Dirac Fermions in the Antiferromagnetic Semimetals

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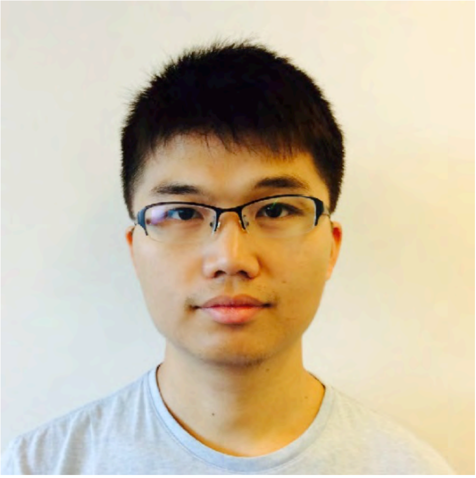
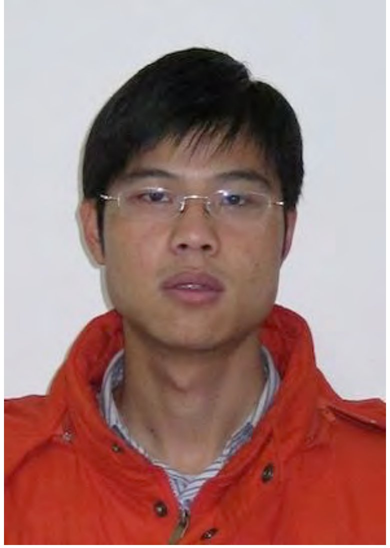
Collaborator:

Prof. Shou-Cheng Zhang @Stanford



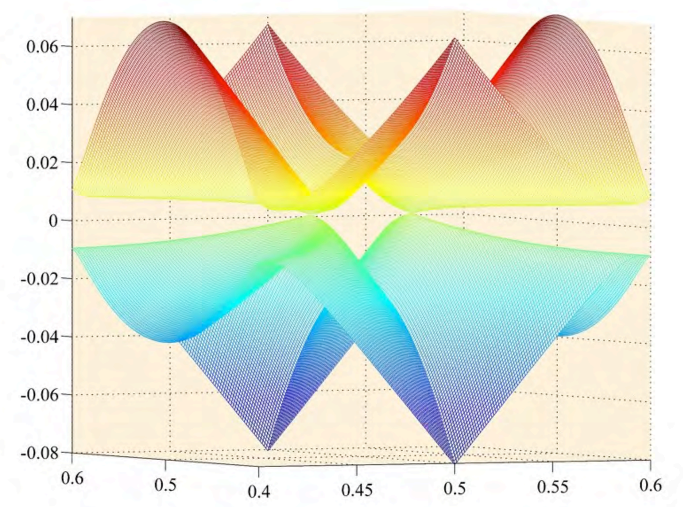
Mr. Quan Zhou @Stanford



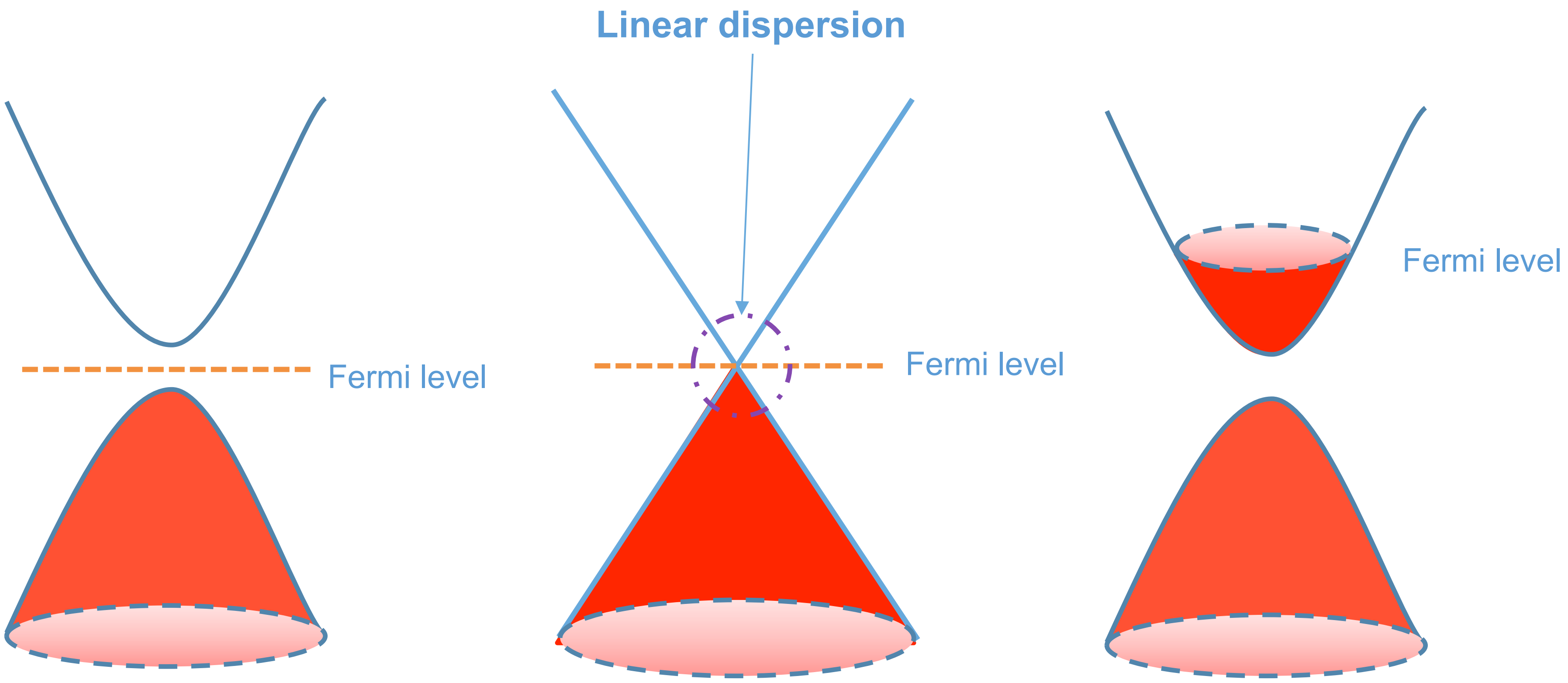
Dr. Gang Xu @Stanford

Outline

- Introduction (Topological semimetal: Dirac, Weyl and Dirac Nodal line)
- Some simple math (Nonsymmorphic group)
- AFM Dirac semimetal ---- CuMnAs && CuMnP
  - Dirac Nodal line
  - Dirac Points
  - Coupled Dirac points
- Conclusion



Introduction



Insulator — No states in the Fermi surface

Semimetal — Single point in the Fermi surface

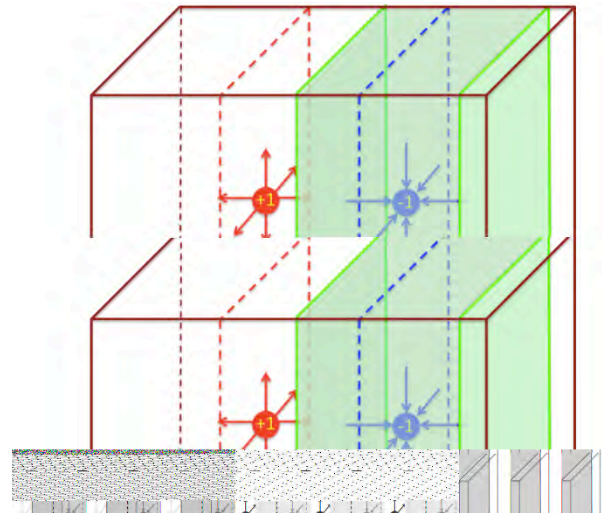
Metal — Filled states in the Fermi surface

What is Weyl semimetal.

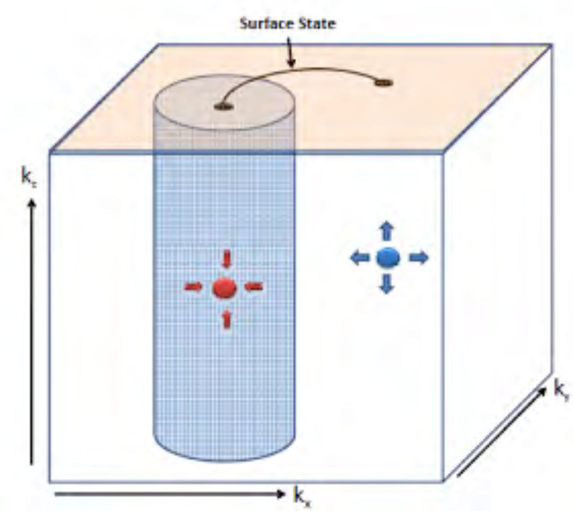
Hamiltonian of the Weyl Fermion in the momentum space:

$$H = \sum_i v_i(\hat{\boldsymbol{n}}_i \cdot \boldsymbol{p})\sigma_i$$ → 2×2 matrix

$$\kappa = sign[\hat{\boldsymbol{n}}_1 \cdot (\hat{\boldsymbol{n}}_2 \times \hat{\boldsymbol{n}}_3)]$$

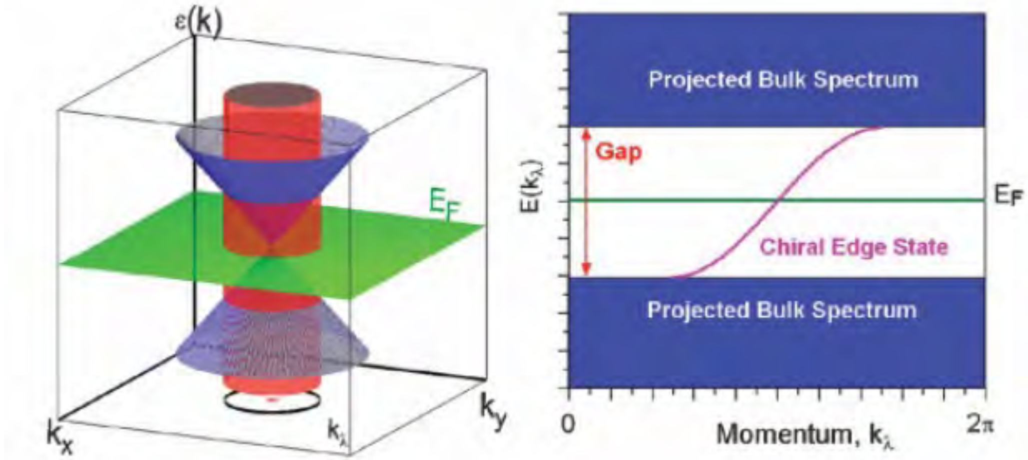


- The total chiral charges should be zero in the solid. The Weyl fermions appear by pairs.
- The Weyl Fermions are robust, small perturbation can not open gap at the Weyl point.
- Chiral anomaly.

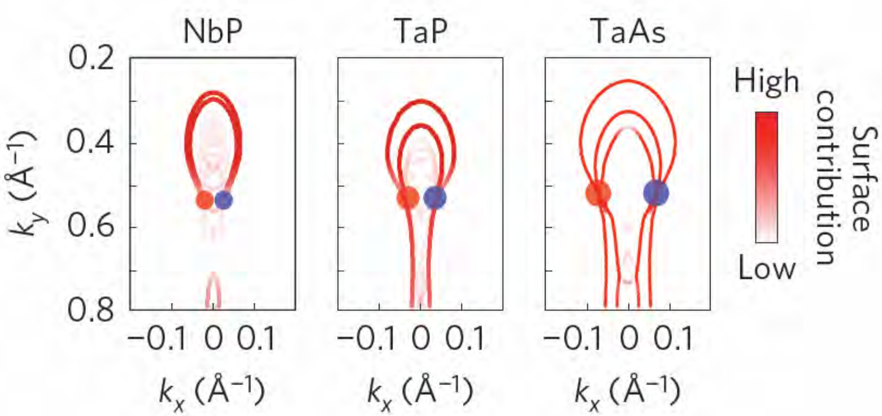


T Breaking: J. Zhang, C. Chang, **P. Tang**, et. al., Science 339, 6127 (2013)
Kurebayashi, et. al., JPSP 83, 063709 (2014),
G. Xu., et. al., PRL 107, 186806 (2011), Wang., et. al., arXiv: 1603.00479 (2016)
P Breaking: Huang., et. al., Nature Comm. 6, 7374 (2015); Weng., et. al., PRX 5, 011029 (2015); Xu., et. al., Science 349, 613 (2015); Yang, et. al., Nature Phys. 11, 728 (2015); Lv., et. al., PRX 5, 031013 (2015); Liu., et. al., Nature Mater. 15, 27 (2016).

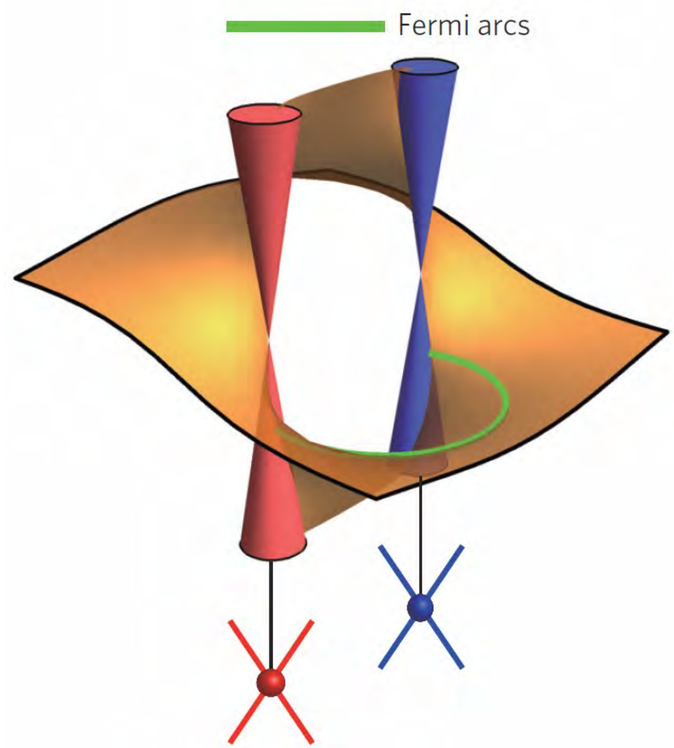
Riemann Surface States on Weyl semimetal.



Wan, et. al., PRB 83, 205101 (2011)

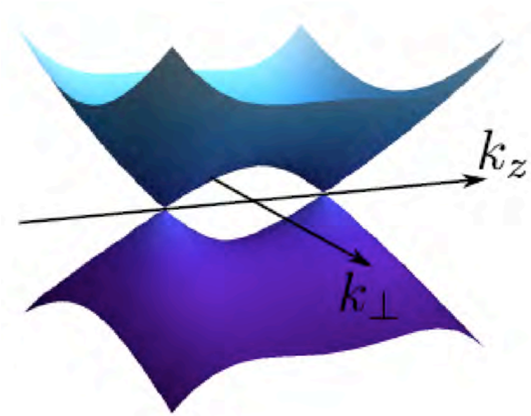


Liu, et. al., Nature Mater. 15, 27 (2016)



Fang, et. al., Nature Phys. doi: 10.1038/nphys3782 (2016)

What is Dirac semimetal

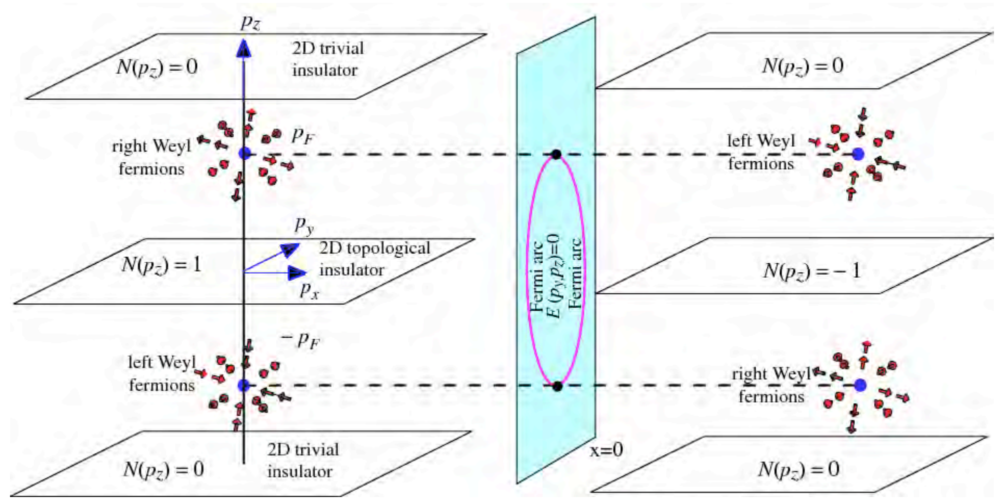


Hamiltonian of the Dirac Fermion in the momentum space:

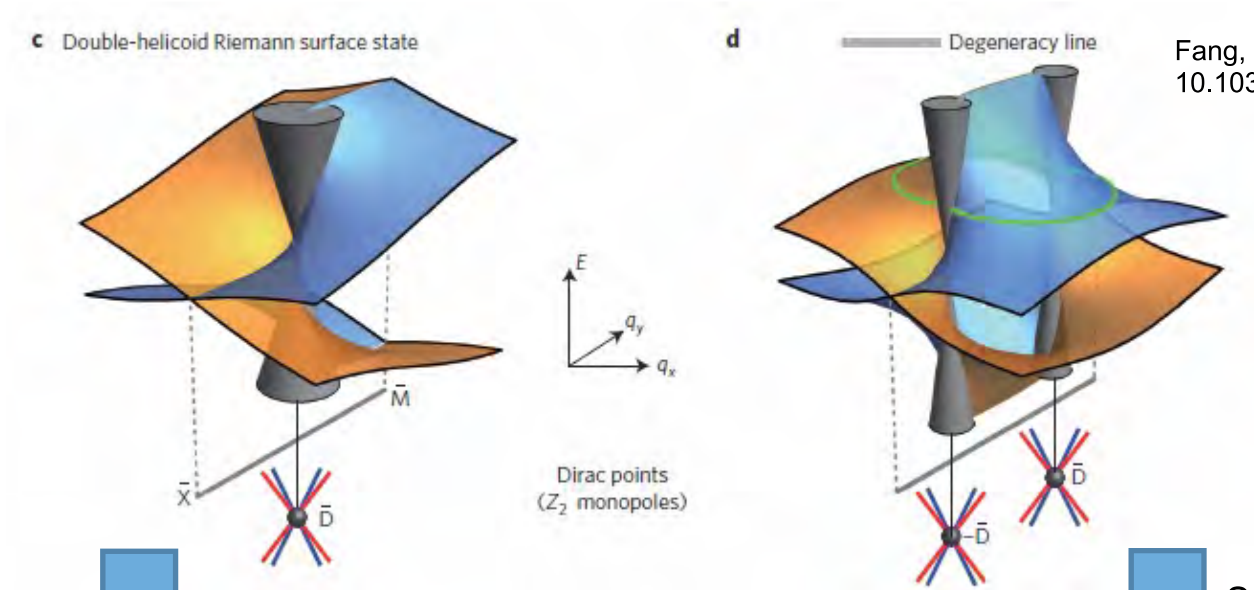
$$H = \begin{pmatrix} \sum_i v_i(\hat{\boldsymbol{n}}_i \cdot \boldsymbol{p})\sigma_i & 0 \\ 0 & \sum_i -v_i(\hat{\boldsymbol{n}}_i \cdot \boldsymbol{p})\sigma_i \end{pmatrix}$$

→ 4×4 matrix

- Dirac points could be regarded as the double of Weyl points. So the similar properties, such as Fermi arc and chiral anomaly, can also could be observed.
- At the crossing point, the states should be fourfold degenerate. Two Weyl points with opposite chirality touch together.
- Additional symmetries are needed to protect the degeneracy, such as rotation symmetries.



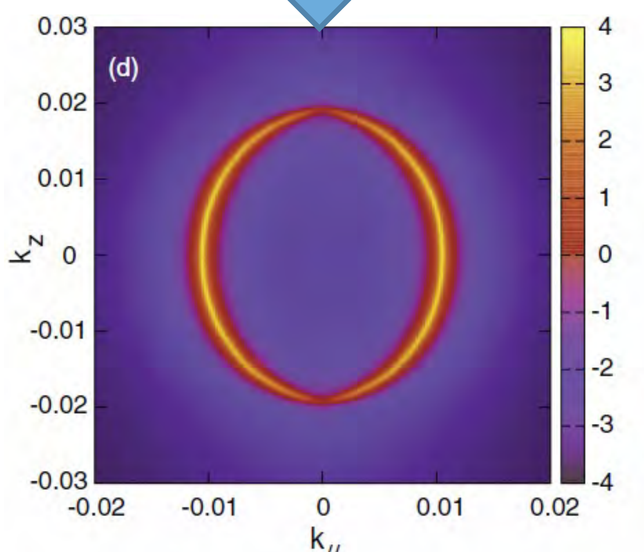
Riemann Surface States on Dirac semimetal.



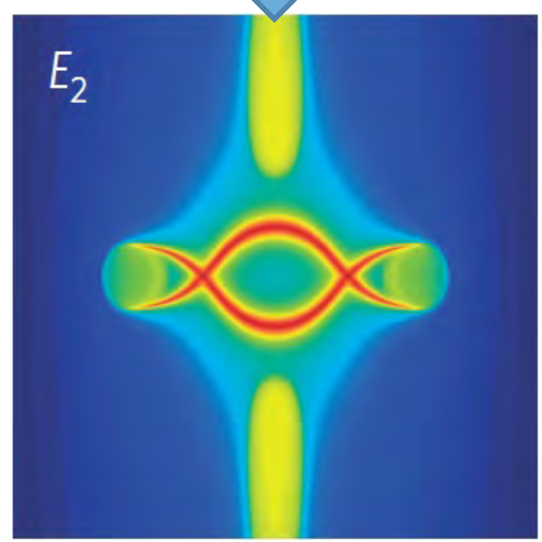
Fang, et. al., Nature Phys. doi: 10.1038/nphys3782 (2016)

No symmetry protection

Symmetry protection

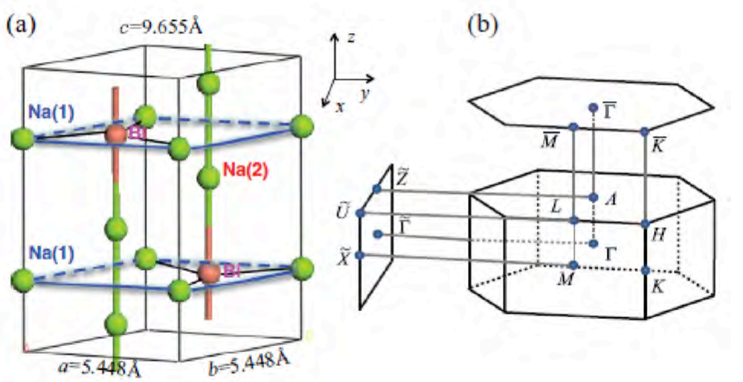


Na_3Bi, Cd_3As_2

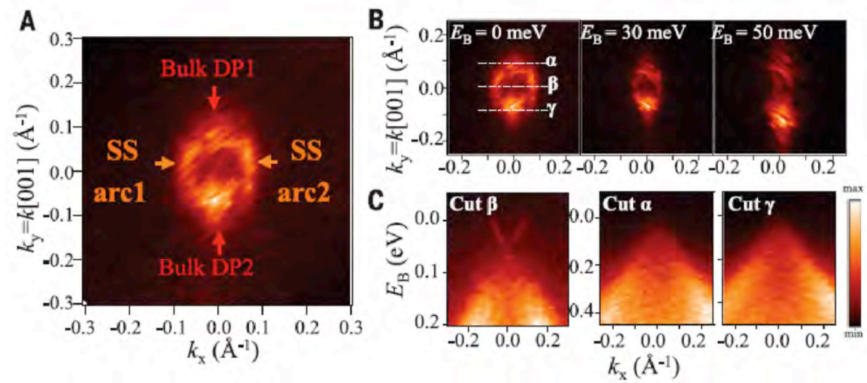


Wang, et. al., PRB 88, 125427 (2013)

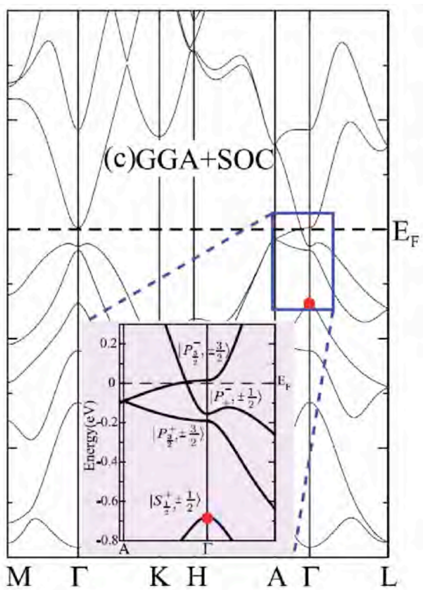
Discovered Dirac SM : Na_3Bi

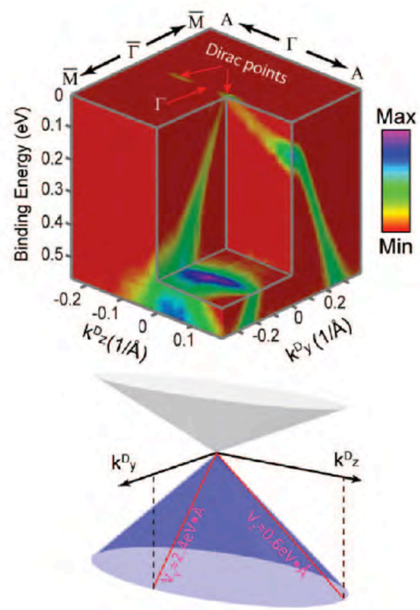


Wang., et. al., PRB 85, 195320 (2012)

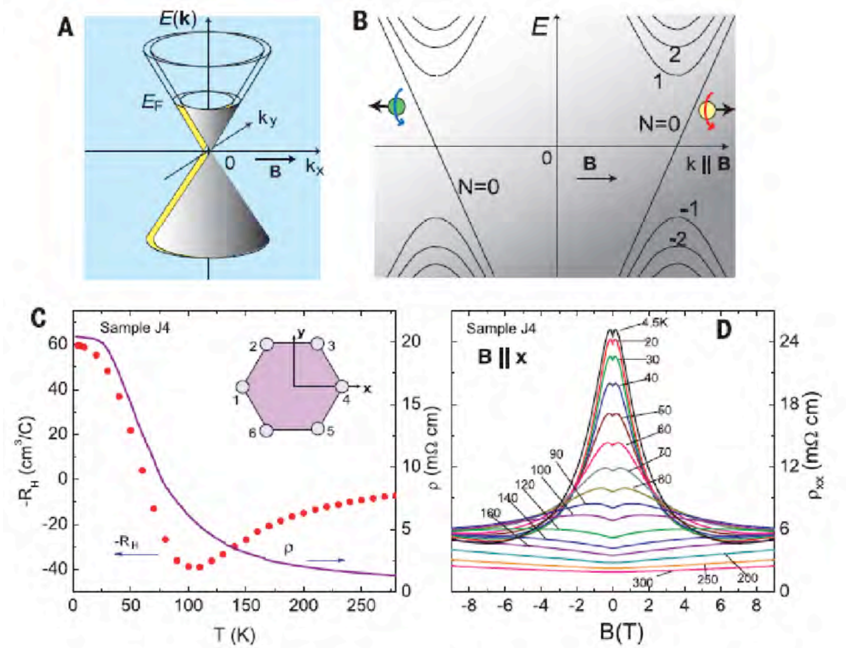


Xu., et. al., Science 347, 6219 (2015)



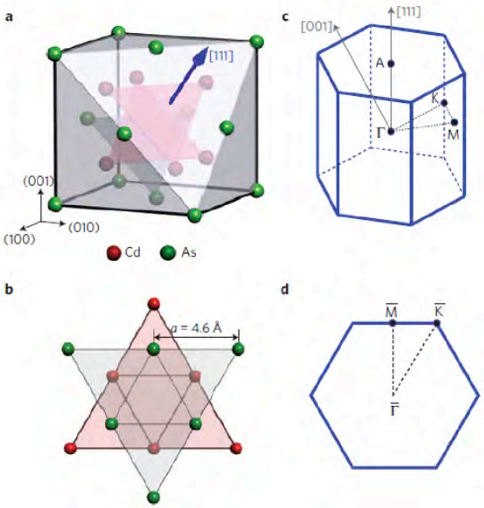


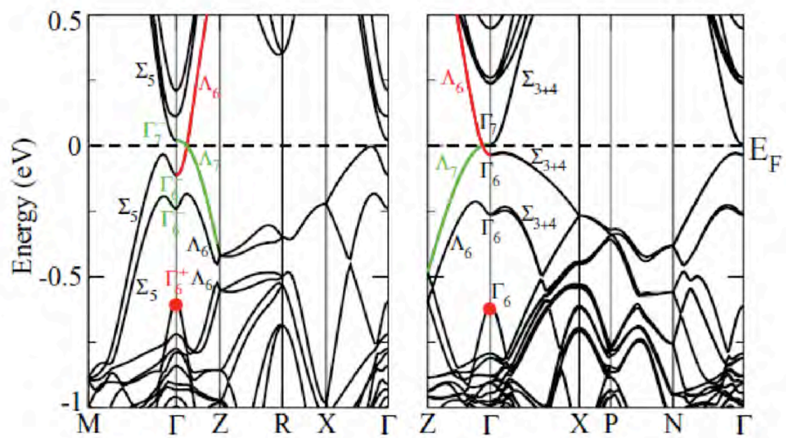
Liu., et. al., Science 343, 864 (2014)



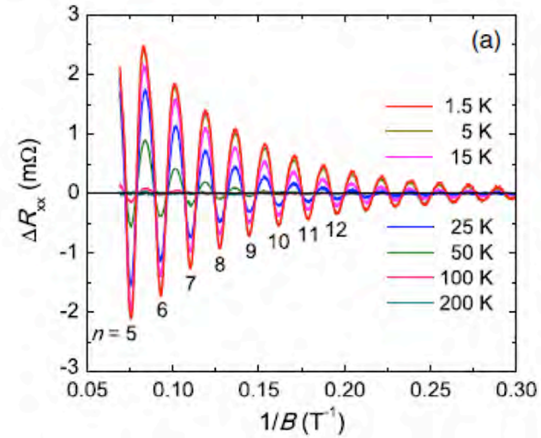
Xiong., et. al., Science 350, 6259 (2015)

Discovered Dirac SM : Cd_3As_2

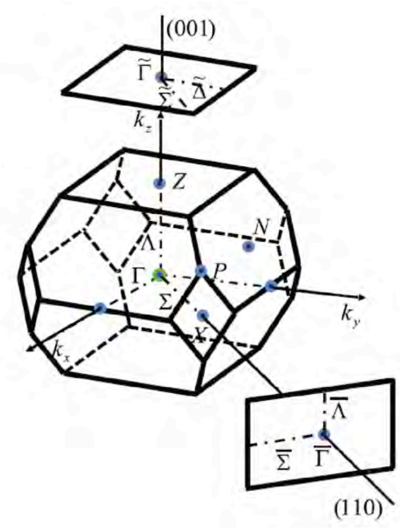


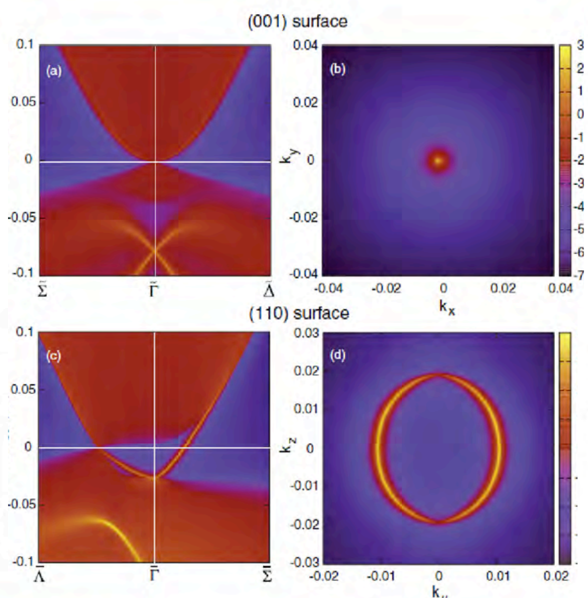


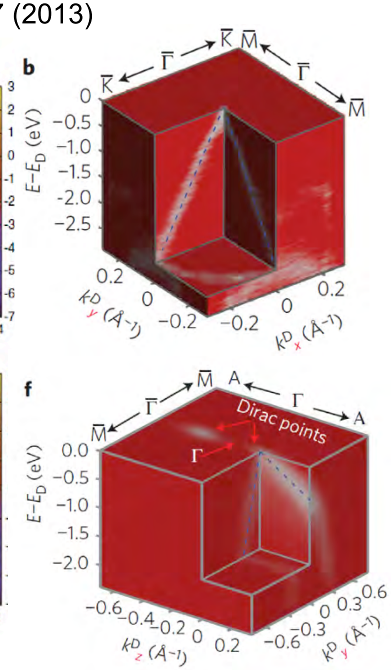
Wang, et. al., PRB 88, 125427 (2013)



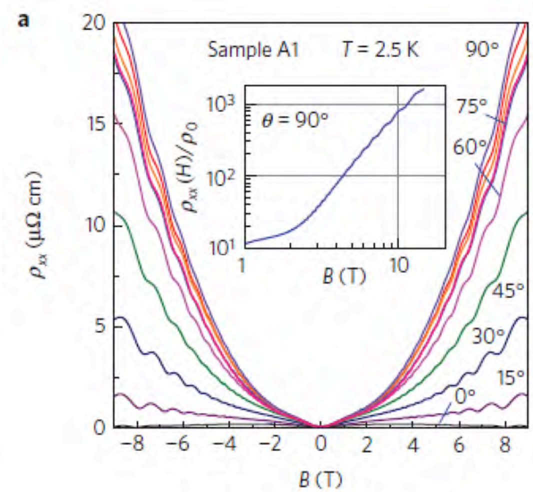
He, et. al., PRL 113, 246402 (2014)







Liu, et. al., Nature Mater. 13, 677 (2014)



Liang, et. al., Nature Mater. 14, 280 (2015)

Results: General argument for AFM Dirac SM

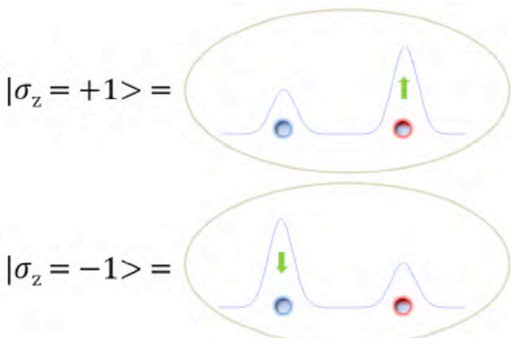
If a system has PT symmetry but do not have P and T, PT symmetry is anti-unitary ($(PT)^2 = -1$), we have:

$$(\mathcal{PT})H(\boldsymbol{k})(\mathcal{PT})^{-1} = H(\boldsymbol{k}).$$

For a Bloch wave $|\psi(k)\rangle$ with energy $\mathrm{E}(k)$ and $H(k)|\psi(k)\rangle = \mathrm{E(k)}\,|\psi(k)\rangle$:

$$H(\boldsymbol{k})\,|\phi(\boldsymbol{k})\rangle = H(\boldsymbol{k})(\mathcal{PT}\,|\psi(\boldsymbol{k})\rangle) = \mathcal{PT}(H(\boldsymbol{k}\,|\psi(\boldsymbol{k})\rangle) = E(\boldsymbol{k})(\mathcal{PT}\,|\psi(\boldsymbol{k})\rangle) = E(\boldsymbol{k})\,|\phi(\boldsymbol{k})\rangle$$

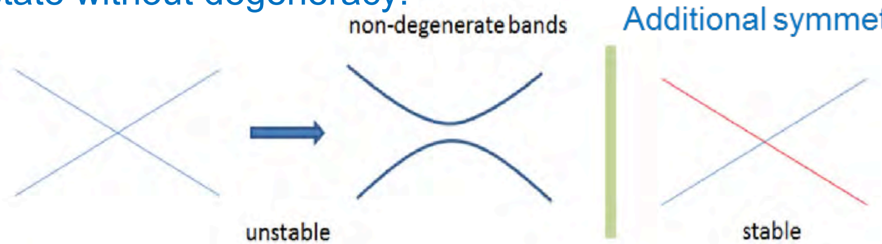
$$\langle\phi(\boldsymbol{k})\,|\,\psi(\boldsymbol{k})\rangle = \langle\mathcal{PT}\psi(\boldsymbol{k})\,|\,\mathcal{PT}\phi(\boldsymbol{k})\rangle = \langle\phi(\boldsymbol{k})|\,(\mathcal{PT})^2\,|\psi(\boldsymbol{k})\rangle = -\,\langle\phi(\boldsymbol{k})\,|\,\psi(\boldsymbol{k})\rangle$$



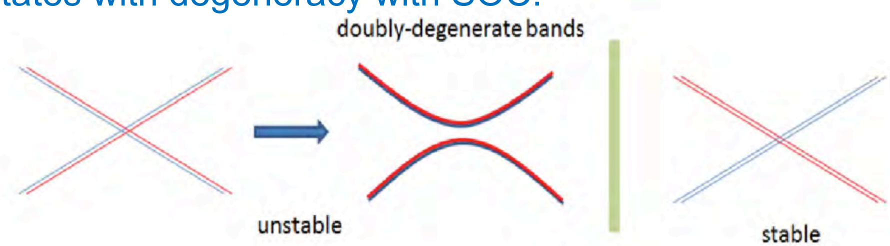
$(PT)|\sigma_z = +1\rangle = |\sigma_z = -1\rangle$

For state without degeneracy:

Additional symmetry: g



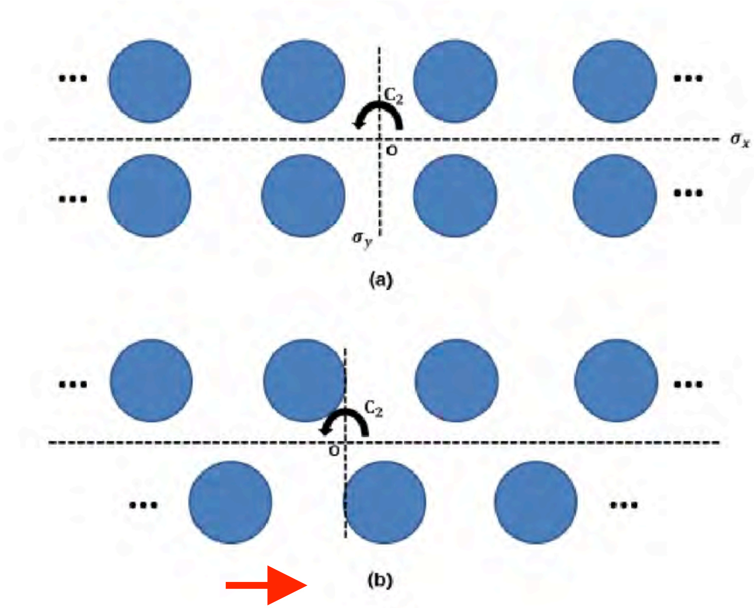
For states with degeneracy with SOC:



$\{g, PT\}$=0

$[g, PT]$=0

Nonsymmorphic group



Define translation vector:

$$\mathbf{t} = t_1\boldsymbol{a_1} + t_2\boldsymbol{a_2} + t_3\boldsymbol{a_3}$$

Seitz operator $\{\alpha|\boldsymbol{\tau}\}$ on a spatial point x:

$$\{\alpha|\boldsymbol{\tau}\}x = \alpha x + \boldsymbol{\tau}$$

$$\boldsymbol{\tau} = \boldsymbol{\upsilon} + \boldsymbol{t}$$

$\boldsymbol{\upsilon}$ is a vector within the primitive cell, it can be regarded as a "fractional" translation vector.

For the nonsymmorphic group, we have: $\{\alpha|\tau_1\}\{\beta|\tau_2\} = \{\alpha\beta|\alpha\tau_2 + \tau_1\}$

so $\{g|\tau\}\{g|\tau\} = \{g^2|g\tau + \tau\}$. If we have $g\tau = \tau = T/2$

$$\{g|\tau\}^2\psi(\boldsymbol{k}) = \{g^2|T\}\,\psi(\boldsymbol{k}) = e^{ikT}g^2\psi(\boldsymbol{k}) = e^{ikT}\lambda^2\psi(\boldsymbol{k}) \qquad \{g|\tau\}|u_k^{\pm}\rangle = \pm\lambda e^{ik\tau}u_k^{\pm}\rangle$$

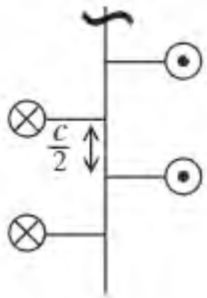
$\{g|\tau\}$:

$$\{g|\tau\}|u_k^{\pm}\rangle = \pm\lambda e^{ik\tau}|u_k^{\pm}\rangle \qquad \boldsymbol{k} = \boldsymbol{G}, e^{ik\tau} = -1$$

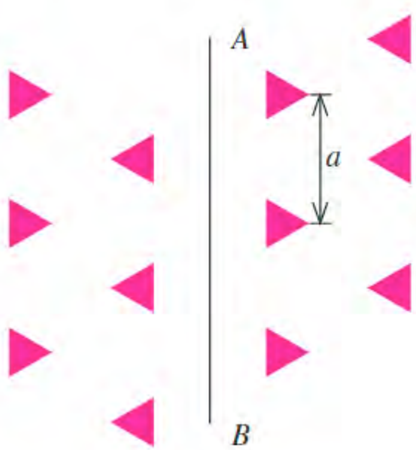
$$|u_{\boldsymbol{k}}^{\pm}\rangle = |u_{\boldsymbol{k}+\boldsymbol{G}}^{\pm}\rangle$$

So, along the line, λ for the blue and red should be different

(a) Diad screw axis



(c) Glide reflection



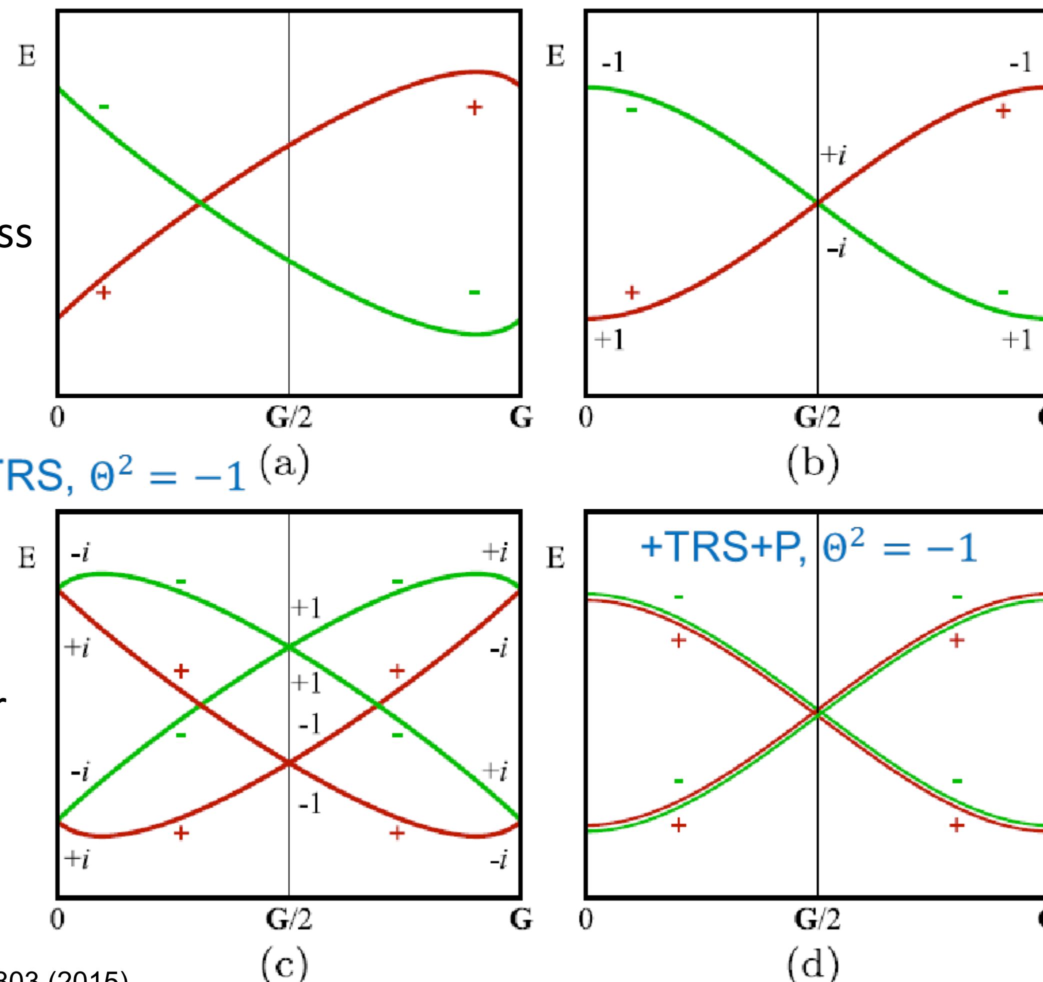
No other symmetry

+TRS, $\Theta^2 = 1$

spinless

+TRS, $\Theta^2 = -1$

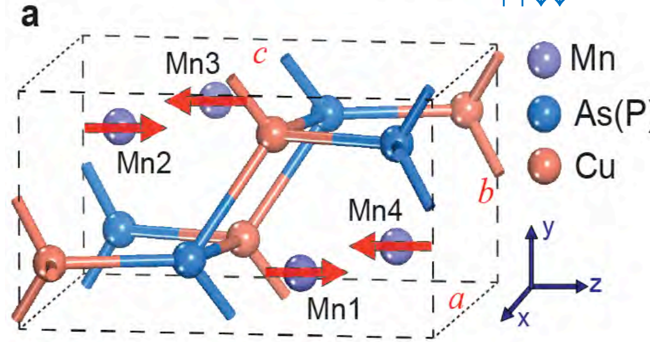
spinor



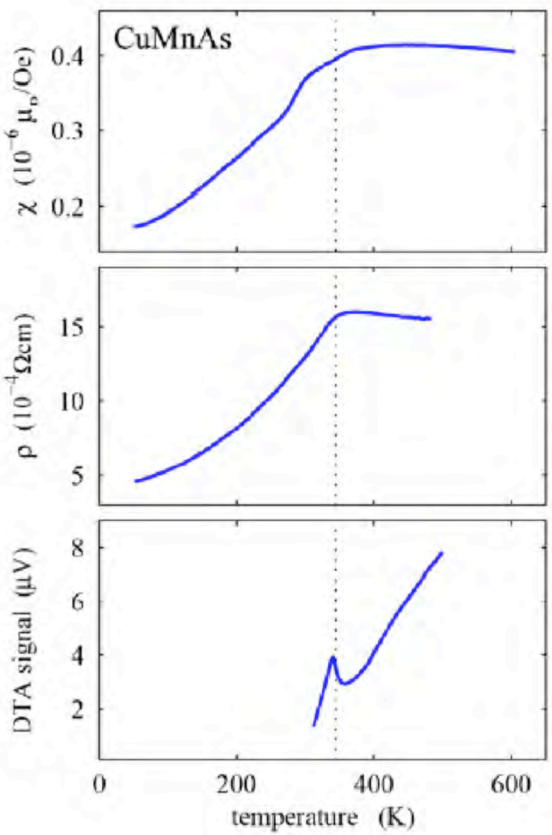
Young, et. al., PRL 115, 126803 (2015)

Results: AFM order

Most stable structure AFM ↑↑↓↓:

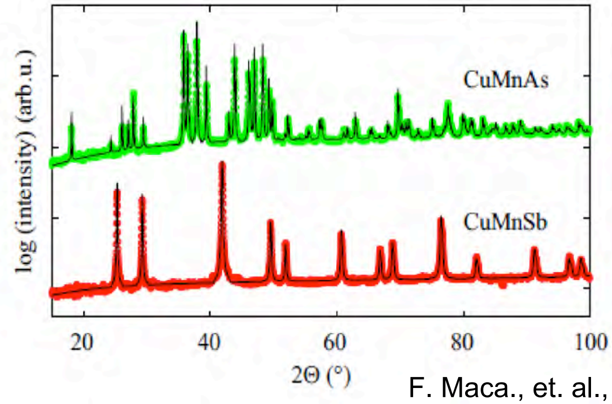


Transport measurement:



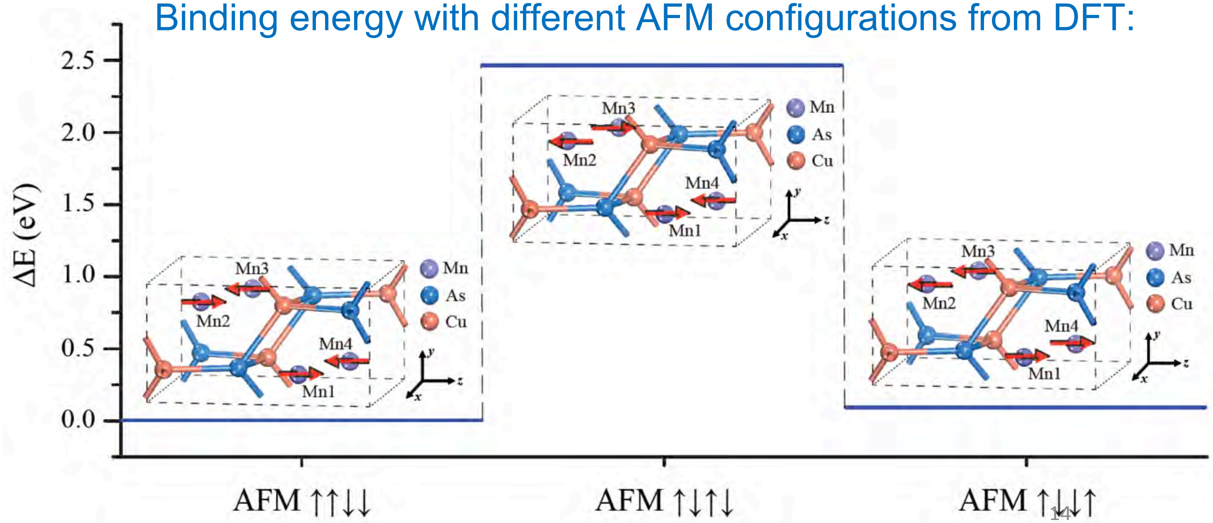
F. Maca., et. al., JMMM 324, 1606 (2012)

XRD:



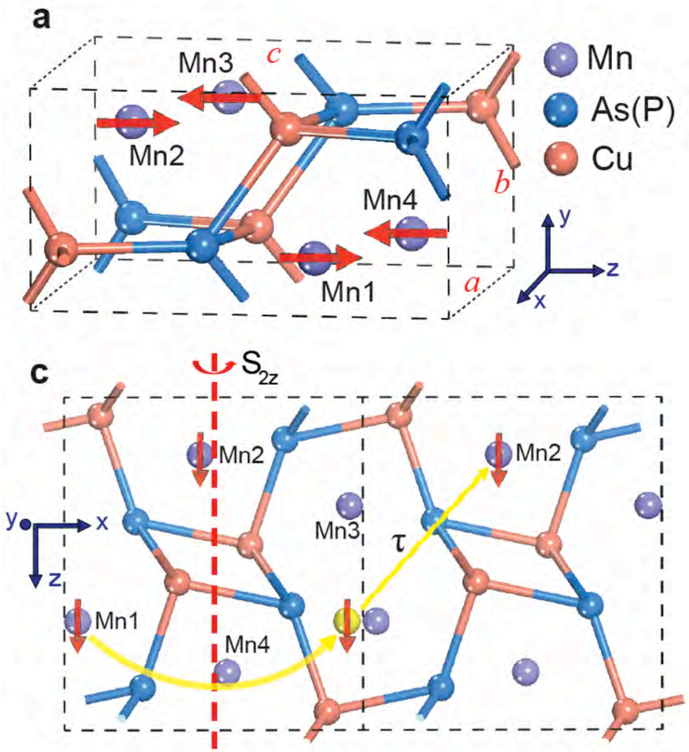
F. Maca., et. al., JMMM 324, 1606 (2012)

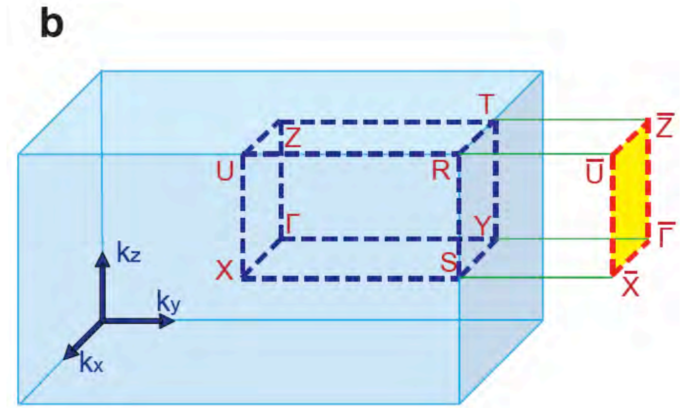
Binding energy with different AFM configurations from DFT:



Results: Structure

3D BZ and projected 2D for orthorhombic CuMnAs(P):





Lattice structure for orthorhombic CuMnAs(P):

d Symmetry for CuMnAs(P):

Symmetry operation	w/o SOC	$\vec{m}//(001)$	$\vec{m}//$other directions
T			
P			
PT	√	√	√
$S_{2z}=\{C_{2z}\vert(0.5,0,0.5)\}$	√	√	
$R_y=\{m_y\vert(0,0.5,0)\}$	√		possible

$$(x,y,z)\xrightarrow{PT}(-x,-y,-z),$$
$$(s_x,s_y,s_z)\xrightarrow{PT}(-s_x,-s_y,-s_z),$$
$$(k_x,k_y,k_z)\xrightarrow{PT}(k_x,k_y,k_z),$$
$$(x,y,z)\xrightarrow{S_{2z}}(-x+\frac{1}{2},-y,z+\frac{1}{2}),$$
$$(s_x,s_y,s_z)\xrightarrow{S_{2z}}(-s_x,-s_y,s_z),$$
$$(k_x,k_y,k_z)\xrightarrow{S_{2z}}(-k_x,-k_y,k_z).$$

$$(x,y,z)\xrightarrow{PT}(-x,-y,-z)\xrightarrow{S_{2z}}(x+\frac{1}{2},y,-z+\frac{1}{2}),$$
$$(s_x,s_y,s_z)\xrightarrow{PT}(-s_x,-s_y,-s_z)\xrightarrow{S_{2z}}(s_x,s_y,-s_z),$$
$$(x,y,z)\xrightarrow{S_{2z}}(-x+\frac{1}{2},-y,z+\frac{1}{2})\xrightarrow{PT}(x-\frac{1}{2},y,-z-\frac{1}{2}),$$
$$(s_x,s_y,s_z)\xrightarrow{S_{2z}}(-s_x,-s_y,s_z)\xrightarrow{PT}(s_x,s_y,-s_z),$$

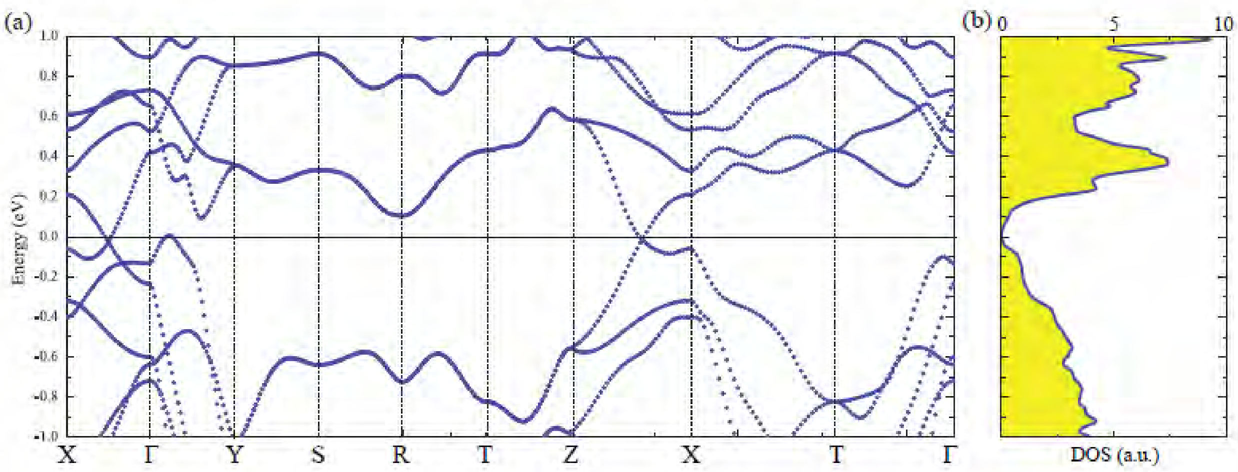
$$S_{2z}^2=-T(0,0,1)=-e^{-ik_z}$$

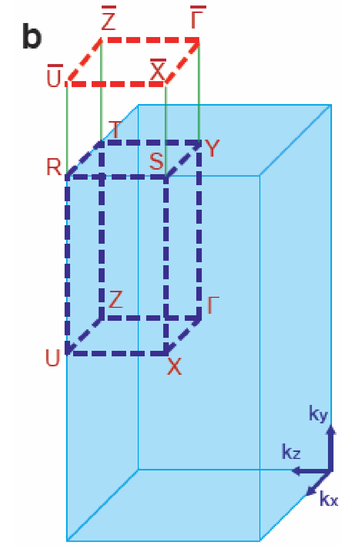
$$S_{2z}\cdot(PT)=T(0{,}1{,}0)(PT)\cdot S_{2z}$$
$$=e^{-ik_x}e^{-ik_z}(PT)\cdot S_{2z}$$

For $k_x=\pi$, $k_z=0$; $[S_{2z},(PT)]=0$

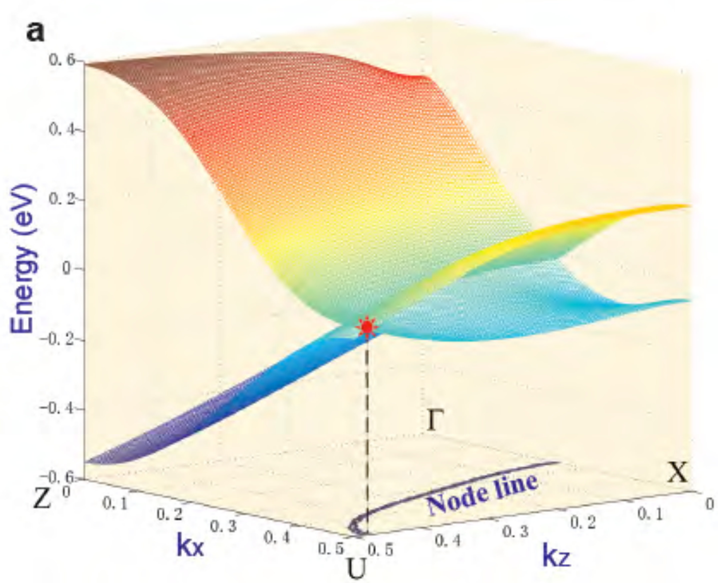
Results: No SOC and No symmetry breaking

3D electronic structures without SOC and symmetry breaking:

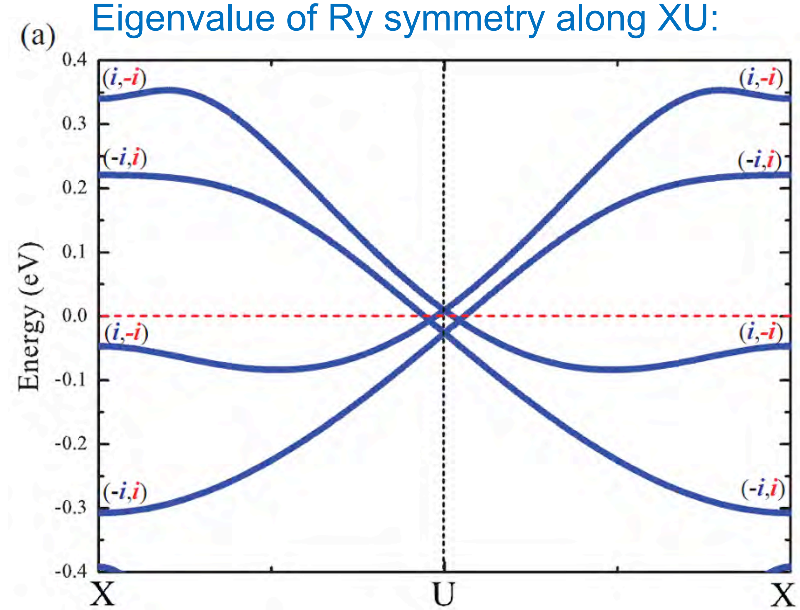




3D bands @ the plane of k_y=0:



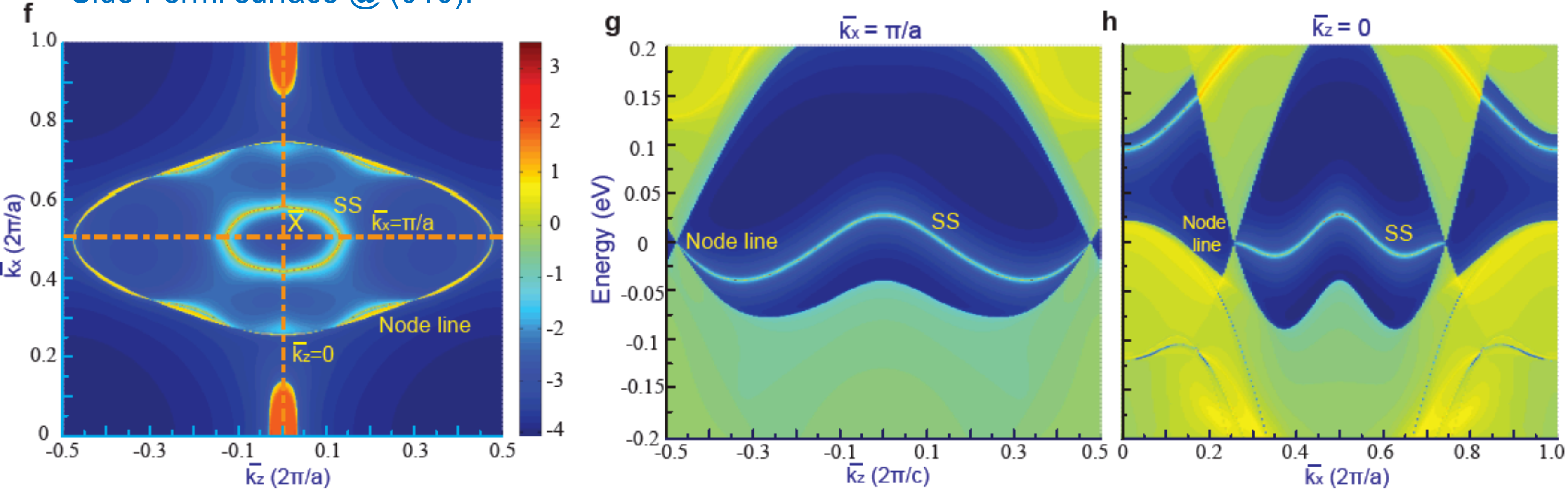
Eigenvalue of Ry symmetry along XU:

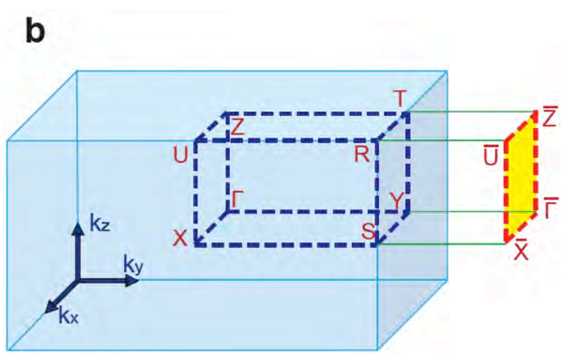


Results: No SOC and No symmetry breaking

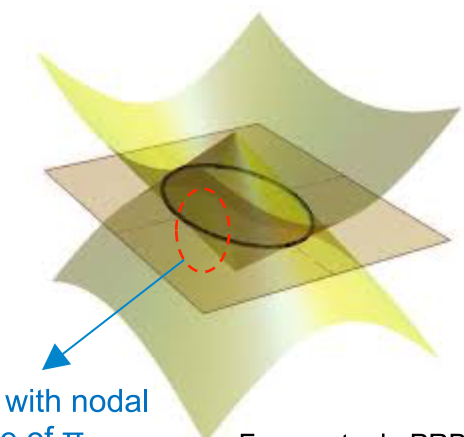
Side Fermi surface @ (010):

Side surface bands @ (010):





3D bulk nodal line in *k* space:



drum-like surface states on the side surface

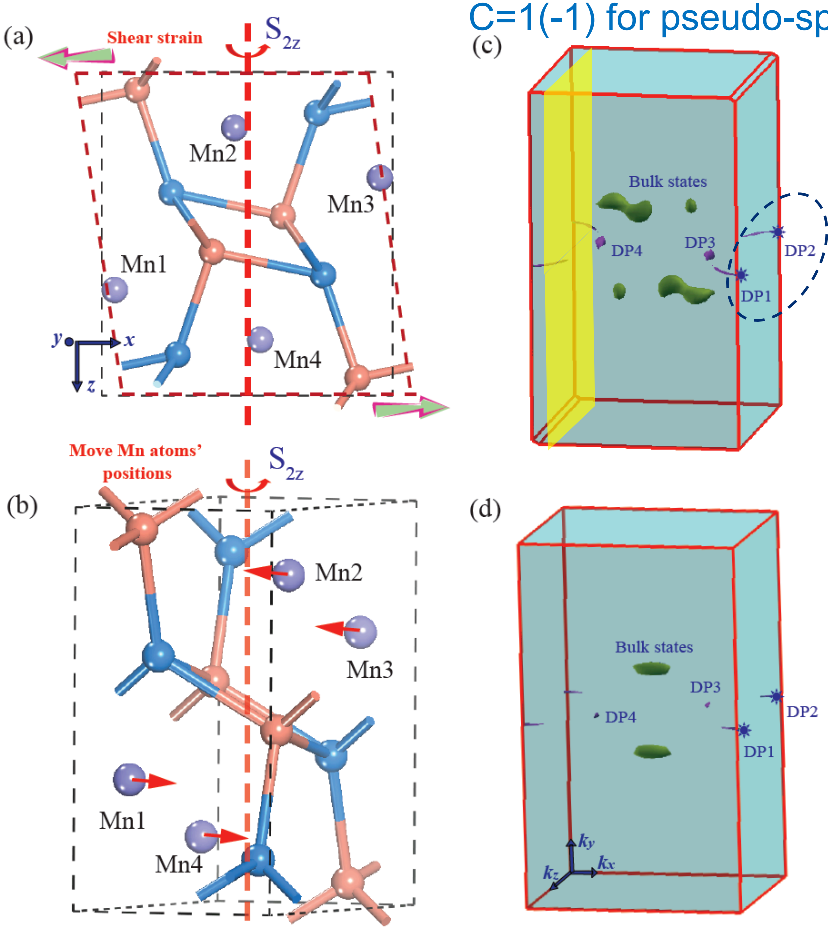
A loop that interlocks with nodal line has a Berry phase of π

Fang., et. al., PRB 92, 081201 (2015)

Results: No SOC and with R_y breaking

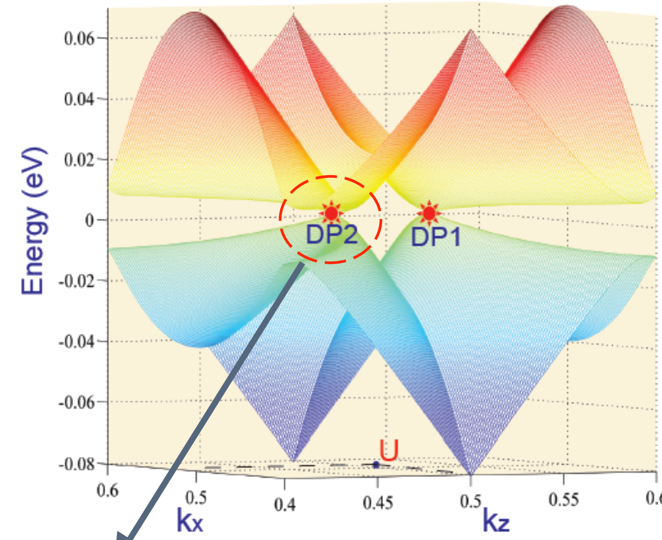
Two method to break R_y symmetry

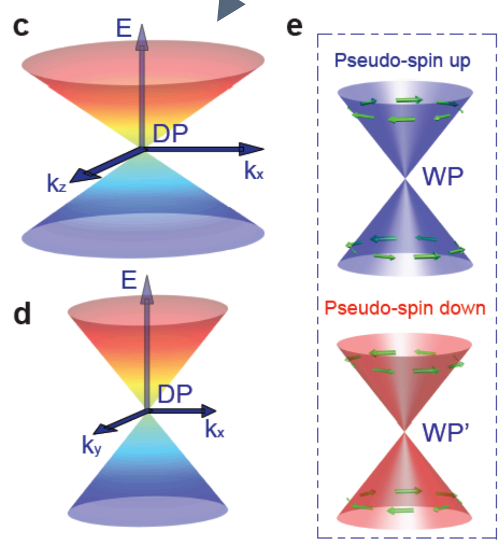
C=1(-1) for pseudo-spin ↑(↓)



3D Fermi surface

3D Bands around Dirac Point





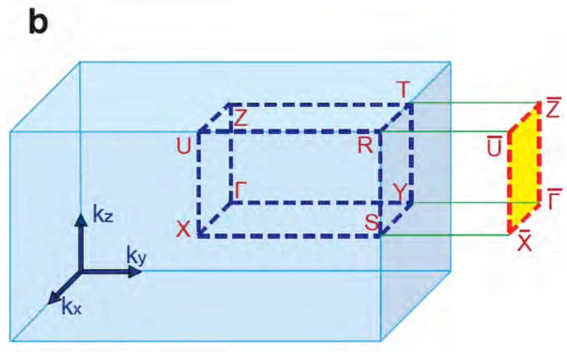
- The Dirac points is anisotropic at 3D k space.
- The Dirac point can be regarded as the copy of the Weyl points.
- The pseudo-spin is coupled with the chirality κ of the Weyl fermion.
- Pseudo-spin is linked with the real spin.

$$\mathcal{H}_{Dirac} = (v_{11}k_x + v_{12}k_y)\tau_x + v_{33}k_z\tau_z + (v_{21}k_x + v_{22}k_y)\tau_y\sigma_z$$

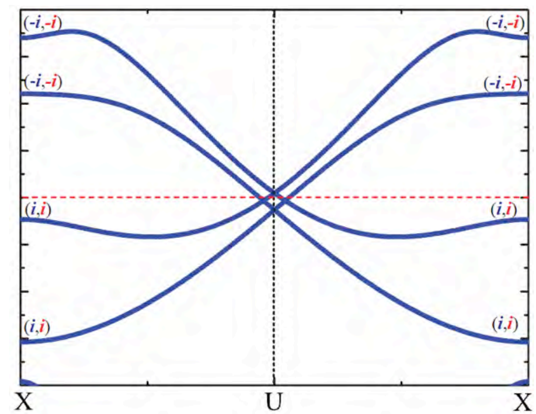
$$\mathcal{H}^{+}_{Weyl} = (v_{11}k_x + v_{12}k_y)\tau_x + v_{33}k_z\tau_z + (v_{21}k_x + v_{22}k_y)\tau_y,$$

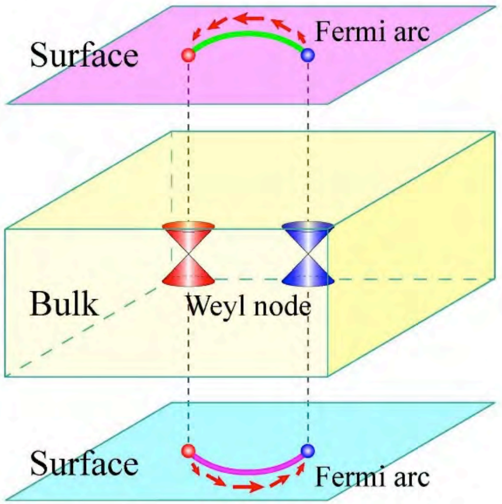
$$\mathcal{H}^{-}_{Weyl} = (v_{11}k_x + v_{12}k_y)\tau_x + v_{33}k_z\tau_z - (v_{21}k_x + v_{22}k_y)\tau_y.$$

Results: No SOC and with R_y breaking

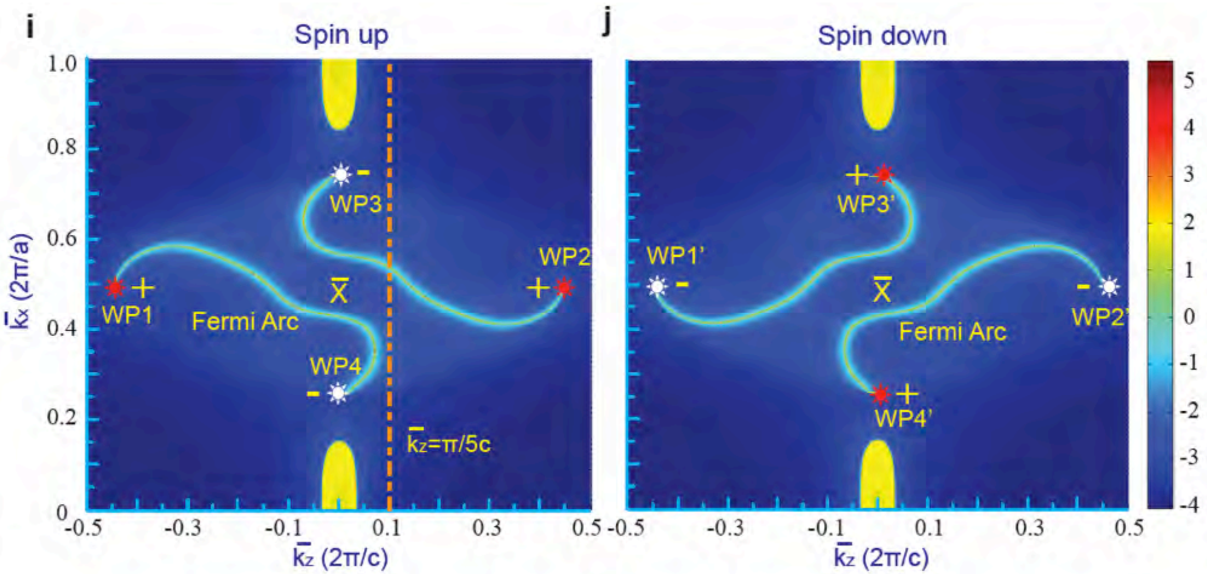


Eigenvalue of S_z symmetry along XU

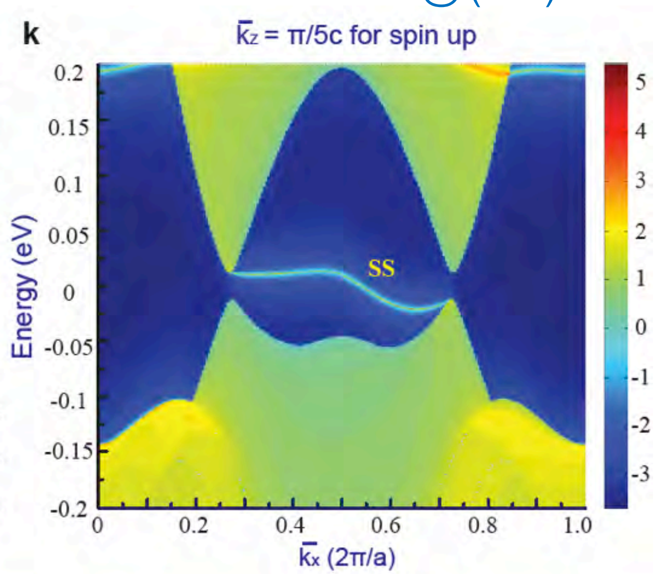




Fermi arc surface states @ (010):

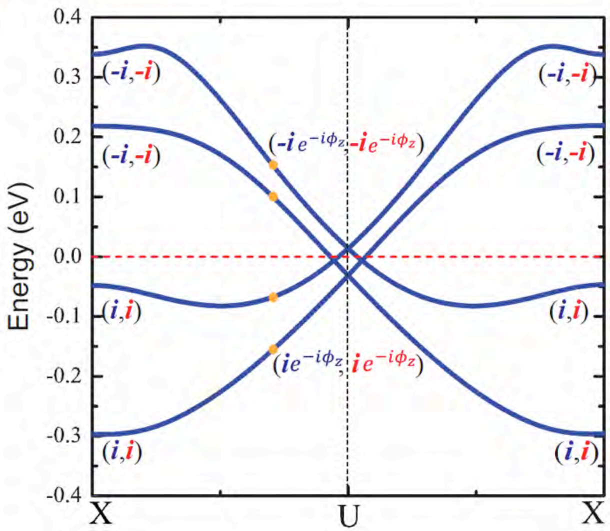


Side surface bands @ (010):

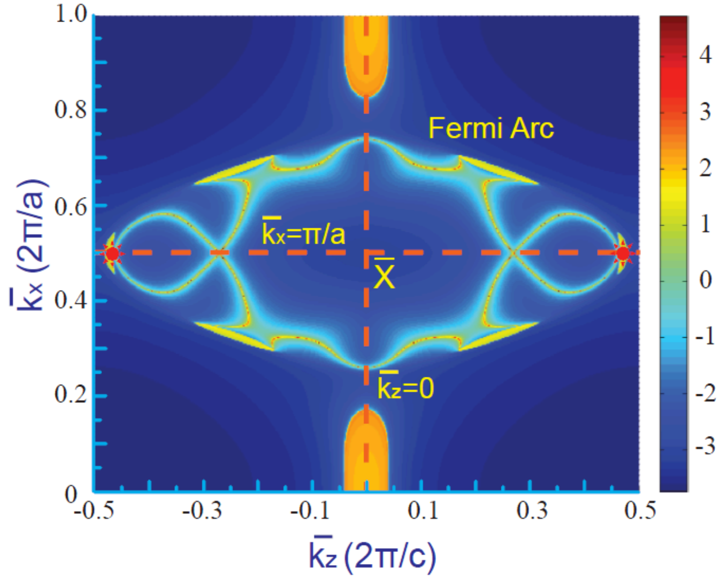


Results: With SOC and m//(001)

a Eigenvalue of S_z symmetry along XU

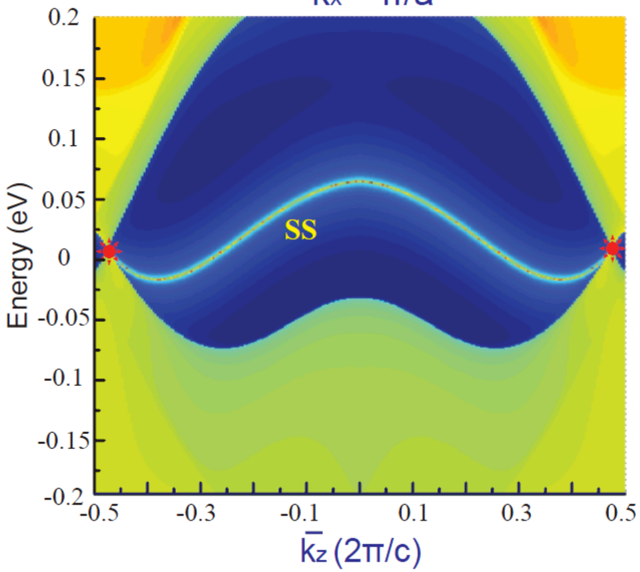


b Side surface states @ (010):

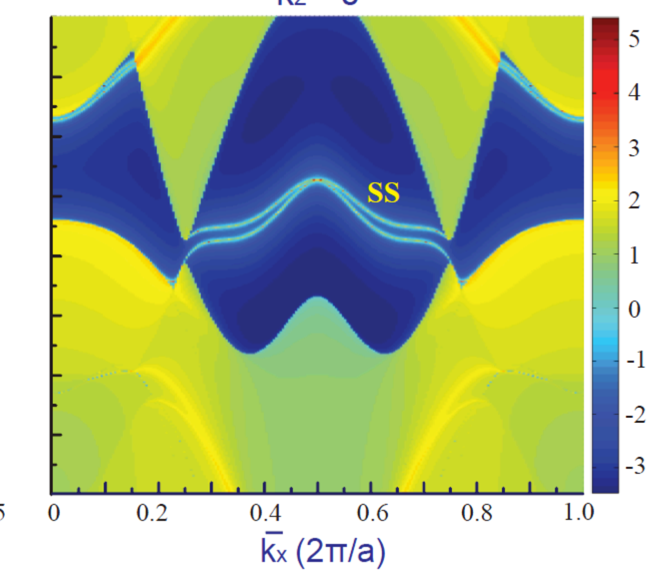


Side surface bands @ (010):

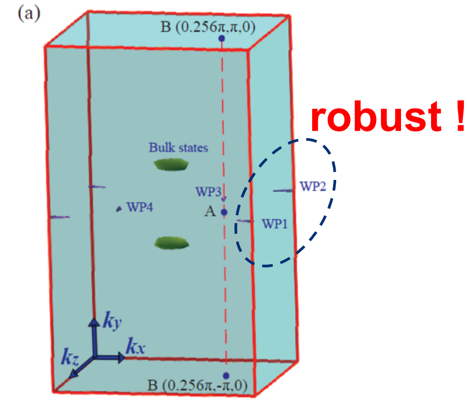
c $\bar{k}_x = \pi/a$



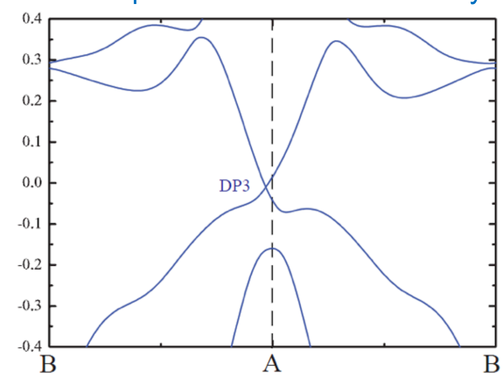
d $\bar{k}_z = 0$



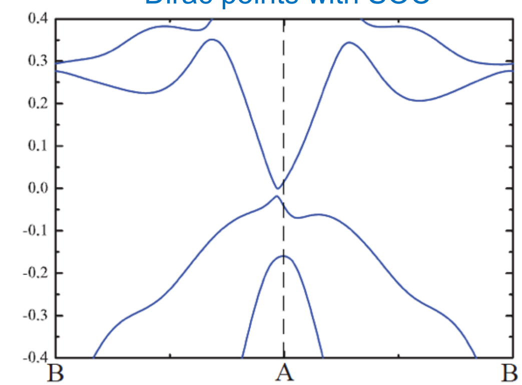
3D Fermi surface without SOC



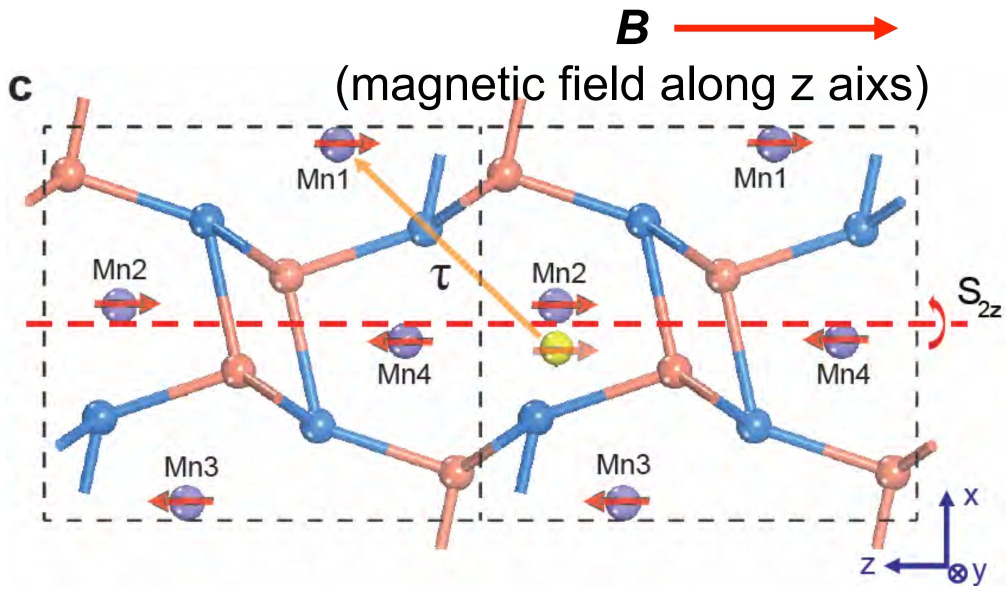
Dirac points without SOC and Ry



Dirac points with SOC

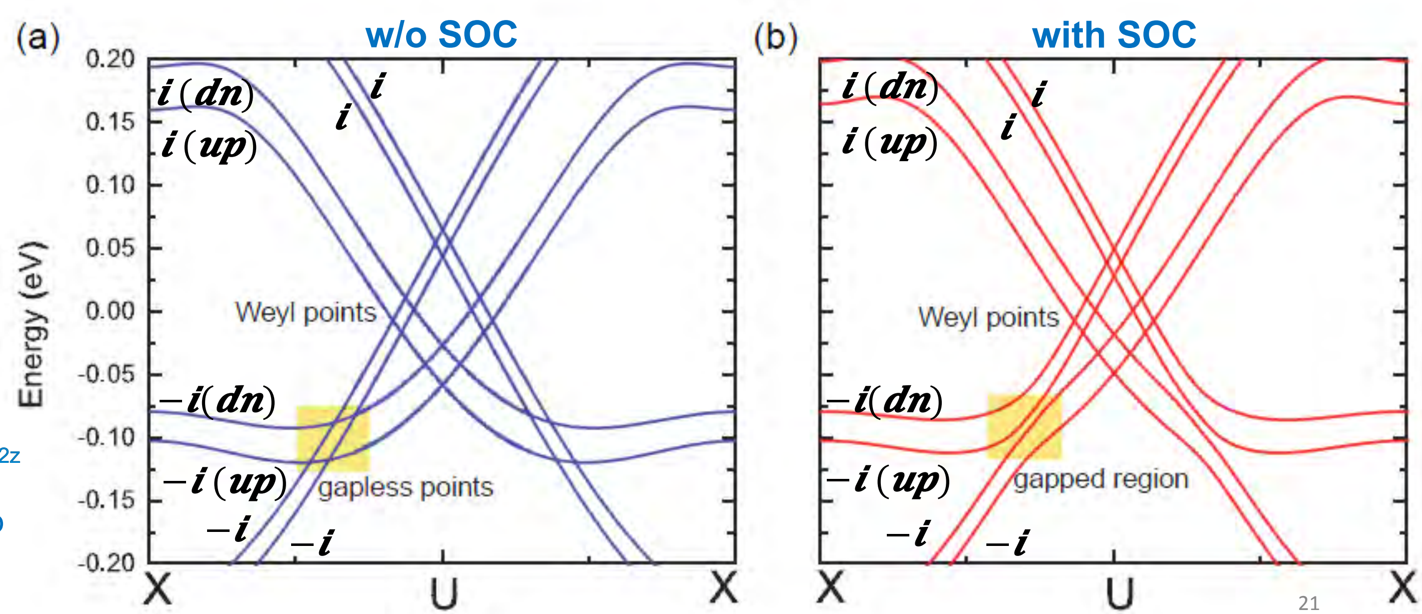


Spin flop Effect in AFM CuMnAs



- Applying ***B*** along z axis will not break S_{2z} symmetry.
- PT symmetry breaking will induce Zeeman Splitting
- The "coupled Weyl points" will split to four Weyl points.

$$\mu\downarrow(Mn1/2) \neq \mu\downarrow(Mn3/4)$$

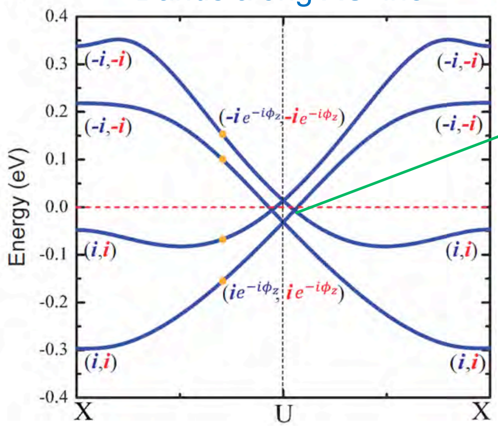


$\pm i$ is the eigenvalue of S_{2z} symmetry. The red and blue stand for the spin-up and spin-down states.

Results: With SOC and m//(001)

a

Bands along XU line



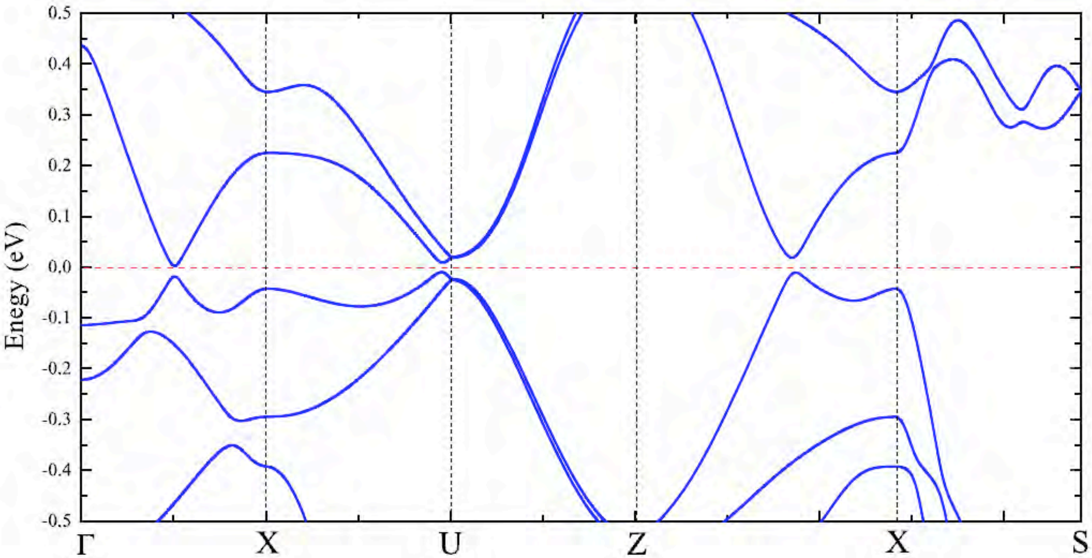
$$\mathcal{H} = \mathcal{H}_{Dirac} + (\delta_1 k_x + \delta_2 k_y)\tau_y\sigma_x + (\delta_3 k_x + \delta_4 k_y)\tau_y\sigma_y,$$

Spin-flip process: SOC

When SOC is considered, the crossing points protected by S_z symmetry are not a Dirac Fermion. They are "*coupled Weyl fermions*".

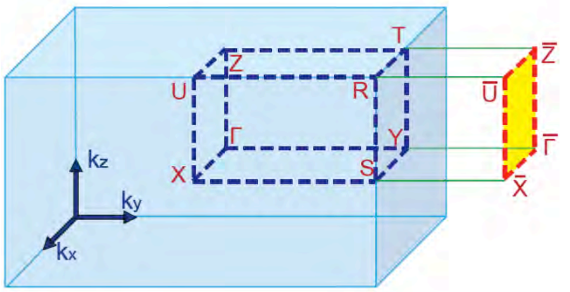
Results: With SOC and m//(111)

3D electronic structures:



R_y symmetry is broken.
S_z symmetry is also broken.

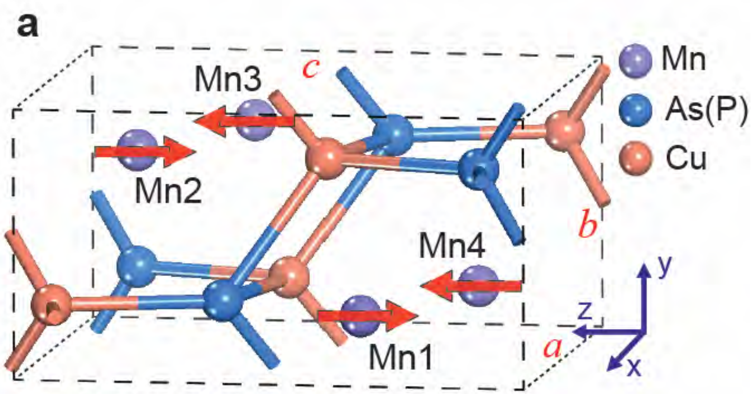
b



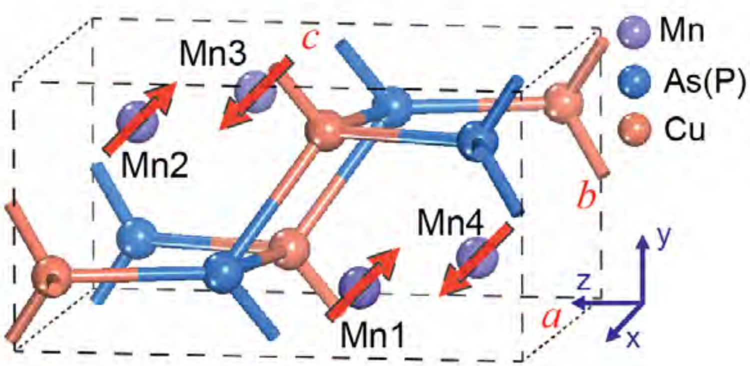
Fully gapped without the Dirac Nodal line and Dirac points.

Magnetic anisotropy in AFM CuMnAs

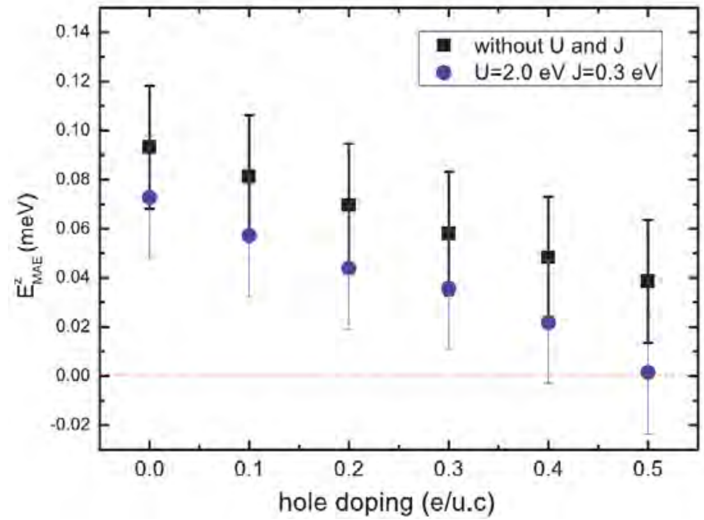
m along *z* direction;



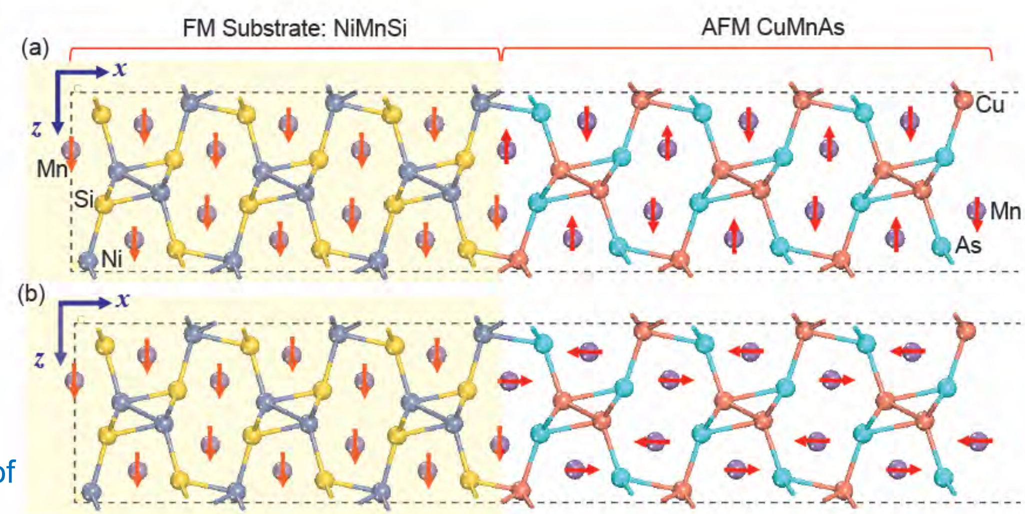
m along *x* direction;



MAE per Mn atom



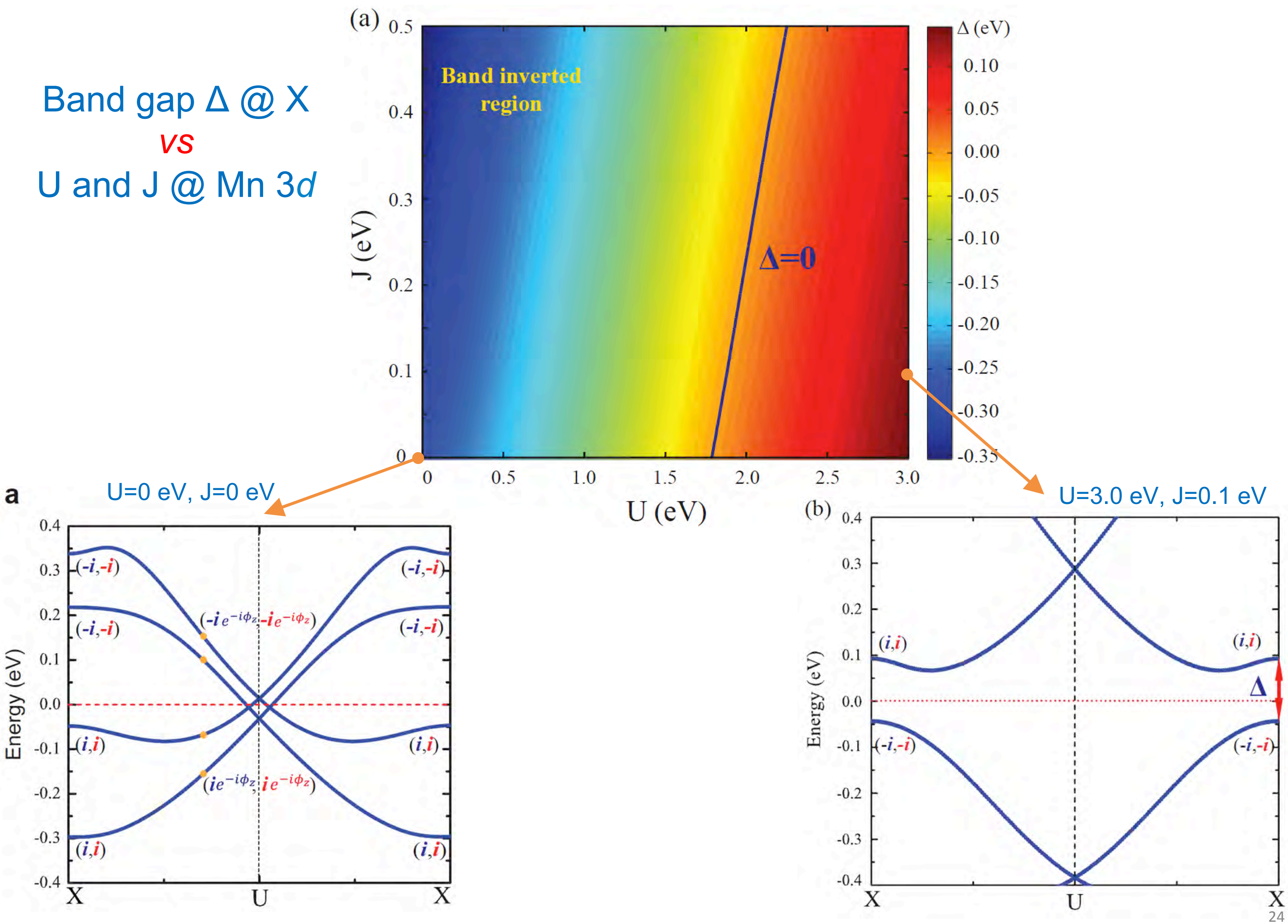
Exchange anisotropy to stabilize ***m*** along *z* direction.



Magnetic easy axis favors along *z* direction with MAE of 7.1 meV per Mn atom.

Results: Electronic structure with interactions

Band gap Δ @ X
vs
U and J @ Mn 3*d*

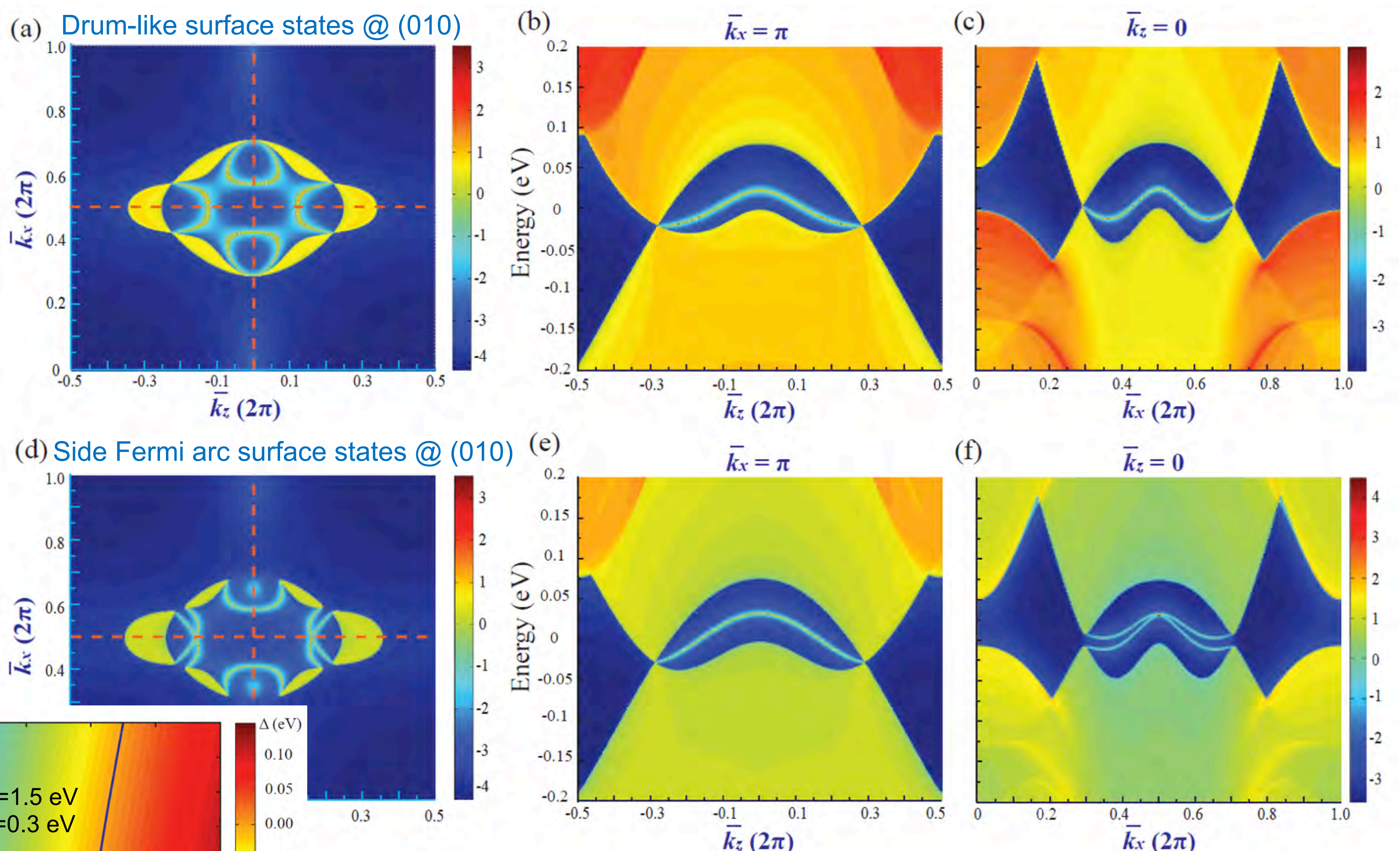


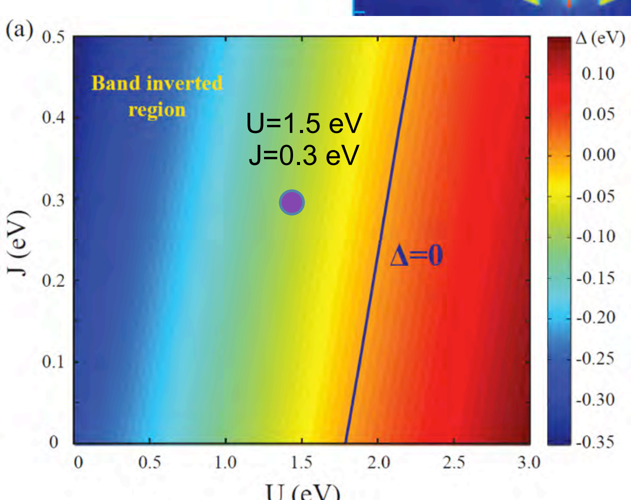
Results: Electronic structure with interactions

Side surface states

No SOC
Keep R_y

With SOC
$\vec{m}$//(001)

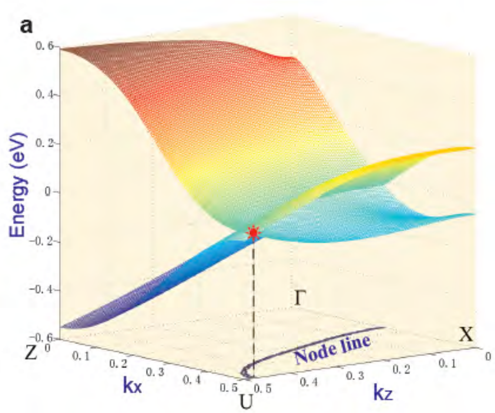


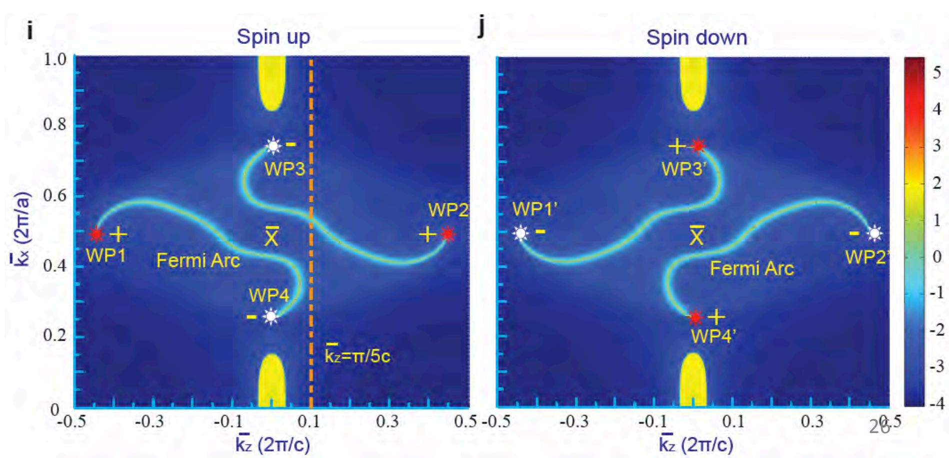


If the band inversion for the symmetry of S_z and R_y occurs, the Dirac nodal line, Dirac fermion and the coupled Weyl fermions are robust.

Summary:

- Develop a general argument for AFM Dirac semi-metal.
- Predict that orthorhombic AFM CuMnAs(P) are topological semi-metal.
  - Dirac Nodal line --- Drum-like surface states (without SOC && Keep R_y)
  - Dirac semi-metal --- Fermi arc (without SOC && Keep S_z)
  - Coupled Weyl Fermions (with SOC && Keep S_z)
  - Semi-metal without band crossing (without SOC && Break S_z)





Thank you very much