\delta_3}\cdot\boldsymbol{k}}\right)$

At K and K', bands degenerate, $\xi(\boldsymbol{k}) = 0$; use to solve for $\delta_{1,2,3}$

Expansion in vicinity of $\pm K$

$$H(\pm K + \boldsymbol{q}) = \hbar v_F \begin{pmatrix} 0 & q_x \pm i q_y \\ q_x \mp i q_y & 0 \end{pmatrix}$$

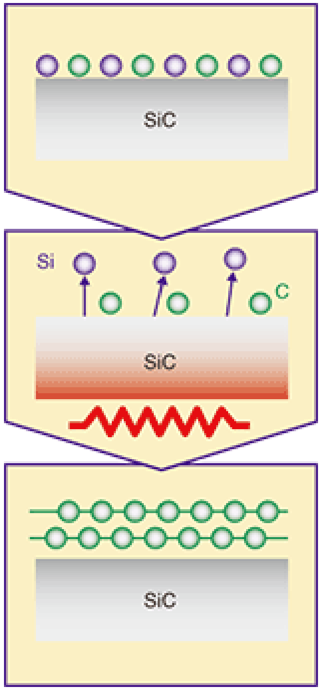
$$H_D = c\boldsymbol{\sigma}\cdot\boldsymbol{p}$$
$$\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$$

Ingredients for Dirac fermions in graphene

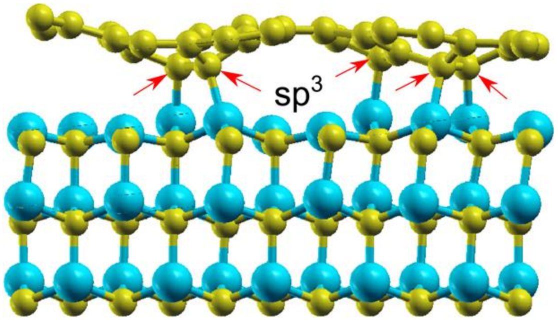
- Destructive interference of three partial hopping amplitudes at $\xi(\boldsymbol{k} = K)$
  →Sublattice symmetry or inversion symmetry
- Time-reversal symmetry (in absence of magnetic field)

Preparation of graphene for surface spectroscopies

- Surface decomposition of SiC (0001)



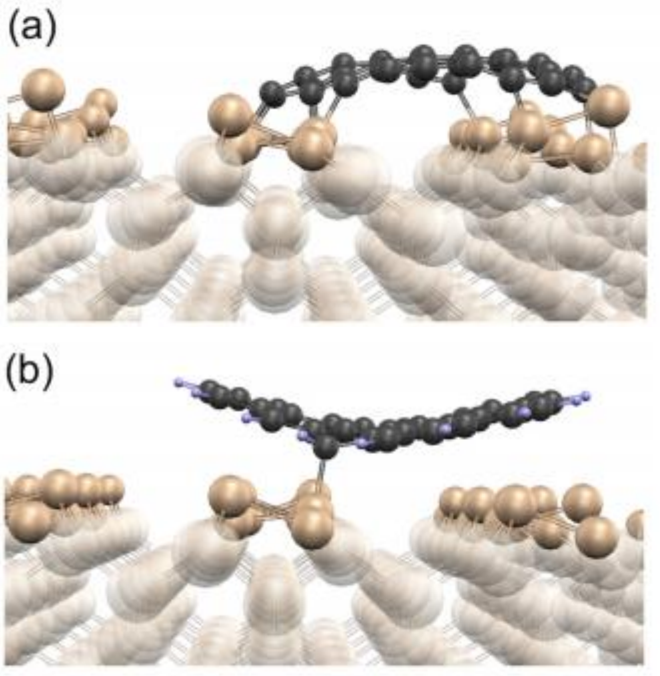
Hidino *et al* NTT Technical review (2010)



Iguchi *et al.* Japn. J. Appl. Phys (2014)

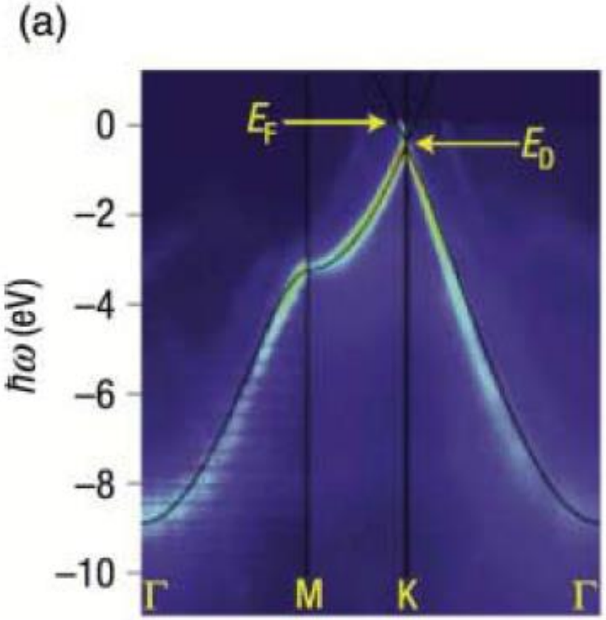
Produces multiple nominally decoupled layers

- MBE or CVD growth on substrate (Si, Ge, SiC)

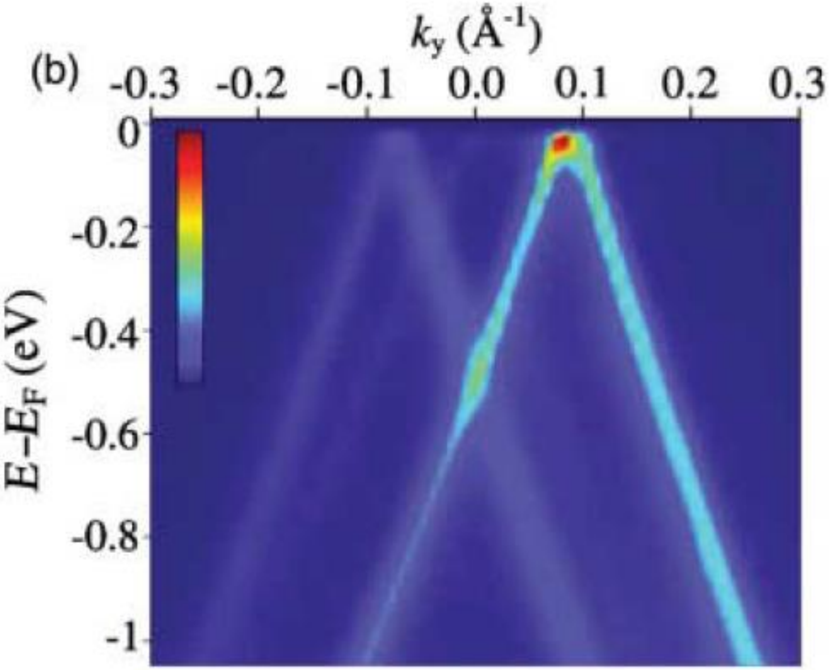


Dabrowski *et al,* arXiv:1604.02315v1

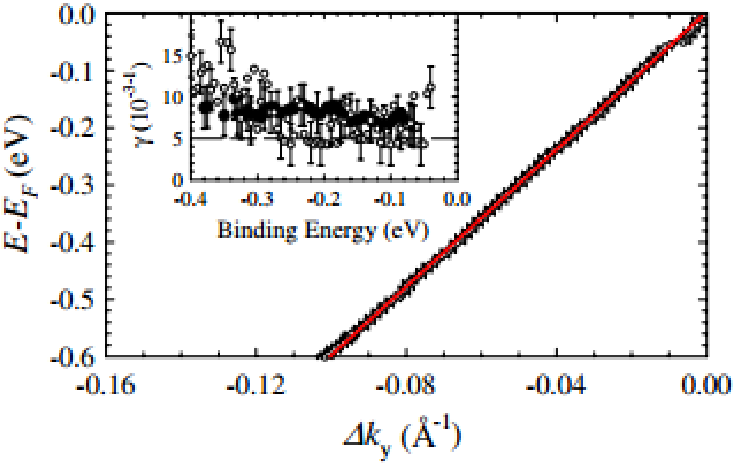
ARPES on isolated graphene



Bostwick *et al,* Nat. Phys. **3** 36 (2007)

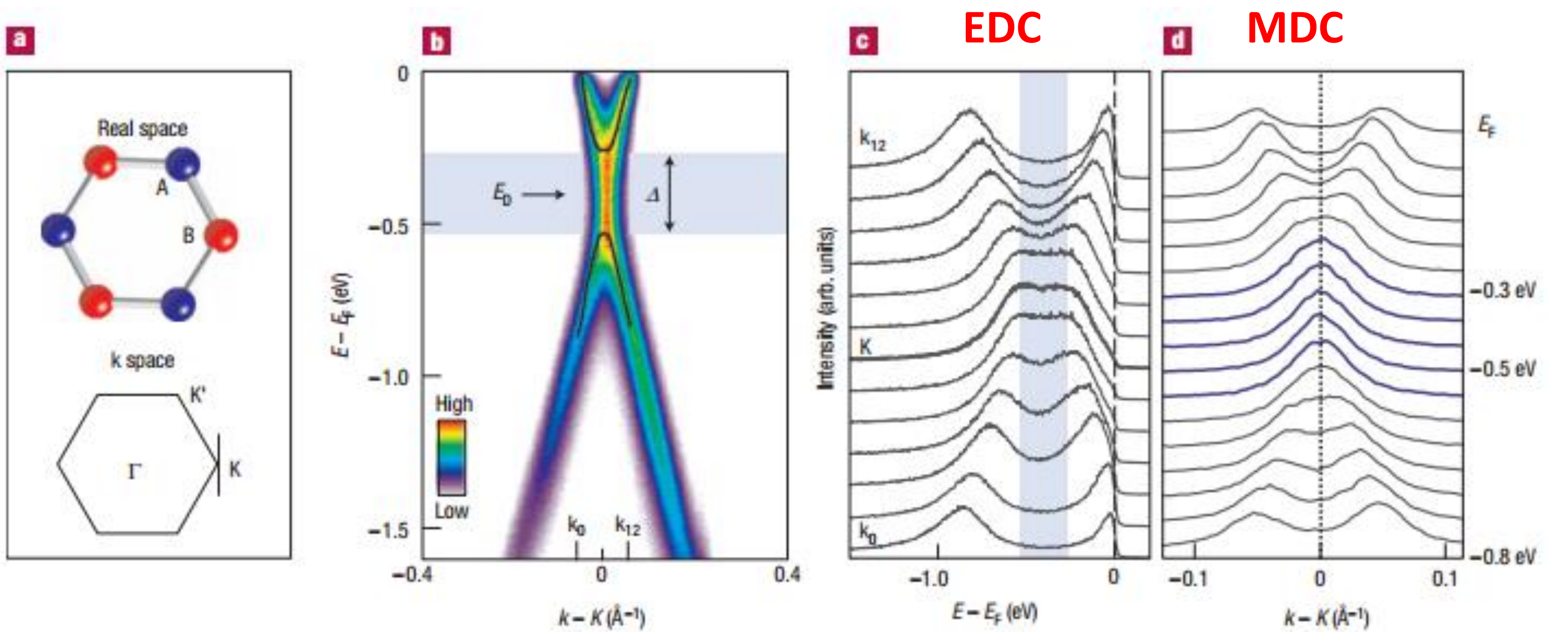


Sprinkle *et al,* PRL 103, 226803 (2009)

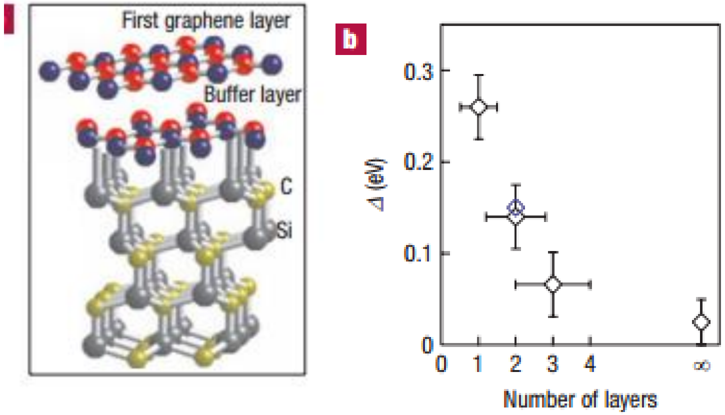


- Extra bands (right) from misoriented layers
- Band dispersion is linear over at least 600 meV

ARPES on not-so-isolated graphene



Zhou *et al.* Nat. Mater. **6** 770 (2007)



- Mass appears in dispersion because of sublattice symmetry breaking due to substrate

$$H_D = c\boldsymbol{\sigma}\cdot\boldsymbol{p} + mc^2\sigma_z$$

$$\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$$

- Total of 36 ways to turn graphene massive (Ryu *et al,* PRB **80**, 205319 (2009))

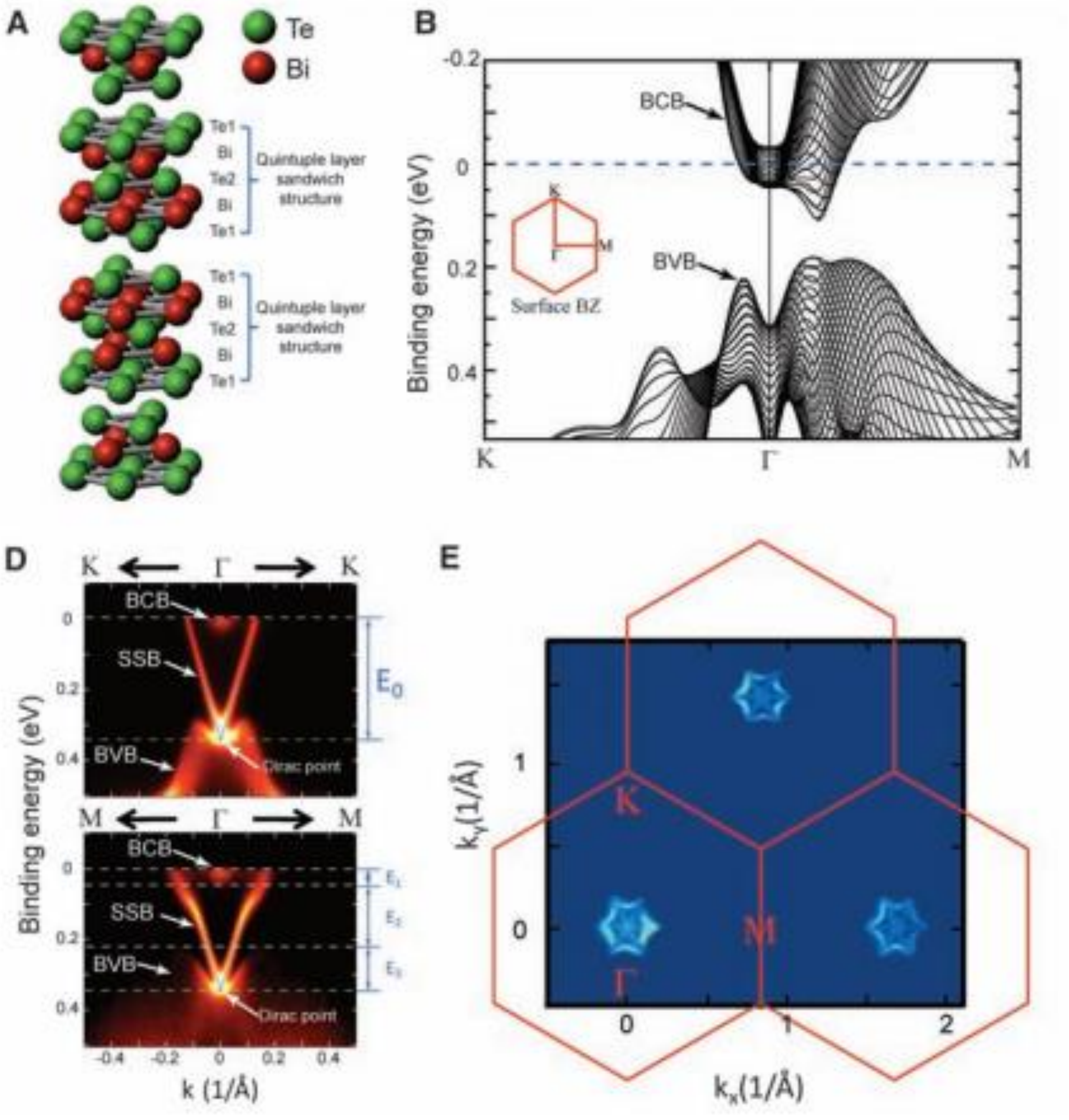
ARPES on graphene summary

- Difficult to prepare samples, but when samples are made ARPES spectra agree well with theory
  - Dirac points at BZ corners
  - Dispersion linear over huge energy range
  - Breaking sublattice symmetry opens a gap
- Common areas of study
  - Coupling of Dirac fermions to phonons and plasmons
  - Inducing superconductivity by intercalating or doping group I or II atoms (e.g. CaC_6)

Topics

- Graphene
- Topological crystalline insulators (TCIs)
- Weyl Semimetals
- Dirac Semimetals

Review: 3D topological insulators



3D Tis:

- Odd number of Dirac cones per BZ (often just one)
- Dirac point protected by TRS

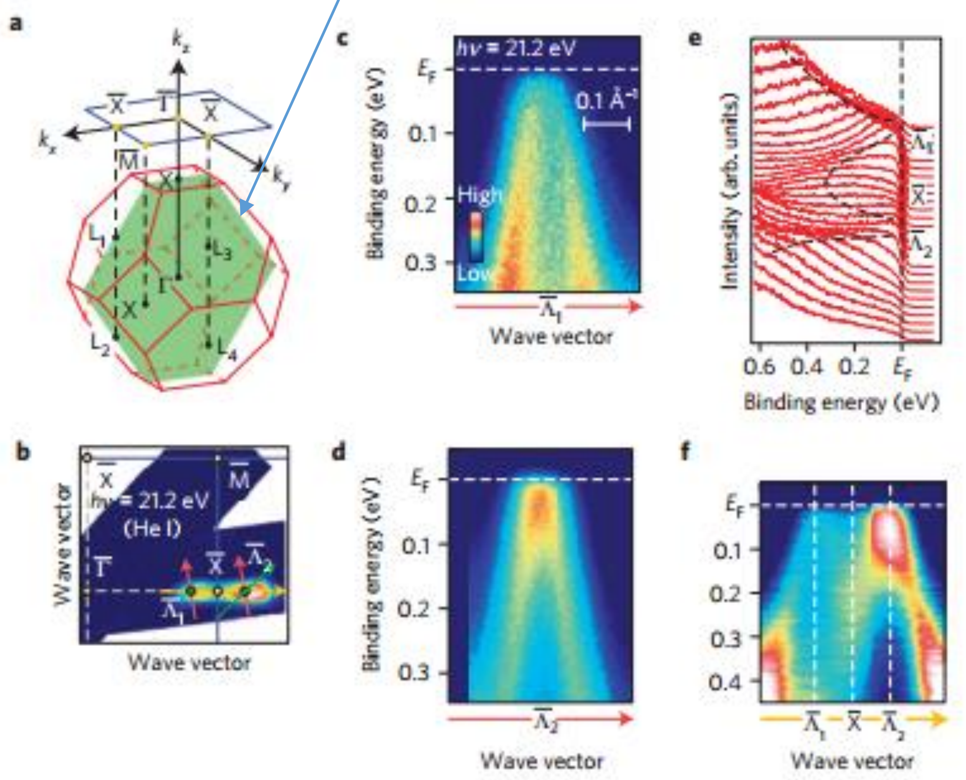
TCIs

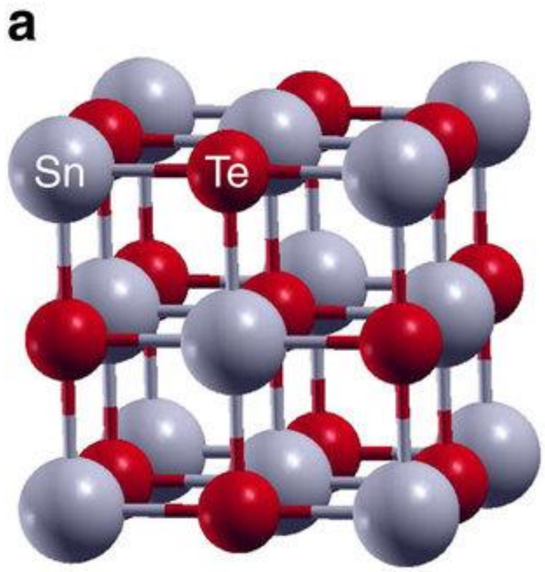
- Even number of dirac cones
- Dirac point protected by mirror symmetry

Chen *et al.* Science **325** July 2009

TCI: SnTe

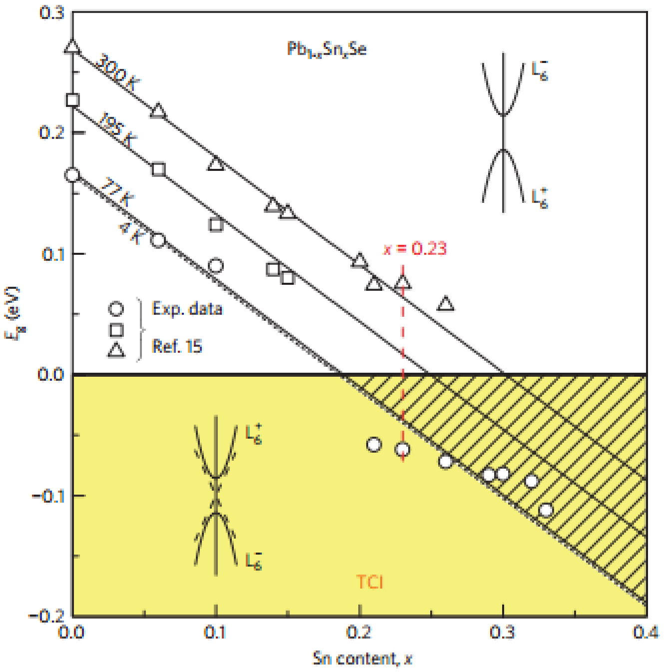
110 mirror plane



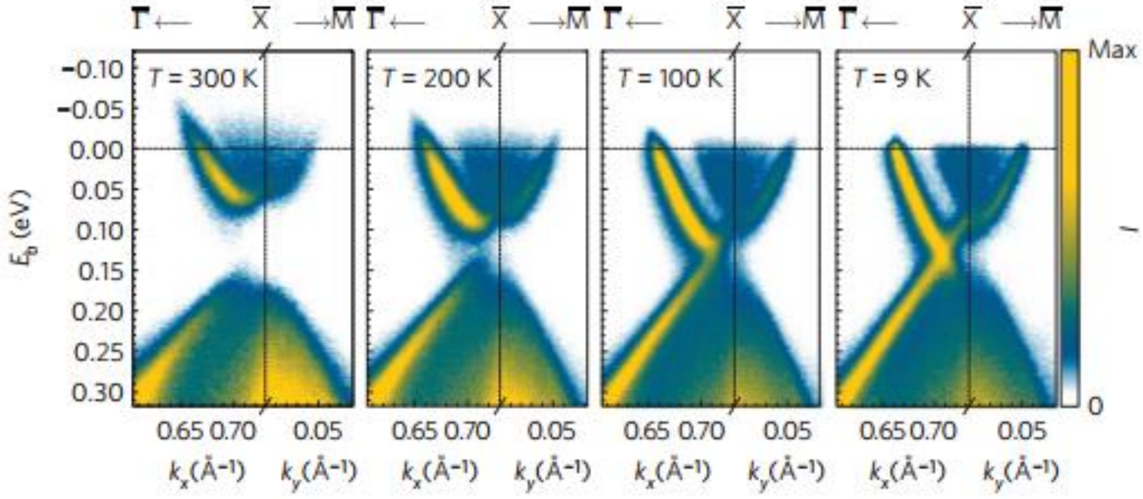


- Prediction of this class of materials: Fu, PRL **106** 106802 (2011)
- Prediction that SnTe is TCI: Hsieh *et al,* Nat. Comm. **3** 982 (2012) (right)
- First ARPES observation: Tanaka *et al.* Nat. Phys. **8** 800 (2012) (left)

Band inversion in $Pb_{1-x}Sn_xTe$ can be tuned by doping or temperature



- Band inversion: first ingredient for topological surface state



- Topological phase transition tuned by temperature!

Dziawa *et al* Nat. Mater. **11** 1023 (2012)

Topics

- Graphene
- Topological crystalline insulators (TCIs)
- **Weyl Semimetals**
- **Dirac Semimetals**

Historically, Dirac Semimetals were discovered first, but they are more easily understood in the context of Weyl semimetals

What is a Weyl semimetal?

- Weyl equation: relativistic wave equation for massless spin ½ particles
- Like 3D graphene in bulk except 'weyl nodes' come in pairs of opposite chirality
- Weyl nodes are protected
- Weyl nodes looks like pseudo-magnetic monopoles in momentum space
- Unusual surface states ('Fermi arcs', no relation to Fermi arcs in cuprates)

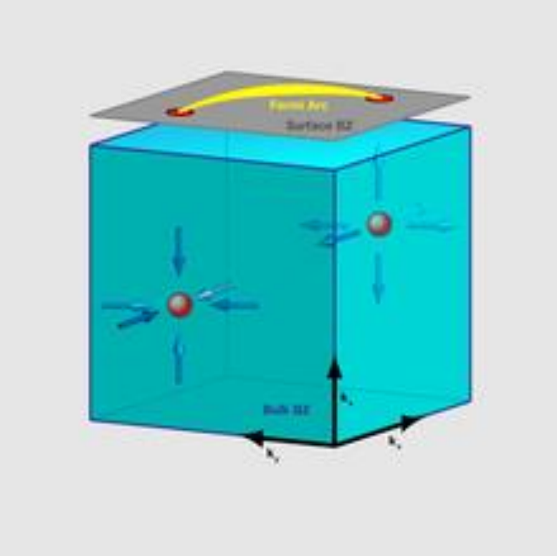
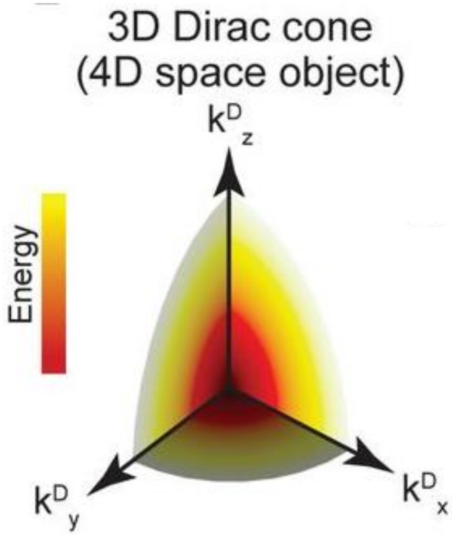


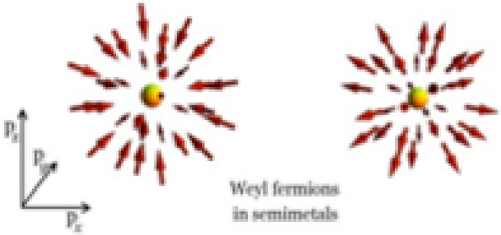
Image source:
https://en.wikipedia.org/wiki/Weyl_semimetal



Liu *et al.* Science (2014)

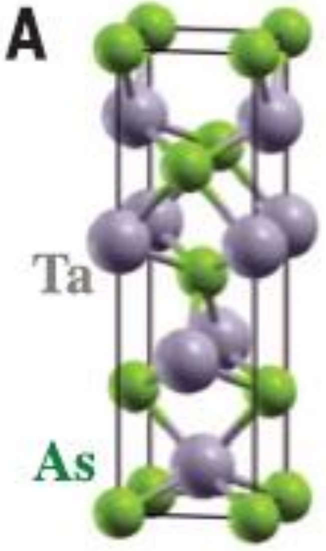
Weyl semimetals: overview

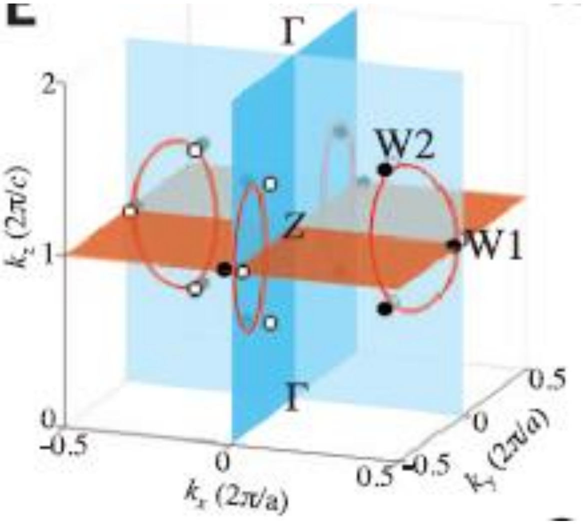
- Low energy dispersion for 3D chiral dirac system:
$$H_{\pm} = \pm\hbar v_F\left(k_x\sigma_x + k_y\sigma_y + k_z\sigma_z\right)$$
- Hamiltonian above uses all three pauli matrices, so there is no 2x2 matrix left over to anticommute with H and open gap
- Velocity is either parallel or opposite to chirality set by pseudospin: $\boldsymbol{v} = \pm\hbar v_F\boldsymbol{\sigma}$
- Energy spectrum around band crossing points: $E = \hbar v_F|\boldsymbol{k}|$
- Weyl points are mathematically like magnetic monopoles (except magnetic field→Berry curvature)
  - Integral around one Weyl node: $\pm 2\pi$
  - Integral over entire BZ: 0
  - Weyl points always come in pairs with opposite chirality
  - The only way to destroy Weyl points is to merge two with opposite chirality
  - Requires broken time reversal or inversion symmetry
- Fermi arcs connect projection of pair of Weyl points to surface

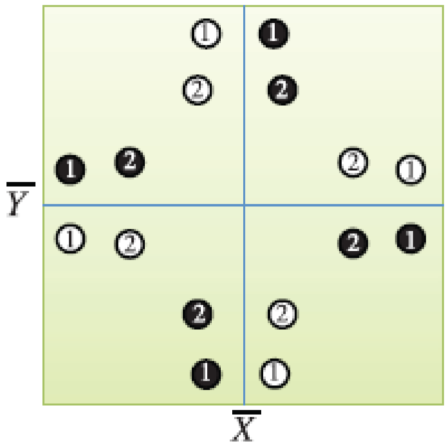


TaAs: first WSM?

- 24 bulk Weyl cones, including 4 pairs with chiral charge ± 2
- Weyl nodes are separated because of boken inversion symmetry
- First observe Fermi arcs, then connect to bulk Weyl nodes



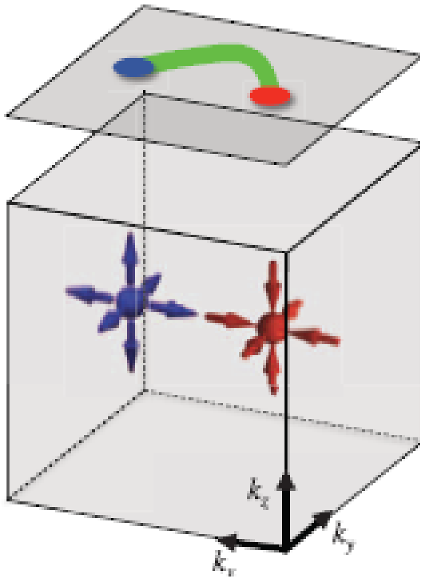




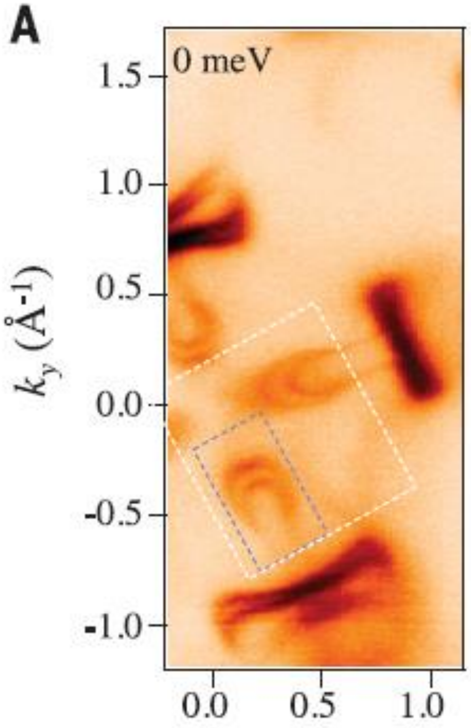
Xu *et al.*
Science **349**
613 (2015)

Demonstrating Fermi arcs in TaAs

Cartoon



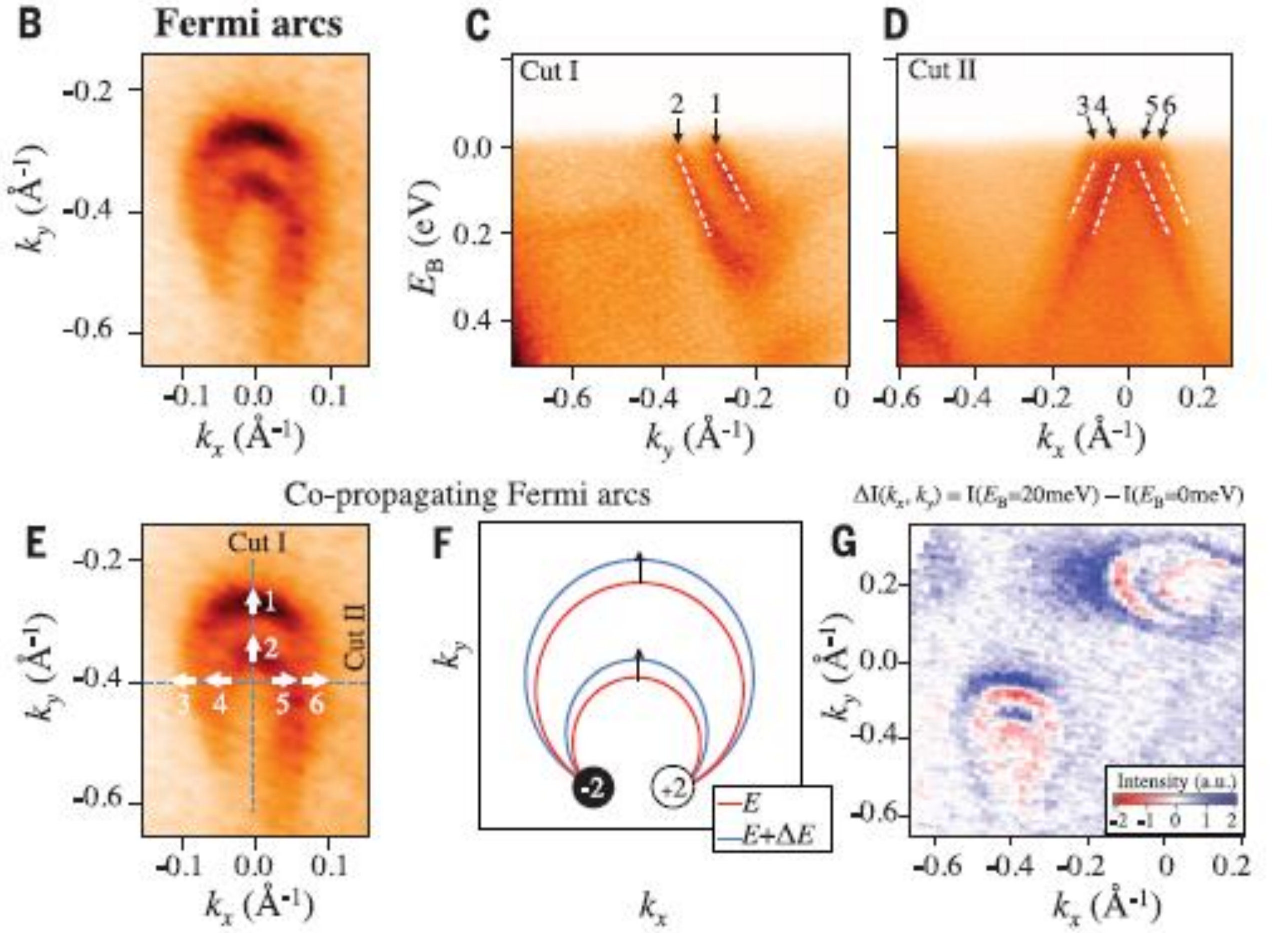
Real life



- Objective: prove that horseshoe-shaped FS is two Fermi arcs, not one weirdly shaped pocket
- Note: a competing paper on this topic came out at the same time (Lv *et al* PRX **5**, 031013 (2015))

Xu *et al.*
Science **349**
613 (2015)

Co-propagating surface states



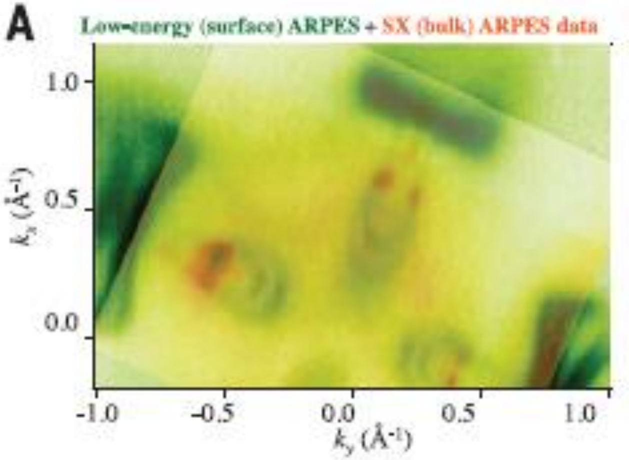
Xu *et al.* Science **349** 613 (2015)

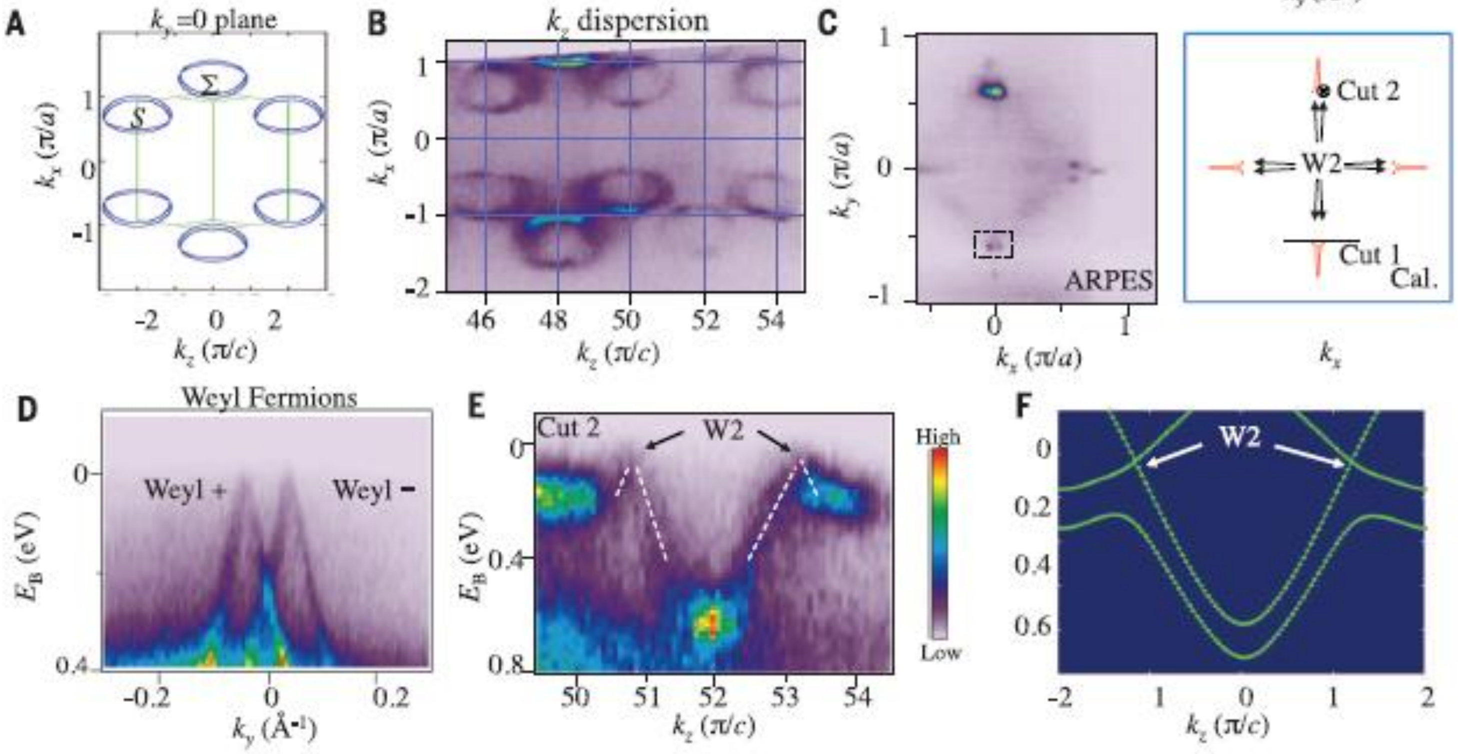
How would panel F look if ‘horseshoe’ feature was a closed pocket?

Bulk Weyl nodes in TaAs

Expectation for spin-integrated ARPES?:

- Band dispersion:
  Dirac cones at specific planes in k-space
- Fermi surface
  Points at specific planes, circles away from these planes





Xu *et al.* Science **349** 613 (2015)

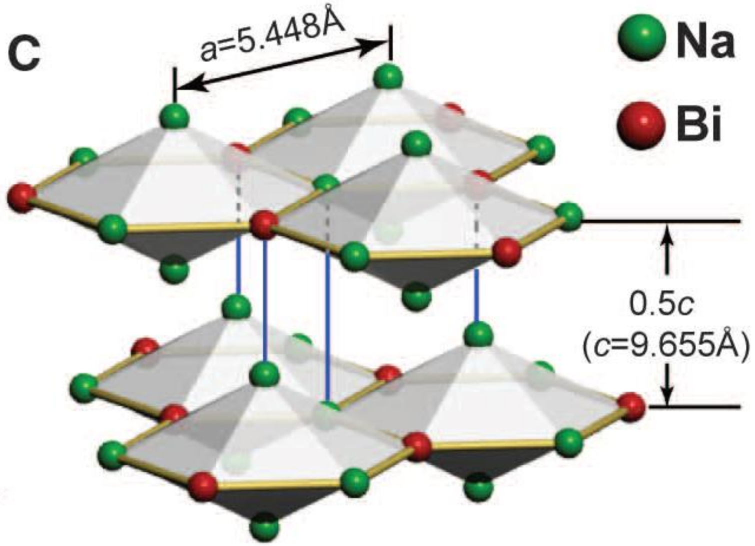
Summary: Evidence that TaAs is WSM

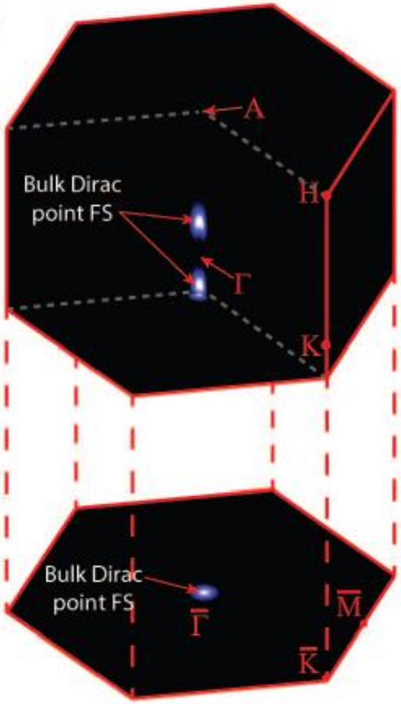
- Theory
- Surface states which are consistent with disconnected Fermi arcs, as opposed to closed pockets
- 3D Dirac dispersions in bulk which project onto termination of surface arcs
- Followup work (not discussed today) showing spin texture of surface state: Xu *et al* PRL 116, 096801 (2016)

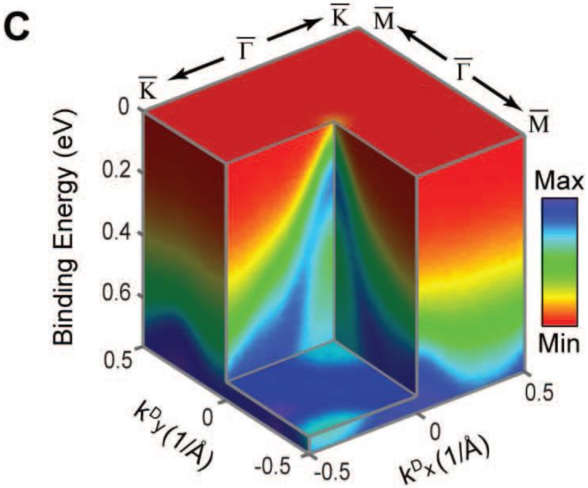
Dirac semimetals

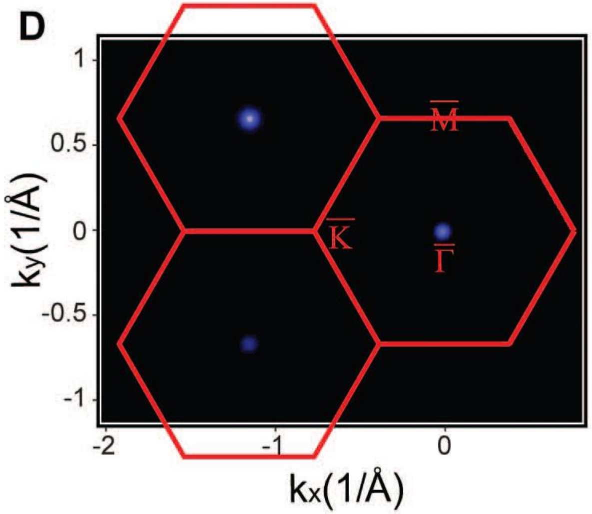
- Non-chiral 3D graphene
- $H = \hbar v_F \begin{pmatrix} \boldsymbol{\sigma} \cdot \boldsymbol{k} & 0 \\ 0 & -\boldsymbol{\sigma} \cdot \boldsymbol{k} \end{pmatrix}$
- This Dirac point is not generally robust against perturbations
- In some specific crystal structures, 3D Dirac point can be protected by certain crystal symmetries

Na_3Bi: a Dirac semimetal





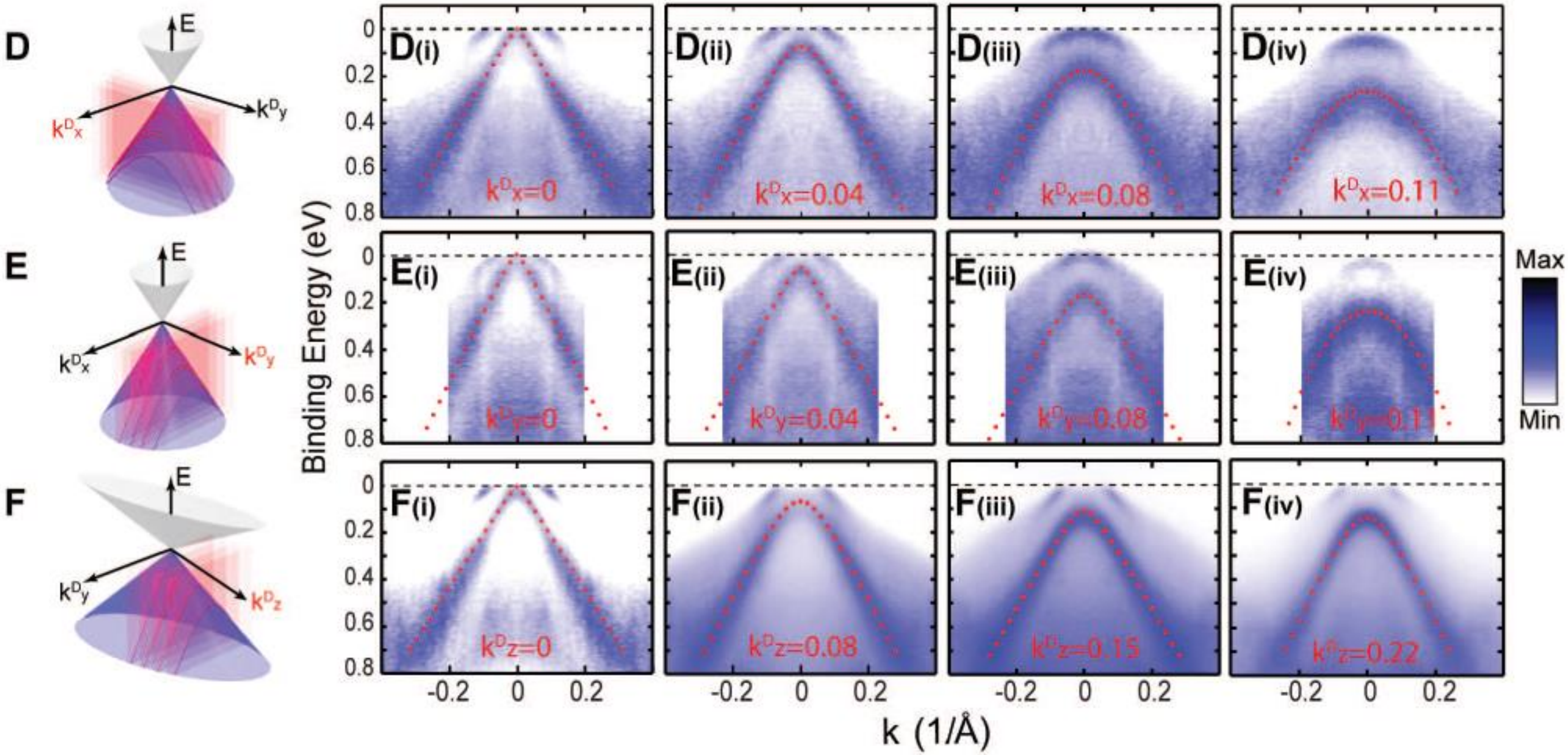




Dirac dispersion and point-like Fermi surface at certain kz

Liu *et al.* Science **343** 864 (2014)

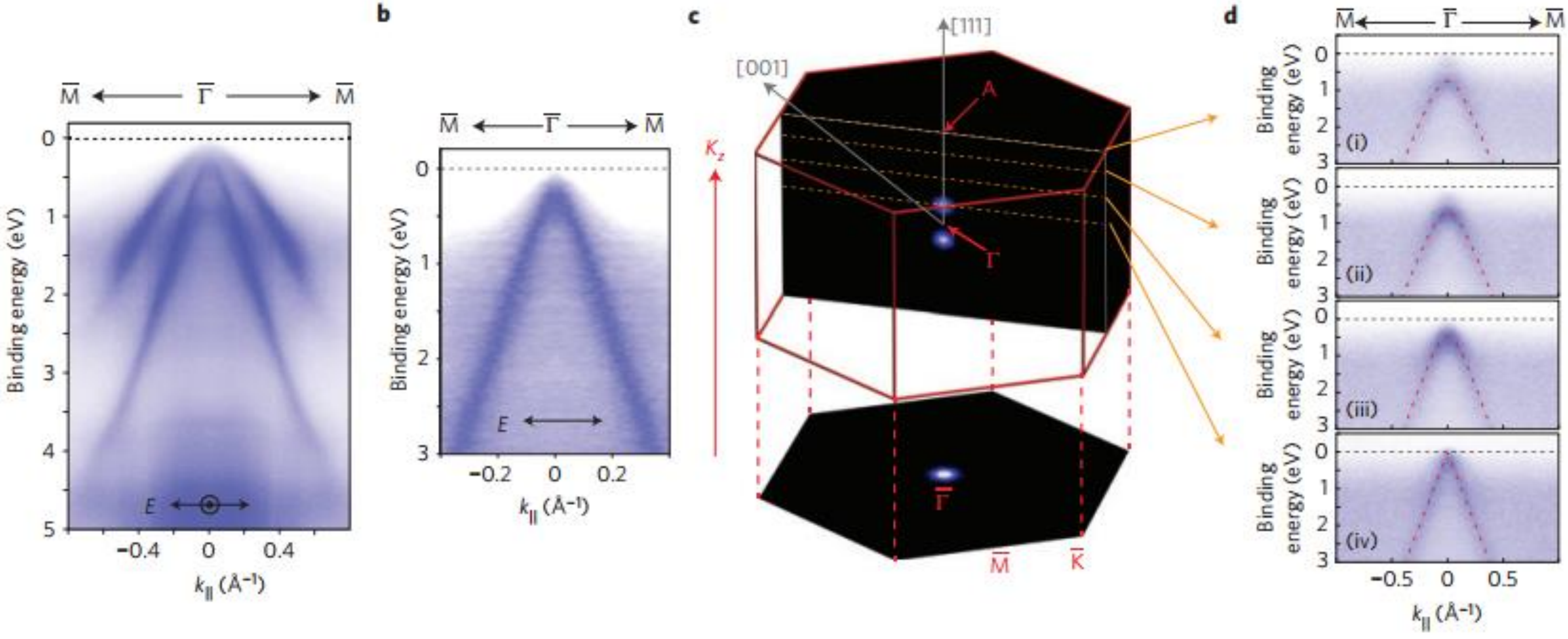
Na_3Bi: a Dirac semimetal



- Dispersion is linear if you slice through Dirac point, but hyperbolic if you miss it
- 3D dirac cone is anisotropic

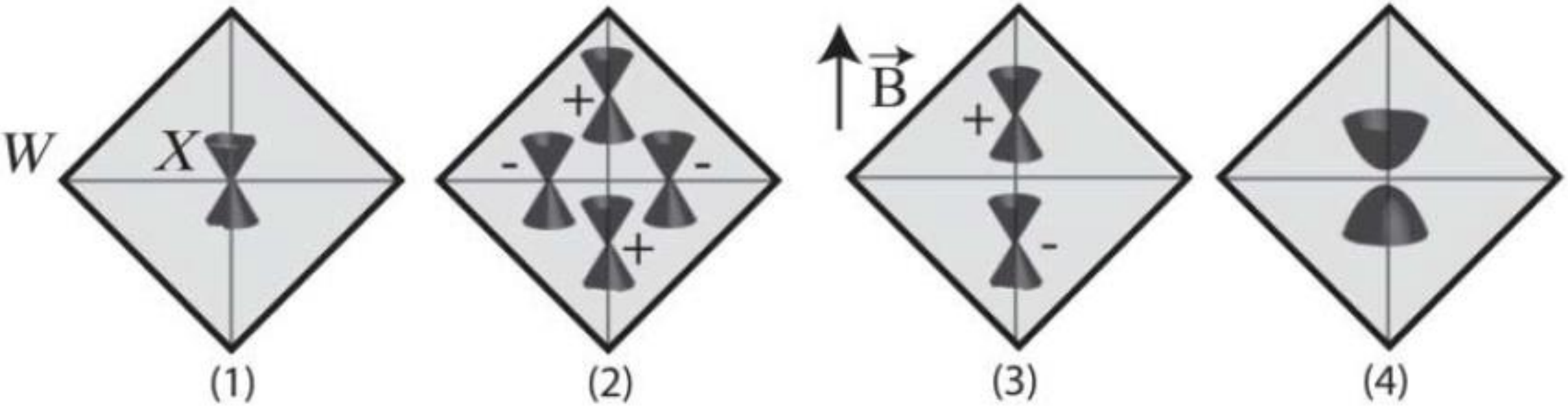
Liu *et al.* Science **343** 864 (2014)

Cd_3As_2: another Dirac Semimetal



Liu *et al,* Nat. Mater. **13** 677 (2014)

Summary: 3D Dirac systems



DSM

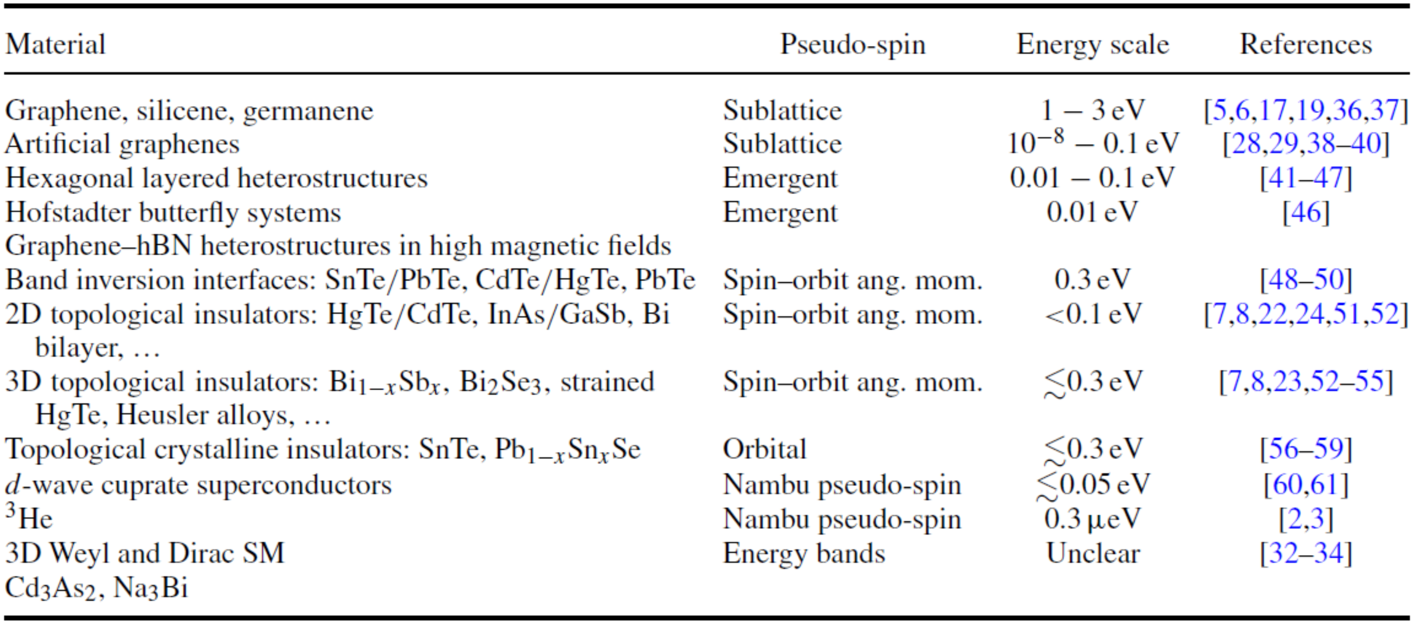
Break inversion symmetry→WSM

Break time reveral symmetry→WSM

Opening a gap in DSM

T. O. Wehling *et al.* Adv. Phys. **63** 1-76 (2014)

Conclusion: many examples of Dirac materials



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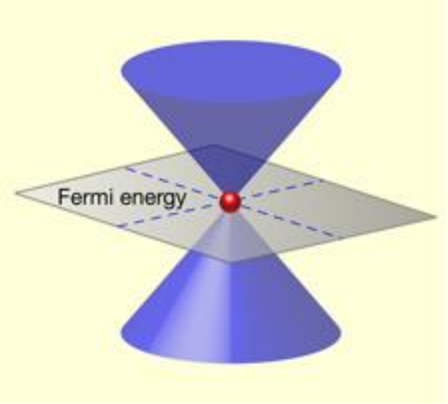

Contributions from ARPES

- Unravel complex 3D Fermiology in multiband materials
- Observe surface states

Resources

- T.O. Wehling *et al.* “Dirac Materials” *Advances in Physics*, **63** p1-76 (2014) http://www.tandfonline.com/doi/abs/10.1080/00018732.2014.927109
- Contemporary Concepts of Condensed Matter Science, Volume 6, Pages 1-324 (2013) **Topological Insulators,** Chapters 1,2, 11 http://www.sciencedirect.com/science/bookseries/15720934/6/supp/C