

## Topology and symmetry in topological semimetals: tutorial

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(a) Weyl semimetal



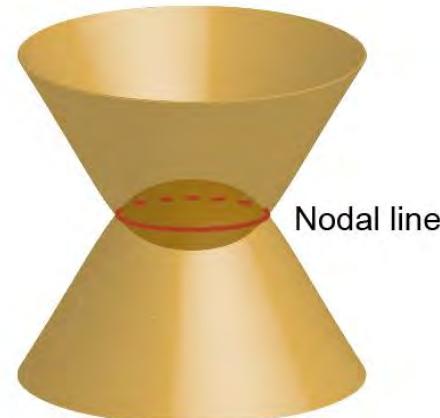
No Kramers degeneracy

(b) Dirac semimetal



Kramers degeneracy

(c) Nodal-line semimetal



Nodal line

## Various topological phases in electronic systems

(1) Bulk is an insulator: “topological insulator” in a broader sense

(1-1) Integer quantum Hall system (Chern insulator)

(1-2) topological insulator

(1-3) topological crystalline insulator

.....

(2) Bulk is a metal: topological metal (topological semimetal)

(2-1) Dirac semimetal

(2-2) Weyl semimetal

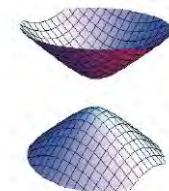
(2-3) nodal-line semimetal

.....

## (2) Bulk is a metal: topological metal (topological semimetal)

Band degeneracy occurs

- at high-symmetry points/lines
- At other general points, bands usually **anticross**.



→ Nevertheless, in some cases, anticrossing does not happen, and band degeneracy occurs at general  $k$  points  
= **topological metal (topological semimetal)**

Weyl semimetal:



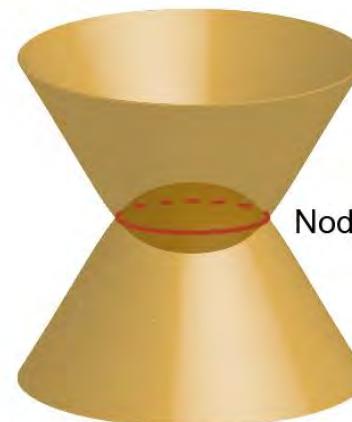
No Kramers degeneracy

Dirac semimetal:



Kramers degeneracy

Nodal-line semimetal:



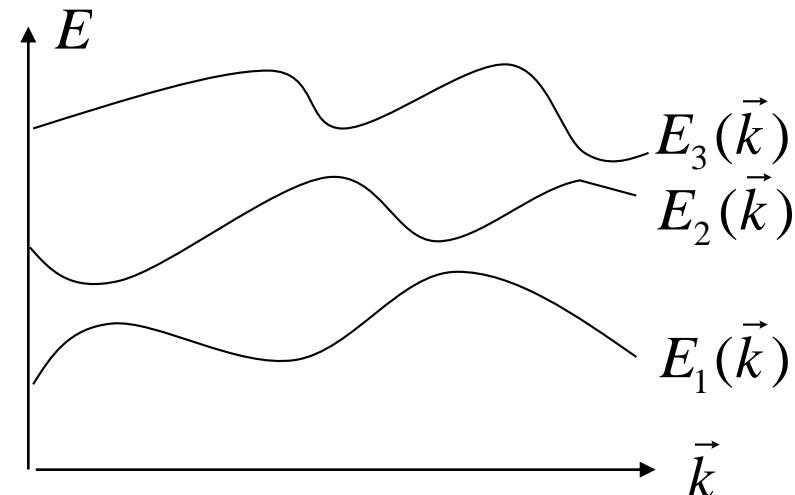
Nodal line

# Degeneracies in electronic states in crystals

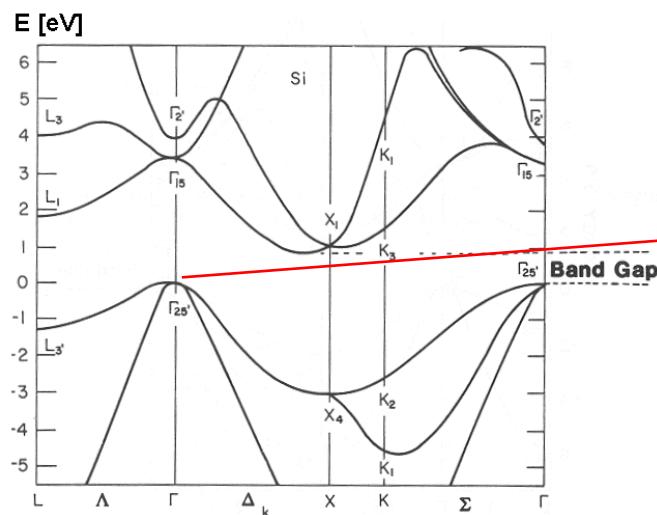
$$H(\vec{k}) \rightarrow E_1(\vec{k}), E_2(\vec{k}), E_3(\vec{k}), \dots$$

- When do degeneracies appear?
- What conditions are required?

$$E_n(\vec{k}) = E_m(\vec{k})$$



Case 1: symmetry: High-dimensional irreducible representation of a little group



At high-symmetry points/lines, there might be degeneracies due to symmetry

# Degeneracies in electronic states in crystals

Case 2: topology    “accidental degeneracy”

Wigner, Herring , Volovik, Murakami, ....

Simple example: general 2\*2 Hamiltonian in k space

$$H(\vec{k}) = \begin{pmatrix} a(\vec{k}) & b(\vec{k}) \\ b^*(\vec{k}) & c(\vec{k}) \end{pmatrix} \quad \begin{array}{ll} a(\vec{k}), c(\vec{k}) & : \text{real} \\ b(\vec{k}) & : \text{complex} \end{array}$$

$$\rightarrow E(\vec{k}) = \frac{a+c}{2} \pm \sqrt{\left(\frac{a-c}{2}\right)^2 + |b|^2}$$

Degeneracy appears when  $\begin{cases} a(\vec{k}) = c(\vec{k}) \\ \operatorname{Re} b(\vec{k}) = 0 \\ \operatorname{Im} b(\vec{k}) = 0 \end{cases}$

In 3D k space: they may have solutions

In 2D k space: they have no solutions (unless there are additional constraints)

**Dimensionality matters !**

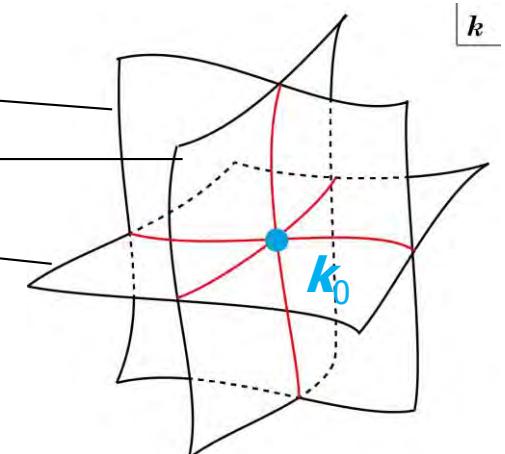
# Degeneracies in electronic states in crystals

## Case 2: topology

$$H(\vec{k}) = \begin{pmatrix} a(\vec{k}) & b(\vec{k}) \\ b^*(\vec{k}) & c(\vec{k}) \end{pmatrix} \rightarrow E(\vec{k}) = \frac{a+c}{2} \pm \sqrt{\left(\frac{a-c}{2}\right)^2 + |b|^2}$$

Degeneracy appears when

$$\begin{cases} a(\vec{k}) = c(\vec{k}) \\ \text{Re } b(\vec{k}) = 0 \\ \text{Im } b(\vec{k}) = 0 \end{cases}$$



In 3D k space: they may have solutions:  
isolated points in k space:  $\mathbf{k}=\mathbf{k}_0$

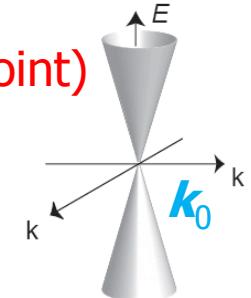
Apart from this degeneracy point at  $\mathbf{k}_0$ ,

energy separation between two bands is linear in wavevector  
= forming a Dirac cone

$\mathbf{k}=\mathbf{k}_0$  : Weyl node (: not necessarily at high-symmetry point)

Note: this Weyl node cannot be removed perturbatively !  
i.e. topologically stable

$$H(\vec{k}) \rightarrow H(\vec{k}) + \delta H(\vec{k})$$



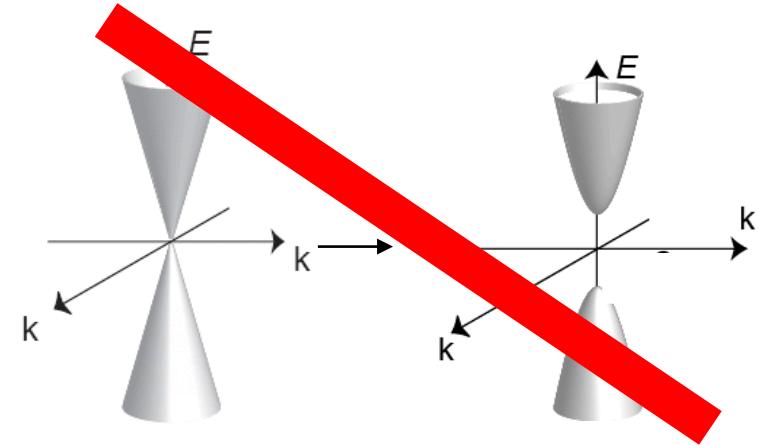
# Weyl nodes in 3D is topologically stable

3D Weyl node :

$$H(\vec{k}, m) = k_x \sigma_x + k_y \sigma_y + k_z \sigma_z + m \sigma_z$$

$$= k_x \sigma_x + k_y \sigma_y + k_z + m \sigma_z$$

Weyl point moves but **gap does not open**  
 $(0,0,0) \rightarrow (0,0,-m)$

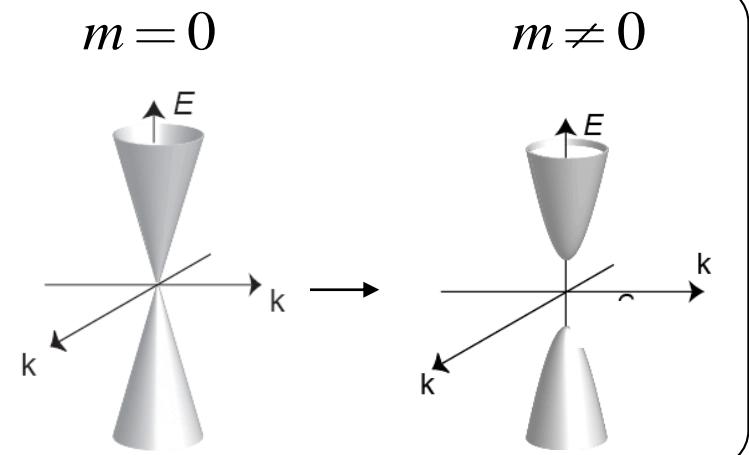


3D Weyl node is topological.

2D Weyl node :

$$H(\vec{k}, m) = k_x \sigma_x + k_y \sigma_y + m \sigma_z$$

parameter  $m$  **opens a gap.**



Apart from 2-band model:

How one can topologically characterize Weyl nodes?

**Berry curvature**

$$\vec{B}_n(\vec{k}) = i \left\langle \frac{\partial u_n}{\partial \vec{k}} \right| \times \left| \frac{\partial u_n}{\partial \vec{k}} \right\rangle$$

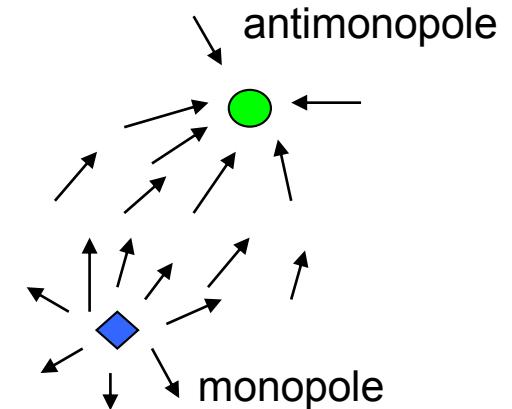
## Berry curvature in k space

### □ Berry curvature

$$\vec{B}_n(\vec{k}) = i \left\langle \frac{\partial u_n}{\partial \vec{k}} \right| \times \left| \frac{\partial u_n}{\partial \vec{k}} \right\rangle$$

$u_{n\vec{k}}$ : periodic part of the Bloch wf.

$$\psi_{n\vec{k}}(\vec{x}) = u_{n\vec{k}}(\vec{x}) e^{i\vec{k} \cdot \vec{x}} \quad (n : \text{band index})$$



### □ Monopole density

: “magnetic field in k-space”

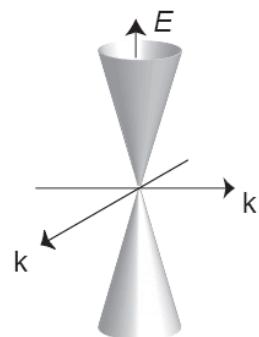
$$\rho_n(\vec{k}) = \frac{1}{2\pi} \nabla_{\vec{k}} \cdot \vec{B}_n(\vec{k})$$

Quantization of monopole charge

$$\rho_n(\vec{k}) = \sum_i q_i \delta(\vec{k} - \vec{k}_i) \quad q_i : \text{integer}$$

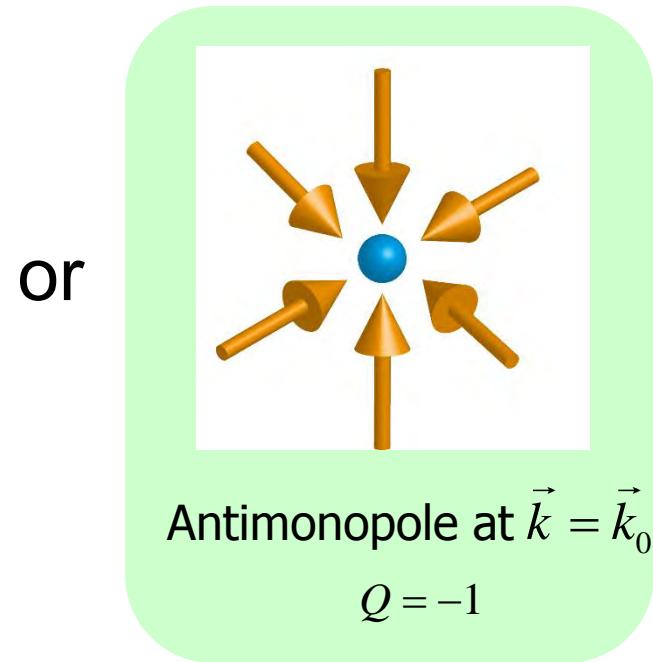
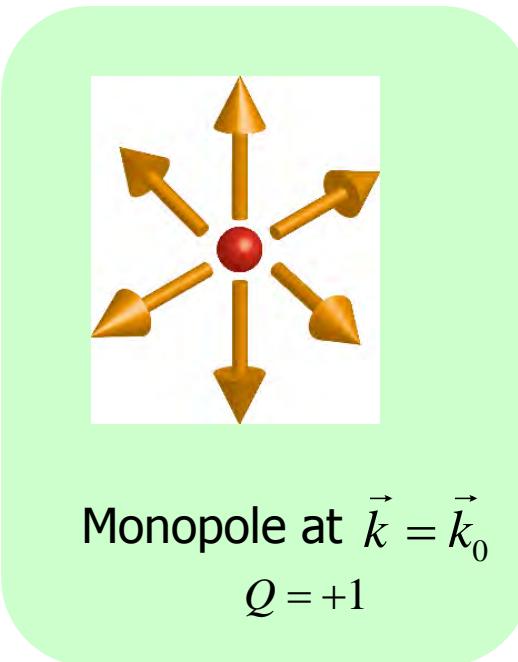
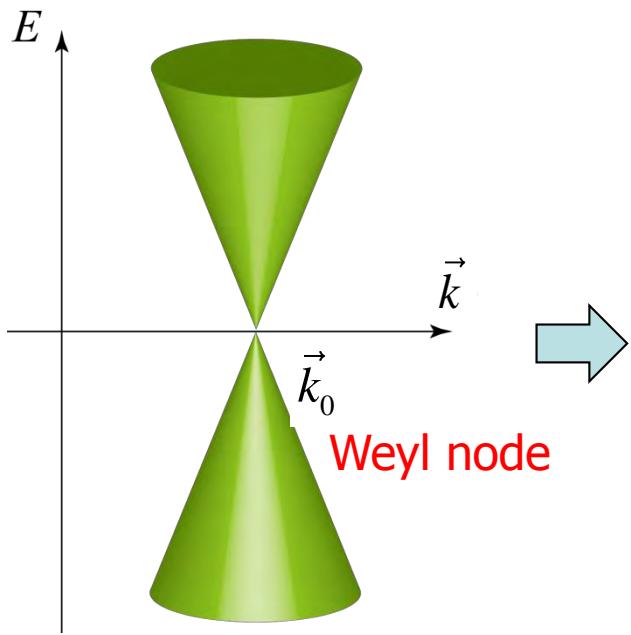


Position of  
Weyl node



# 3D Weyl nodes = monopole or antimonopole for Berry curvature

$$\begin{cases} B_n(\vec{k}) = i \left\langle \frac{\partial u_{nk}}{\partial k} \right| \times \left| \frac{\partial u_{nk}}{\partial k} \right\rangle & : \text{Berry curvature} \\ \rho_n(\vec{k}) = \frac{1}{2\pi} \nabla_{\vec{k}} \cdot \vec{B}_n(\vec{k}) & : \text{monopole density} \end{cases}$$



- Weyl nodes are either monopole or antimonopole
- Quantization of monopole charge  
→ Weyl nodes can be created only as a monopole-antimonopole pair

C. Herring, Phys. Rev. 52, 365 (1937).

G. E. Volovik, The Universe in a Helium Droplet (2007).

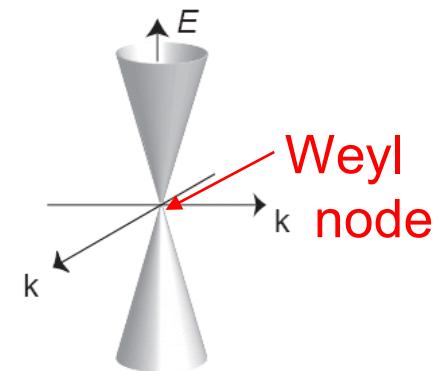
S. Murakami, New J. Phys. 9, 356 (2007).

## Weyl semimetal and Fermi arc

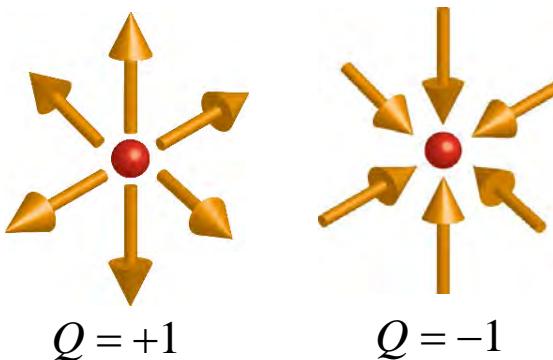
# Weyl semimetal

Murakami, New J Phys. (2007)  
Wan et al., Phys. Rev. B (2011)

= Bulk 3D Dirac cones **without** degeneracy at or around the Fermi energy



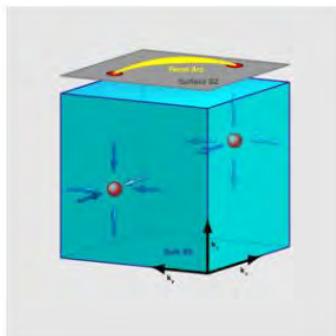
- Weyl nodes are either monopole or antimonopole for Berry curvature



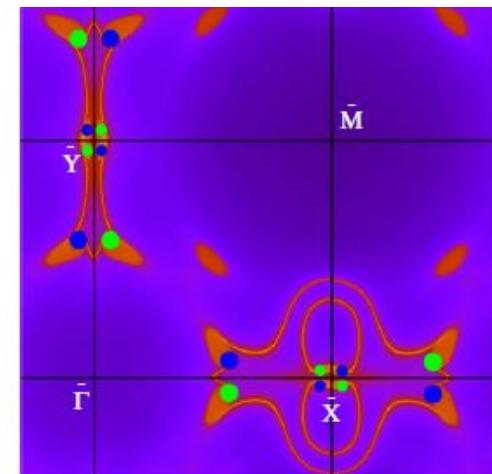
$$B_n(\vec{k}) = i \left\langle \frac{\partial u_{nk}}{\partial k} \right\rangle \times \left\langle \frac{\partial u_{nk}}{\partial k} \right\rangle$$

$$\rho_n(\vec{k}) = \frac{1}{2\pi} \nabla_{\vec{k}} \cdot \vec{B}_n(\vec{k})$$

- Surface Fermi arc
  - connecting between Weyl nodes



TaAs surface Fermi arc  
(Xu et al., Lv et al., Yang et al. '15)



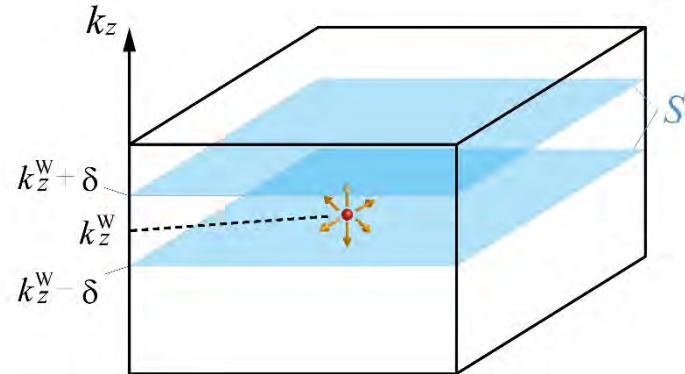
## 3D system with Weyl node

Even in 3D, one can consider the plane,  $k_z=\text{const.}$ , to be a 2D system and consider its Chern number.

$$Ch_{(n)}(k_z) = \frac{1}{2\pi} \int_{k_z=\text{const}} \vec{B}(\vec{k}) \cdot \vec{n} dS$$

This Chern number depends on  $k_z$

When a monopole (Weyl node with  $Q=1$ ) is at  $k_z^W$  the Chern number jumps by +1



E.g.  $\begin{cases} Ch_{(n)}(k_z^W - \delta) = 0 \\ Ch_{(n)}(k_z^W + \delta) = 1 \end{cases}$ , chiral surface states exist not at  $k_z < k_z^W$

but at  $k_z > k_z^W$

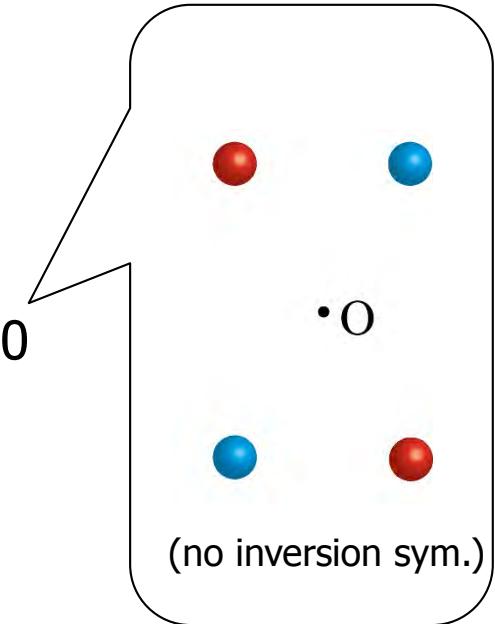
→ Surface states starting from the Weyl node projection = **Fermi arc**

Wan et al. (2011)

## Symmetry and monopole density

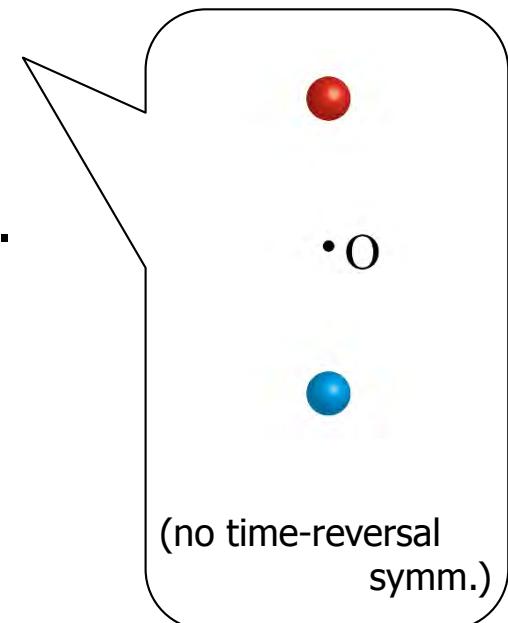
- Time-reversal symmetry

→ Monopoles distribute symmetrically w.r.t.  $k=0$



- Inversion symmetry

→ Monopoles distribute antisymmetrically  
with respect to  $k=0$



- Total monopole charge in the whole BZ vanishes.

- Inversion + Time-reversal

→ monopoles do not exist

→ Weyl semimetal cannot be realized  
(Dirac semimetal is possible)

# Topological metals with bulk Dirac cones

Dirac semimetals =

bulk 3D Dirac cone with Kramers degeneracy

Both inversion- or time-reversal symmetry are required

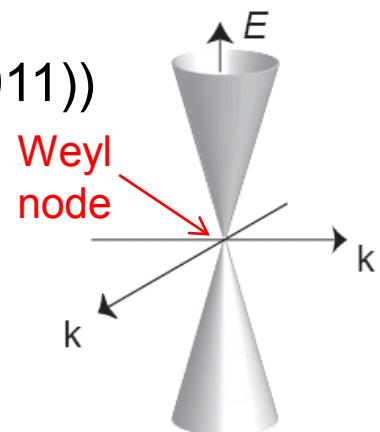
- $\beta\text{-BiO}_2$  (Young et al., (2011))
- $A_3\text{Bi}$  ( $A = \text{Na, K, Rb}$ ) (Wang et al., (2011))
- $\text{Cd}_3\text{As}_2$  (Wang et al., (2012))
- NI/TI multilayer (Burkov, Balents)

Weyl semimetals=

bulk 3D Dirac cone without Kramers degeneracy

Either inversion- or time-reversal symmetry should be broken

- pyrochlore iridates  
(Wan et al., PRB (2011), Yang et al., PRB(2011))
- NI/TI multilayer (Burkov, Balents)
- TaAs
- YbMnBi<sub>2</sub> ...



# Effective model : insulator – Weyl semimetal

Okugawa, Murakami, Phys. Rev. B 89, 235315 (2014)

$$H = \gamma(k_x^2 - m)\sigma_x + v(k_y\sigma_y + k_z\sigma_z)$$

## Bulk dispersion

$$E = \pm \sqrt{\gamma^2(k_x^2 - m)^2 + v^2k_y^2 + v^2k_z^2}$$

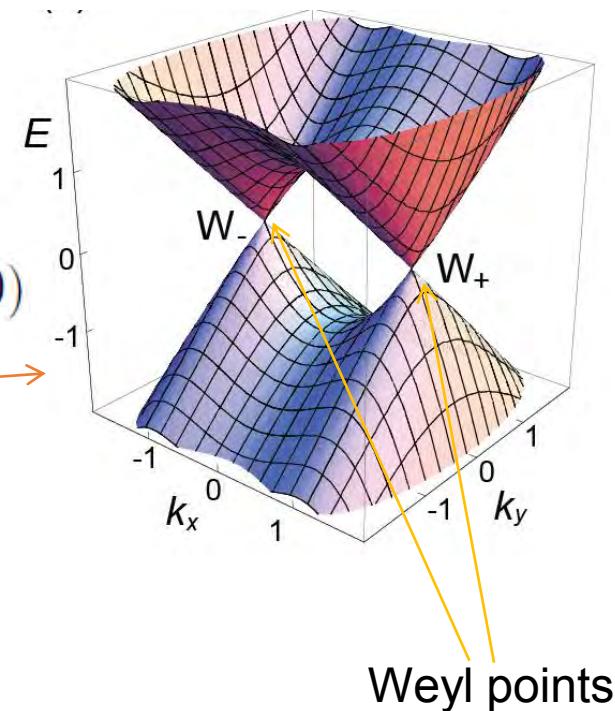
$m < 0$ : bulk gap =  $2\gamma|m|$

= topological or normal insulator

$m > 0$ : bulk is gapless

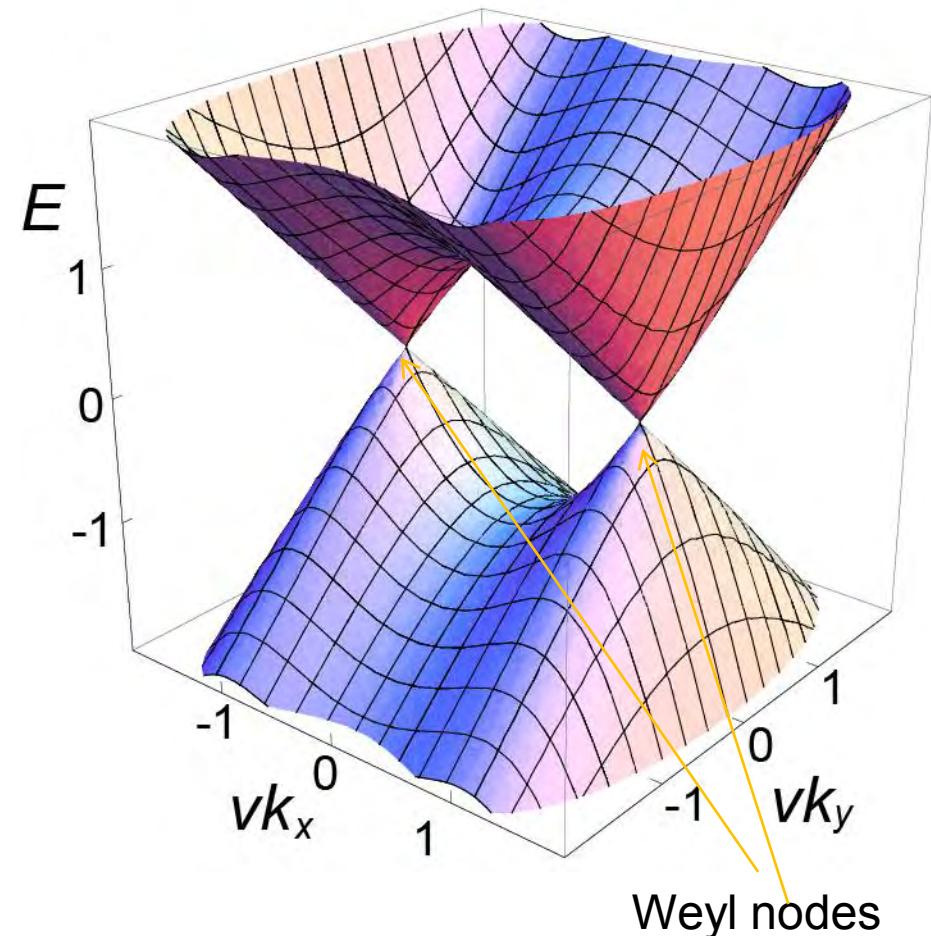
gap closed at  $\mathbf{W}_\pm$ :  $\mathbf{k} = (\pm\sqrt{m}, 0, 0)$

= Weyl semimetal

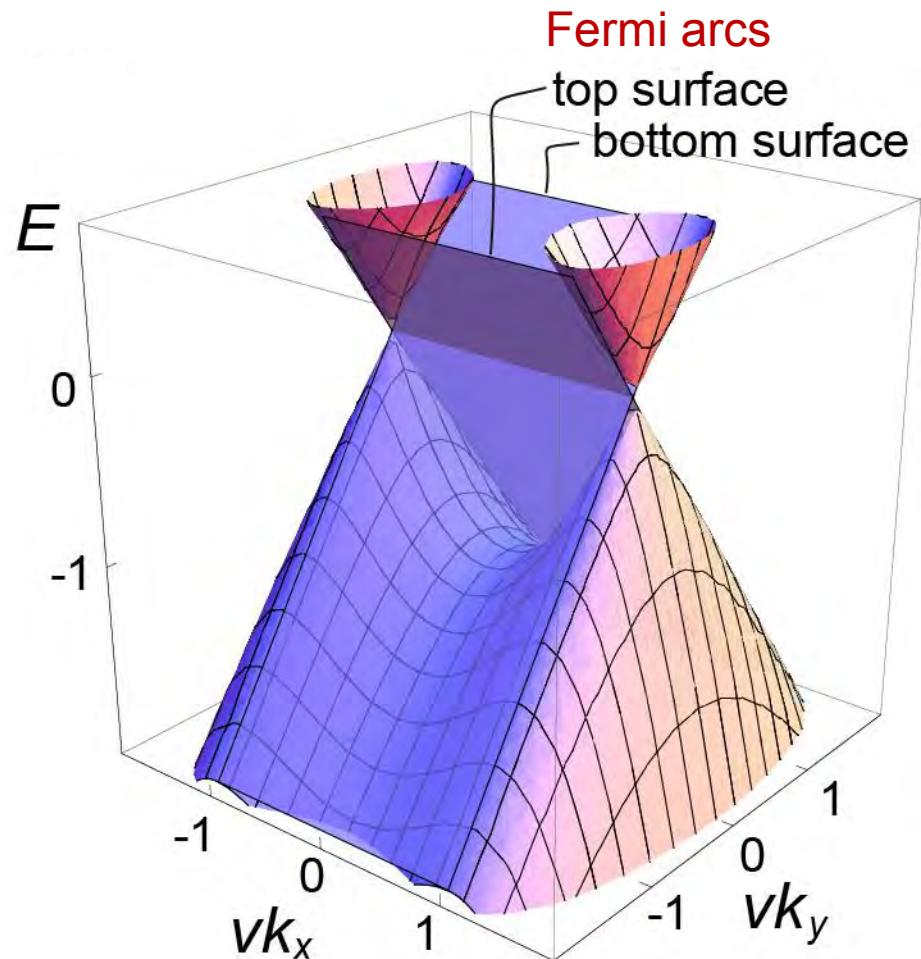


## Surface Fermi arc : effective model calc.

Bulk band structure



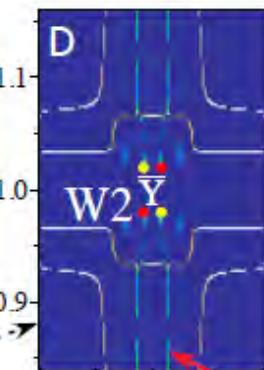
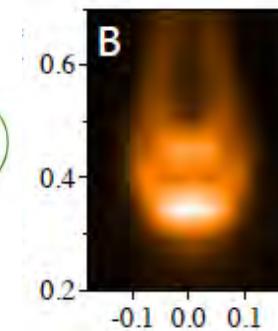
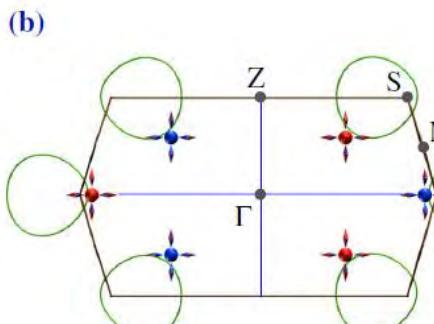
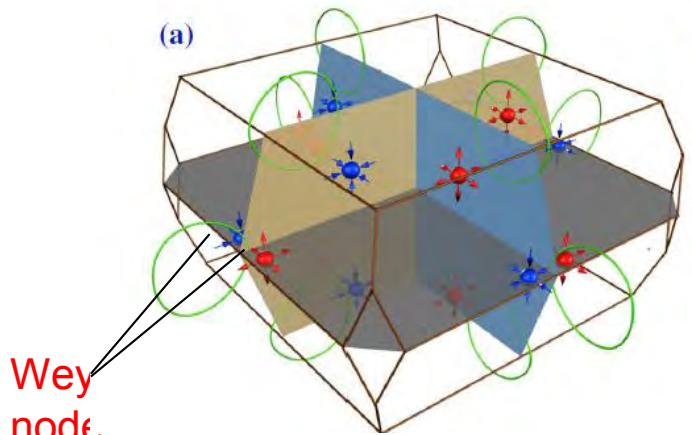
Bulk + surface



Okugawa, Murakami, Phys. Rev. B 89  
235315 (2014)

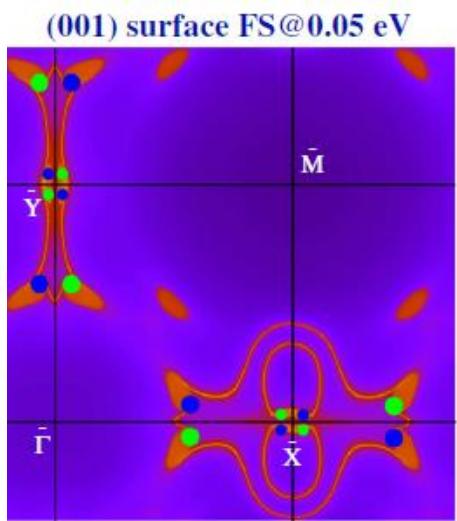
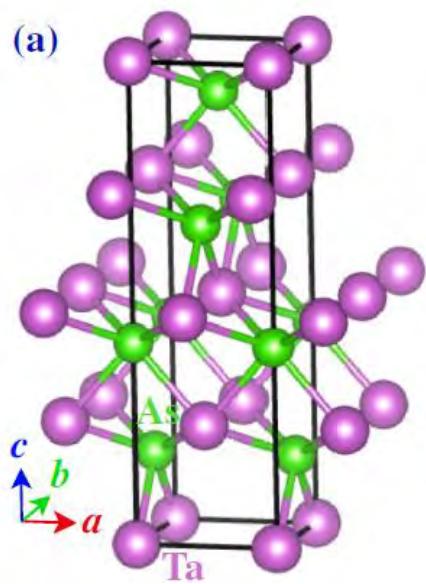
# Weyl semimetal TaAs

Lv et al., Xu et al. (2015):

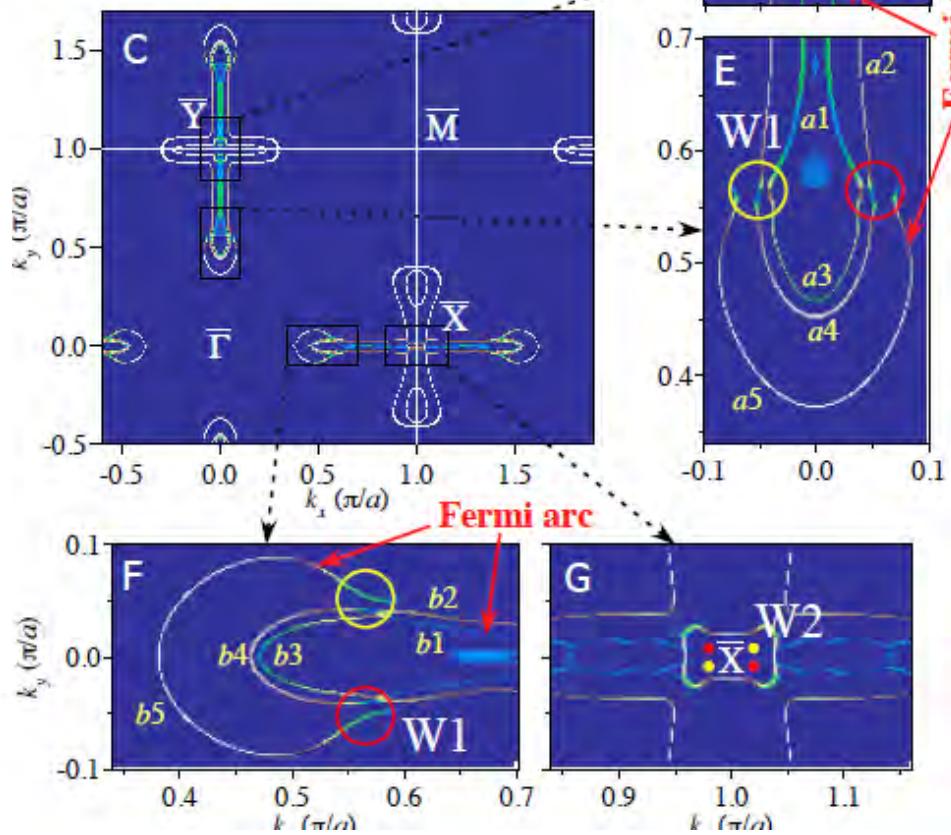


Wey  
nodes

Weng et al., PRX (2015): theory



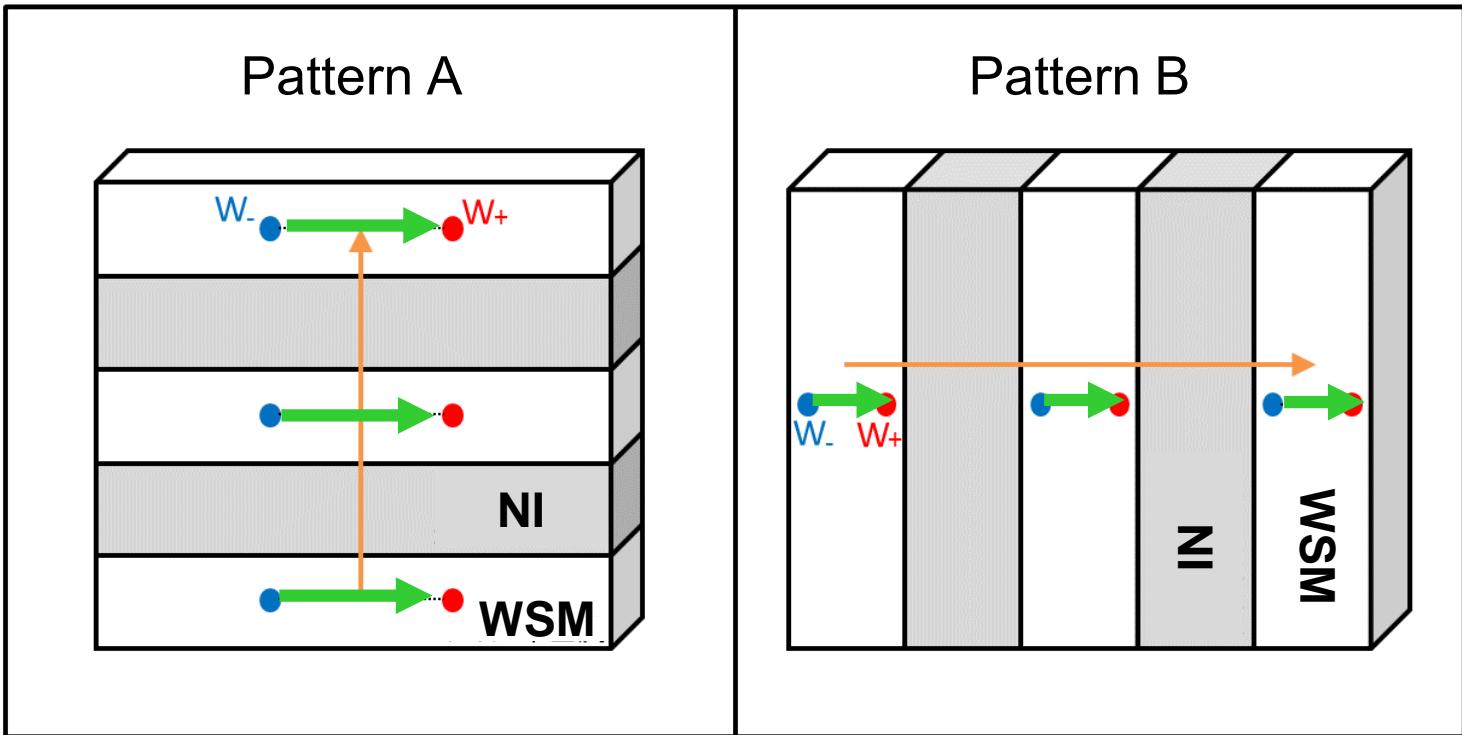
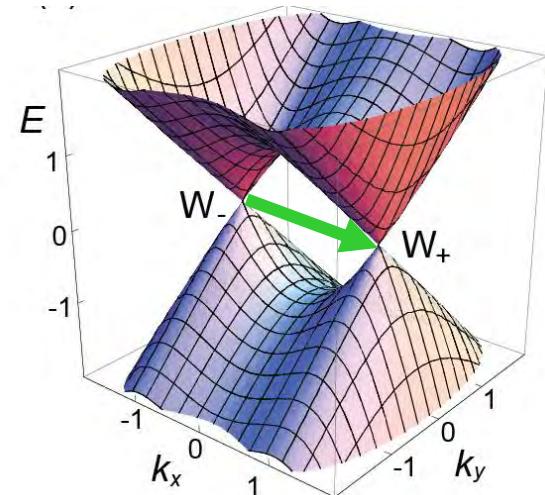
Fermi arc



# Multilayers of a Weyl semimetal and a normal insulator

K. Yokomizo and S. Murakami

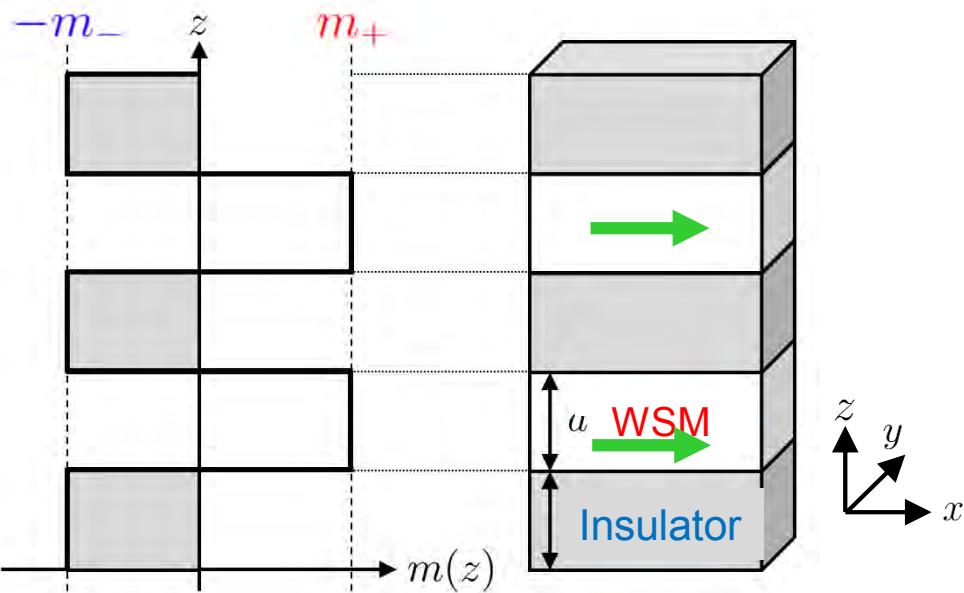
Phys. Rev. B 95, 155101 (2017)



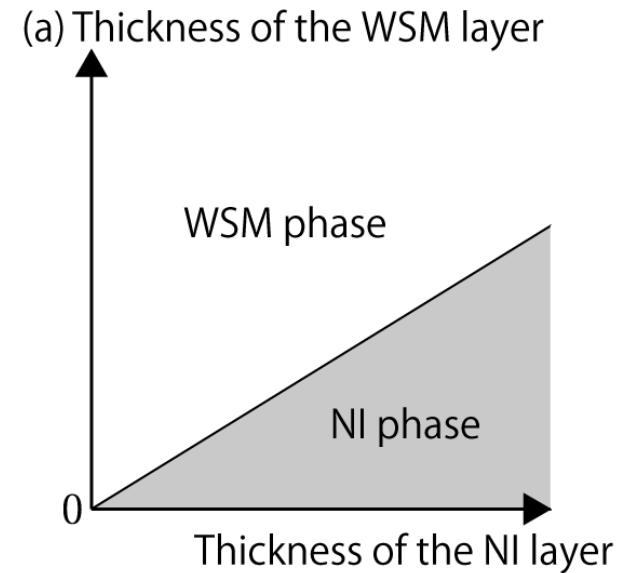
# Multilayer (Pattern A)

$$H = \gamma (k_x^2 - m(z)) \sigma_x + v (k_y \sigma_y - i \partial_z \sigma_z)$$

Spatial modulation



Phase diagram of the multilayer



The multilayer becomes the WSM phase  
by increasing the thickness of the WSM layer

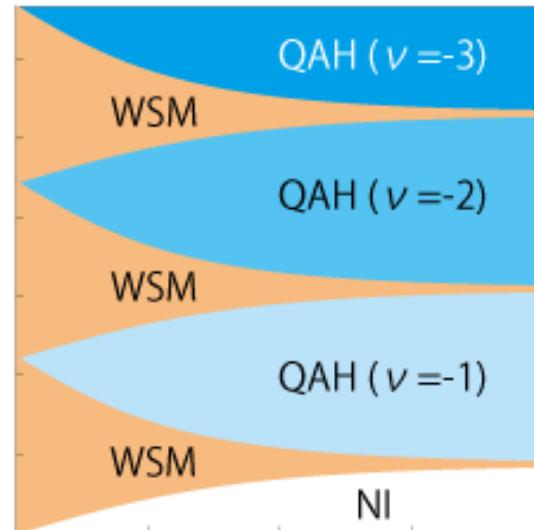
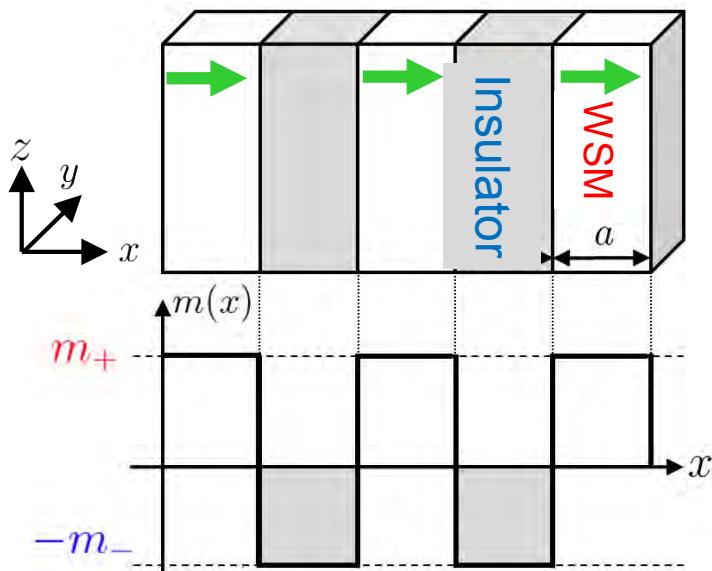
# Multilayer (Pattern B)

Phase diagram of the multilayer

Hamiltonian

$$H = \gamma \left( -\partial_x^2 - \underline{m(x)} \right) \sigma_x + v (k_y \sigma_y + k_z \sigma_z)$$

Spatial modulation



Thickness of the WSM layer

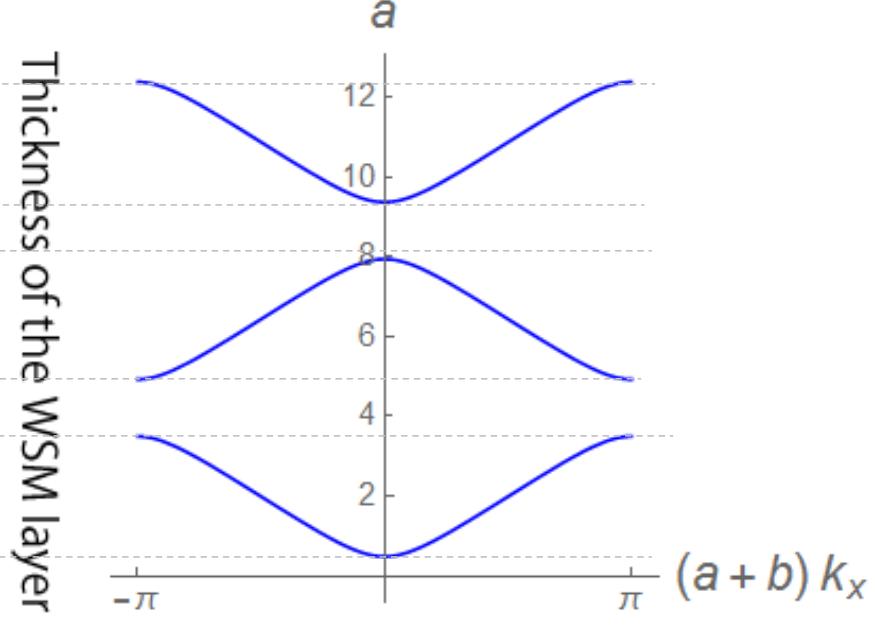
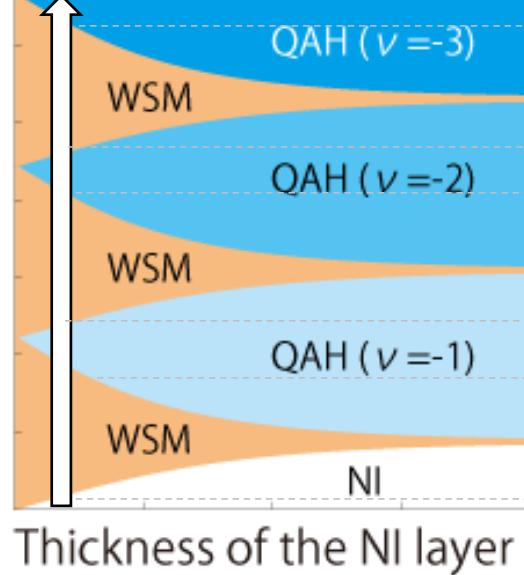
Thickness of the NI layer

- (1) WSM phases periodically emerge
- (2) Quantum anomalous Hall (QAH) phases which have different Chern number periodically emerge

# Trajectory of the Weyl nodes in multilayer (Pattern B)

thickness of the WSM layer: increase

thickness of the NI layer: const

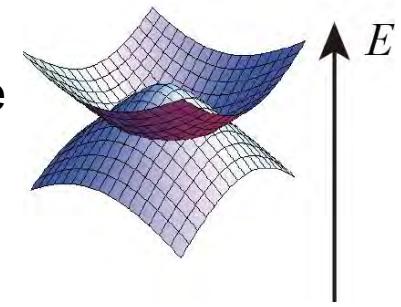


K. Yokomizo and S. Murakami

Phys. Rev. B 95, 155101 (2017)

Nodal-line semimetal

Nodal-line semimetal: bulk gap closes along a loop in k space



## 2 typical mechanisms

### (i) Mirror symmetric system:

Mirror eigenvalues are different

between the valence and the conduction bands

$$\begin{cases} \text{spinless (SOC=0)} & M = \pm 1 \\ \text{spinful (nonzero SOC)} & M = \pm i \end{cases}$$

→ No anticrossing between the two bands  
(← prohibited hybridization)

→ **Nodal line on a mirror plane**

#### Dirac line node

- Carbon allotropes
- Cu<sub>3</sub>PdN
- Ca<sub>3</sub>P<sub>2</sub>
- LaN
- CaAgX (X=P,As)

#### Weyl line node

- HgCr<sub>2</sub>Se<sub>4</sub>
- TiTaSe<sub>2</sub>

## 2 typical mechanisms

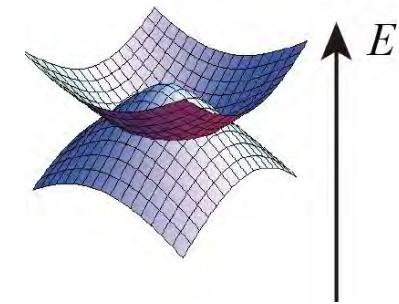
### (ii) Spinless (SOC=0) & time-reversal sym. & inversion symm.

topological nodal line at generic position in k space

(Example)

$$H(\vec{k}) = \begin{pmatrix} a(\vec{k}) & b(\vec{k}) \\ b^*(\vec{k}) & c(\vec{k}) \end{pmatrix}$$

$a(\vec{k}), c(\vec{k})$  : real  
 $b(\vec{k})$  : complex



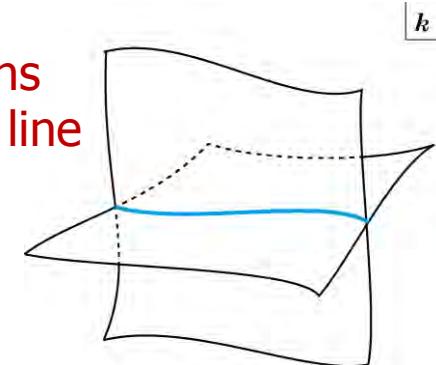
With the above 3 conditions  $\rightarrow$  Hamiltonian is a **real** matrix.

$b(\vec{k})$  : real

Degeneracy appears when

$$\begin{cases} a(\vec{k}) = c(\vec{k}) \\ \text{Re } b(\vec{k}) = 0 \end{cases}$$

2 conditions  
 $\rightarrow$  nodal line

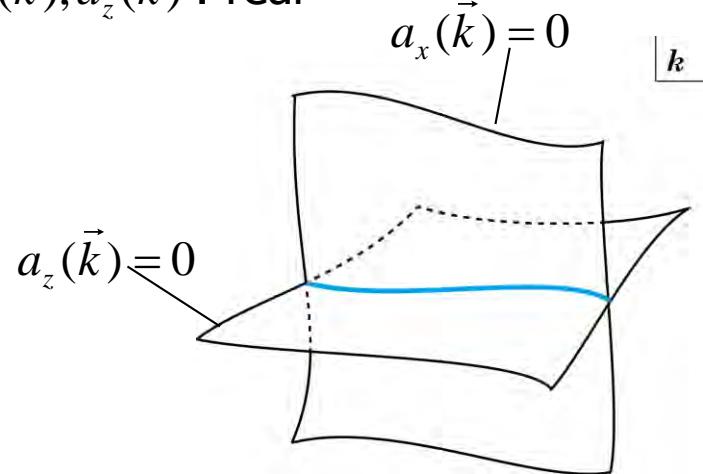


Topological characterization:  
 $\pi$  Berry phase around the nodal line

(Example)

Rewrite the matrix in terms of Pauli matrices. Omit the trace part.

$$H(\vec{k}) = \begin{pmatrix} a_z(\vec{k}) & a_x(\vec{k}) \\ a_x(\vec{k}) & -a_z(\vec{k}) \end{pmatrix} \quad a_x(\vec{k}), a_z(\vec{k}) : \text{real}$$



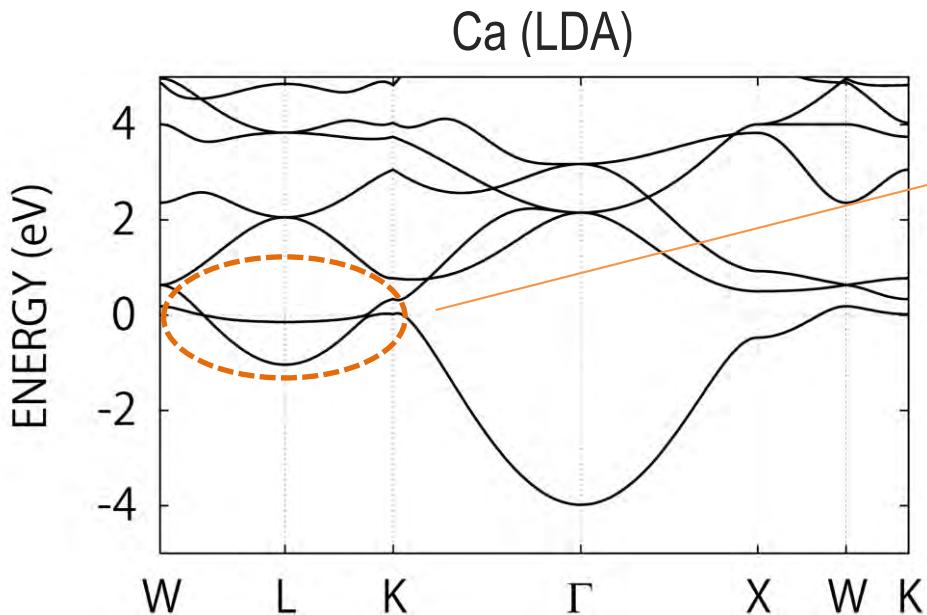
Phase of  $z(\vec{k}) \equiv a_x(\vec{k}) + ia_z(\vec{k})$  winds by  $2\pi$  around the nodal line.  
 → Nodal line is topological

In general systems, the nodal line is characterized by  $\pi$  Berry phase.

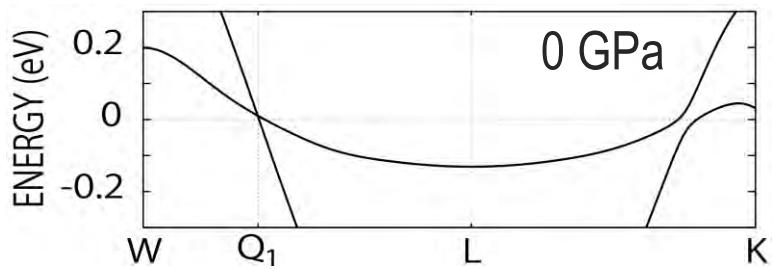
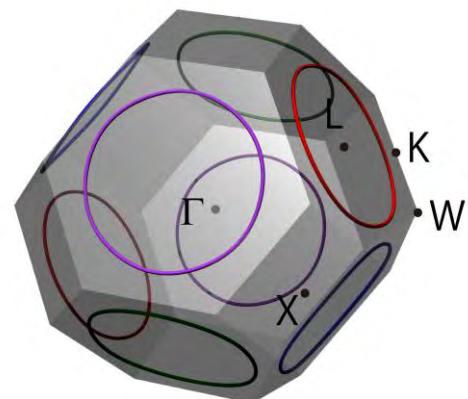
$$\phi = -i \oint_C d\vec{k} \cdot \left\langle u_n(\vec{k}) \left| \frac{\partial}{\partial \vec{k}} \right| u_n(\vec{k}) \right\rangle = \pi$$

# Ca have nodal lines near $E_F$

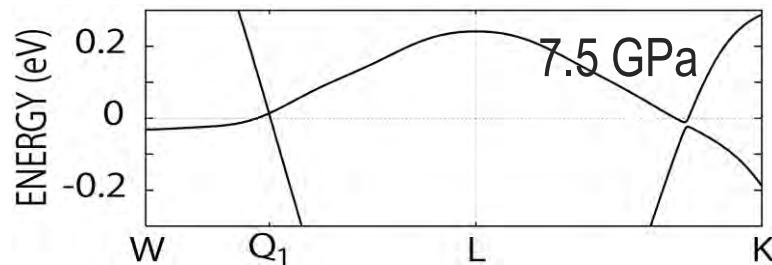
Hirayama, Okugawa, Miyake, Murakami  
Nat. Commun.8, 14022 (2017)



Nodal line around Fermi energy



Not semimetal at 0 GPa



Nodal line semimetal at 7.5GPa

(cf.) previous works

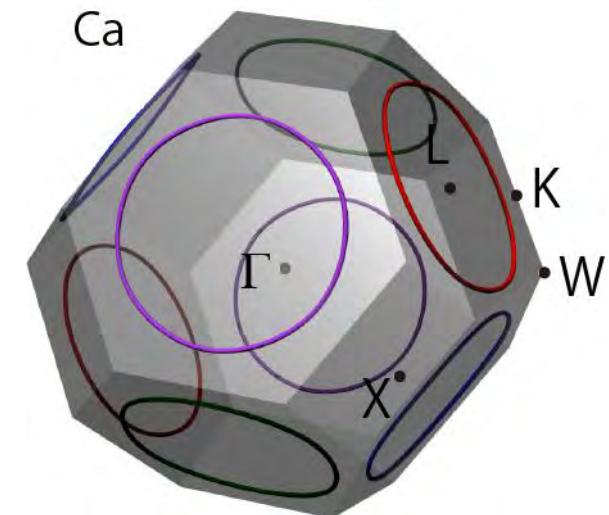
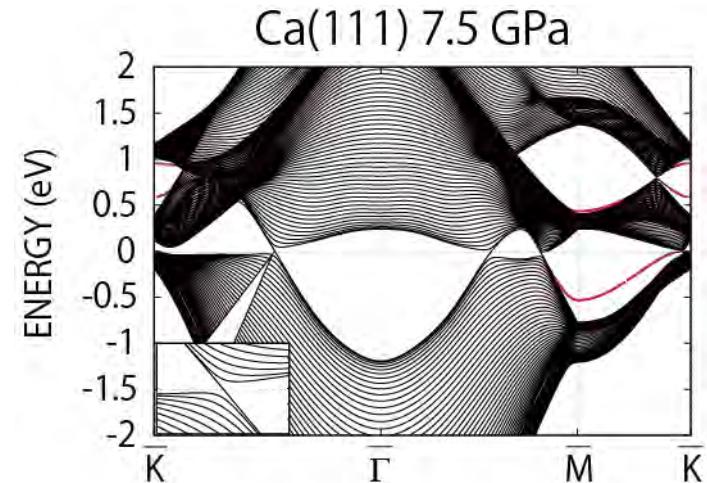
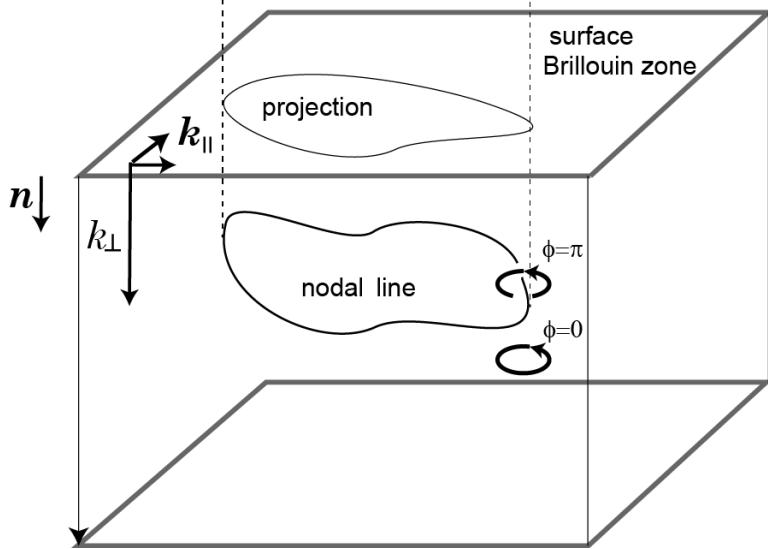
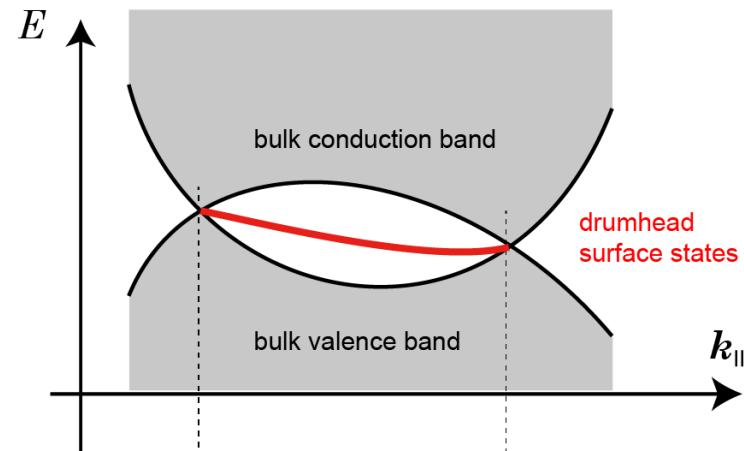
Vasvari, Animalu, Heine, Phys. Rev. 154, 535 (1967).

Vasvari, Heine, Phil. Mag. 15, 731–738 (1967).

# nodal-line semimetal : drumhead surface states

Surface state often appears within the region surrounded by the nodal line

- Similar to the flat-band edge states in graphene zigzag ribbon.



# Nodal-line and Zak phase

Zak phase (Berry phase) for a given  $\vec{k}_{\parallel}$  (= surface wavevector)

$$\theta(k_{\parallel}) = -i \sum_n^{\text{occ.}} \int_0^{2\pi/a_{\perp}} dk_{\perp} \left\langle u_n(k) \left| \frac{\partial}{\partial k_{\perp}} \right| u_n(k) \right\rangle$$

$$\theta(\vec{k}_{\parallel}) = 0 \text{ or } \pi$$

← Inversion+ time-reversal symmetries

Zak phase  $\theta(\vec{k}_{\parallel})$  jumps by  $\pi$   
at the nodal line

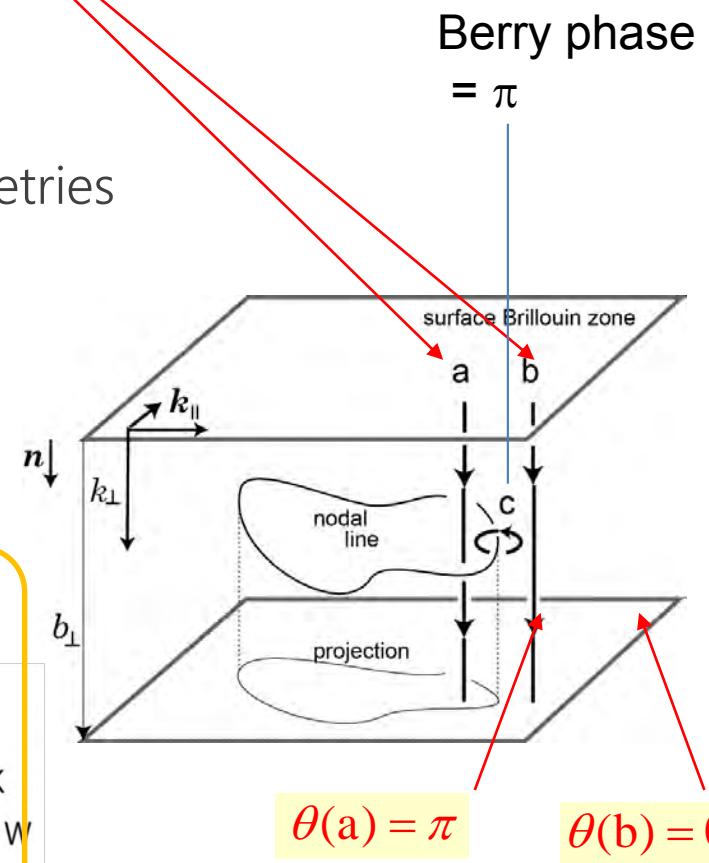
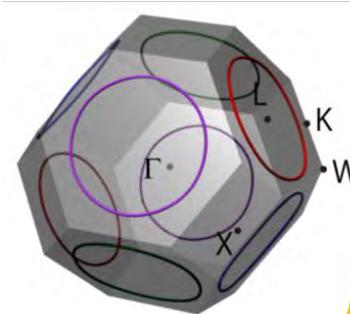
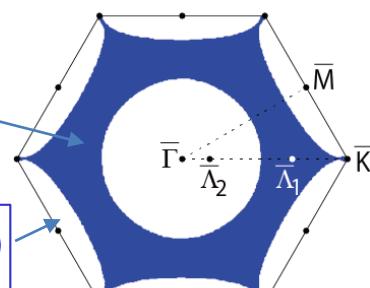
(111) Surface Brillouin zone in Ca

Zak phase

$$\theta(\vec{k}_{\parallel}) = \pi$$

Zak phase

$$\theta(\vec{k}_{\parallel}) = 0$$



# Zak phase and charge polarization

In 1D system:

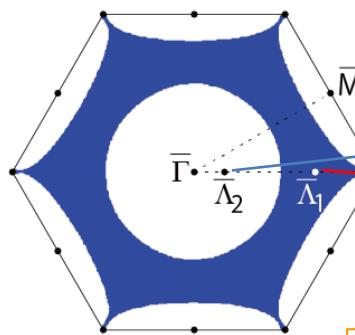
$$\text{Polarization } \sigma = \frac{e}{2\pi} \text{Zak phase} \theta(\vec{k}_{\parallel}) \quad (\text{mod } e)$$

"modern theory of polarization"

(Vanderbilt,  
King-Smith, PRB,1993)

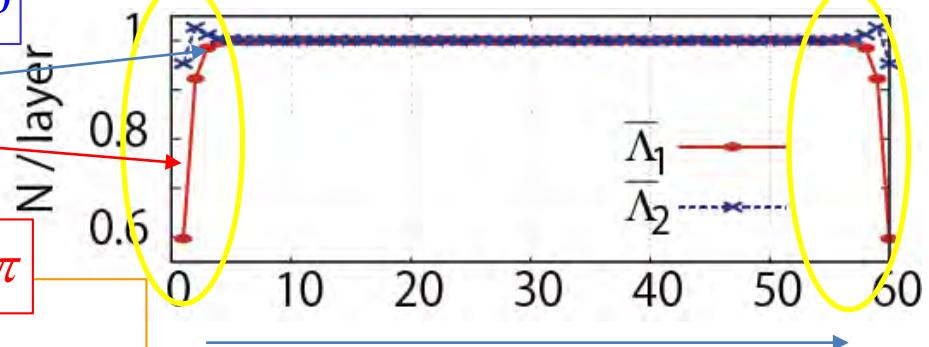
Total polarization for 3D system (=surface polarization charge density)

$$\sigma = \int \frac{d^2 \vec{k}_{\parallel}}{(2\pi)^2} \sigma(\vec{k}_{\parallel}) \quad (\text{Note: only for insulators})$$



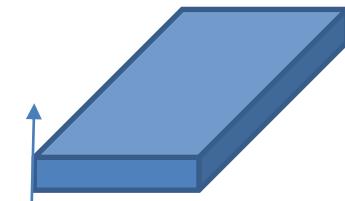
$$\theta(\vec{k}_{\parallel}) = 0$$

Charge profile in a slab  
along thickness direction

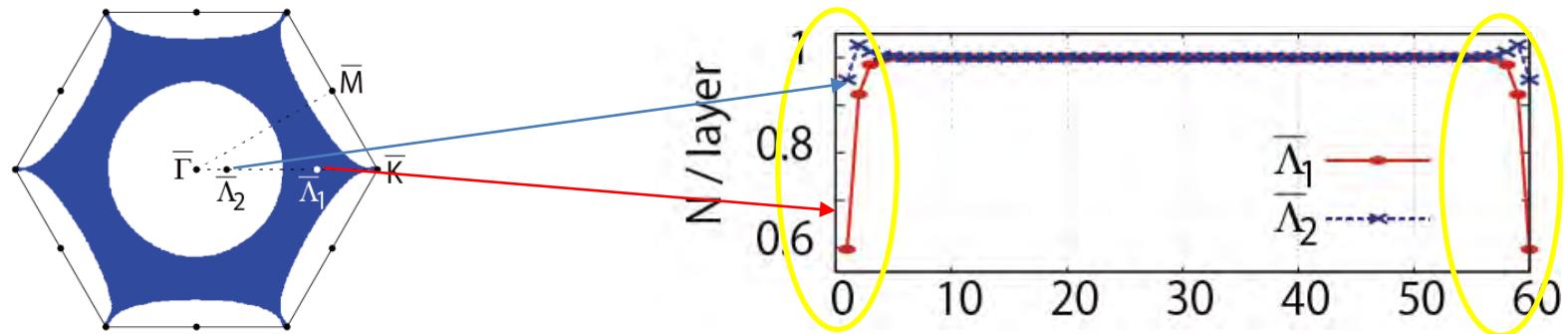


$$\theta(\vec{k}_{\parallel}) = \pi$$

Charge is depleted  
by  $e/2$

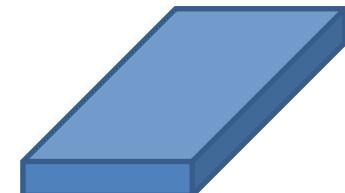


# Surface charge



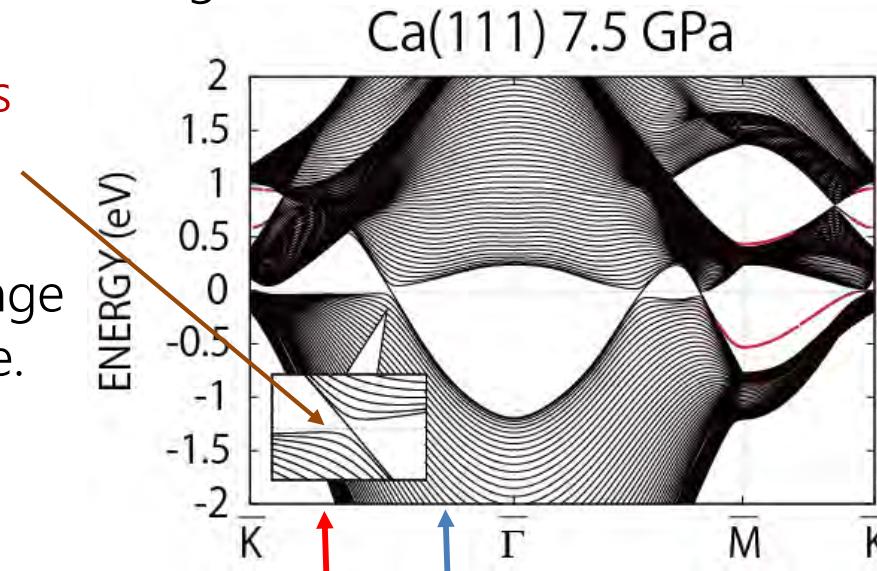
Remarks:

- It is not ferroelectric  $\leftarrow$  centrosymmetric FCC
- Where is the missing charge at  $\pi$  Zak phase region ?

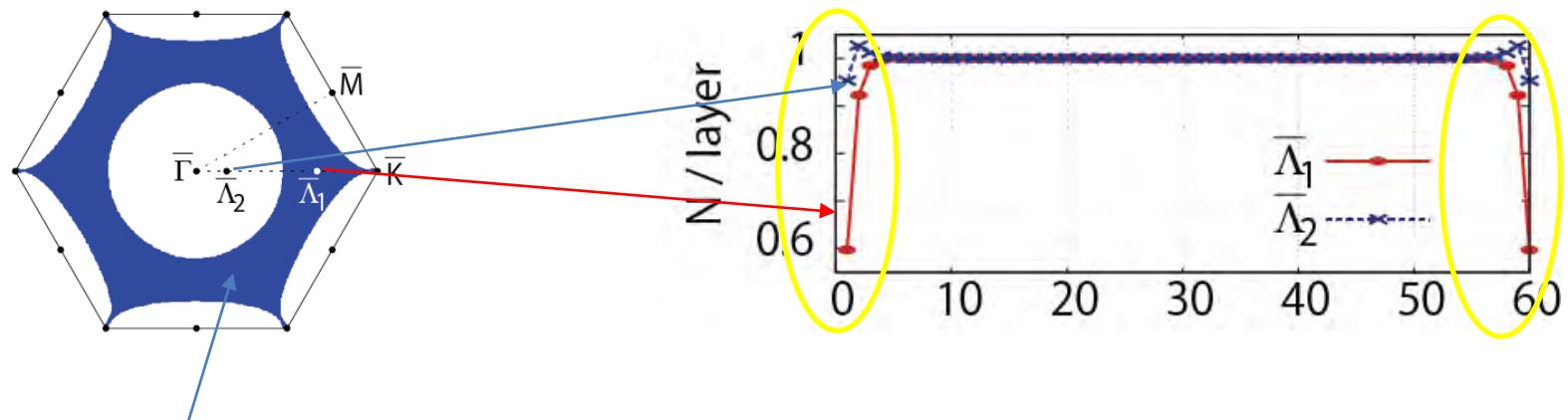


The number of bulk occupied bands  
change at the nodal lines

Chemical potential will slightly change  
to accommodate missing charge.



# Nodal-line and Berry phase



$$\text{Area} = 0.485 * \text{BZ}$$

$$\rightarrow \text{surface charge density} = 0.485 \cdot \frac{e}{2} \text{ per surface unit cell}$$

Huge surface polarization charge

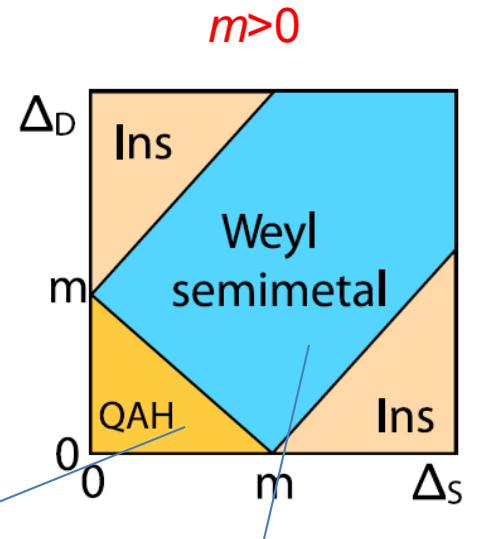
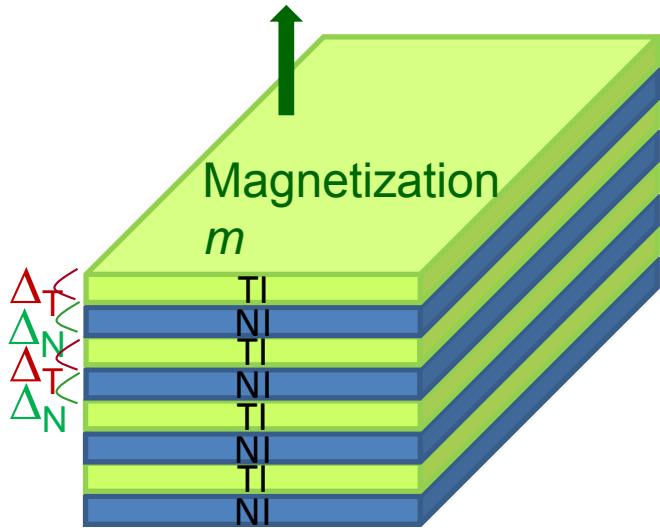
→ In metals this charge is screened by carriers and lattice

→ Charge imbalance & lattice relaxation at the surface

Topological metals often appears between  
various topological insulator phases

# Topological insulator multilayer without time-reversal symmetry

Burkov, Balents, PRL 107, 127205 (2011)



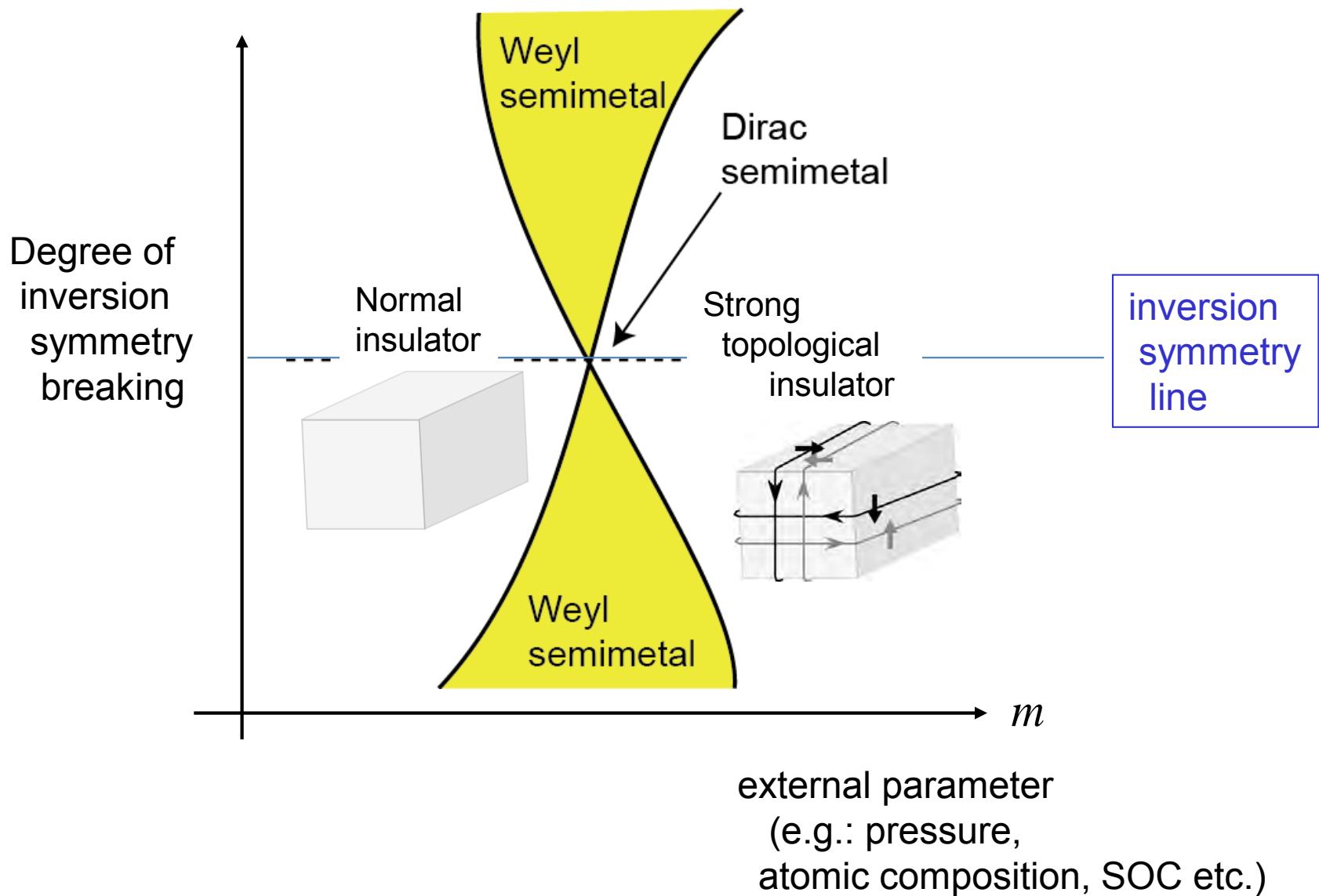
Quantum anomalous Hall:  
Ch=1 for all  $k_z$   
=Chiral surface state for  
all  $k_z$

Weyl semimetal:  
Ch=1 for  $k_z$  between the two Weyl  
nodes. = **Fermi arc**  
Ch=0 otherwise

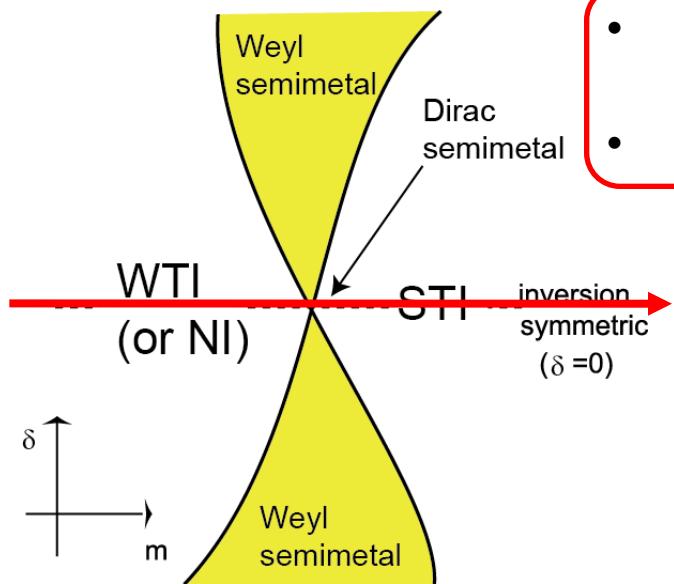
- By changing parameters, the Weyl nodes move in k-space.
- When they meet, they are annihilated in pair and the system becomes an insulator in the bulk (i.e. either QAH phase or an insulator phase).

# NI-TI universal phase diagram in 3D

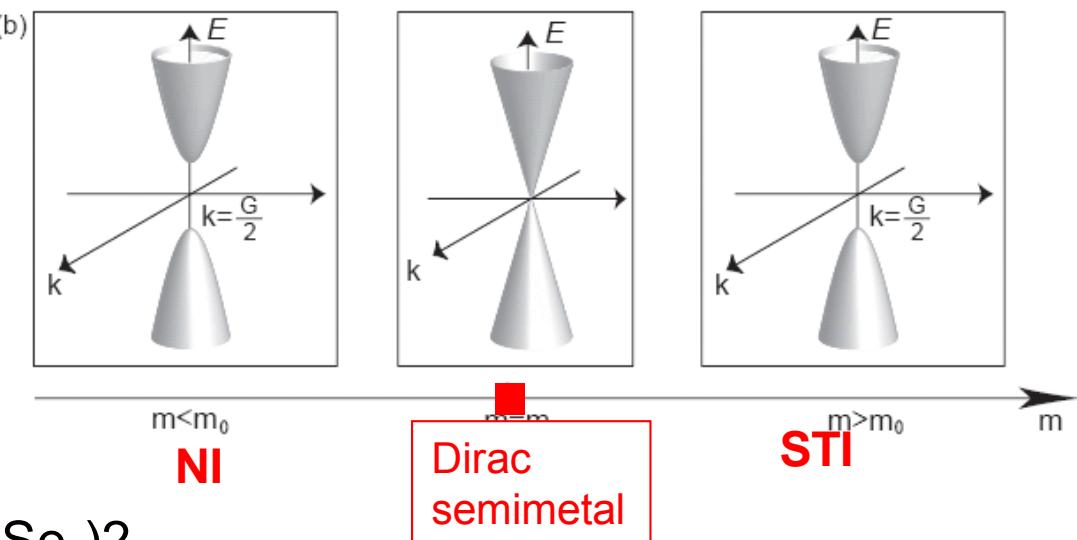
SM, New J. Phys. ('07).  
SM, Kuga, PRB ('08)  
SM, Physica E43, 748 ('11)



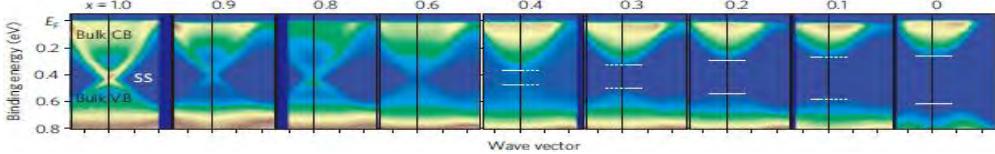
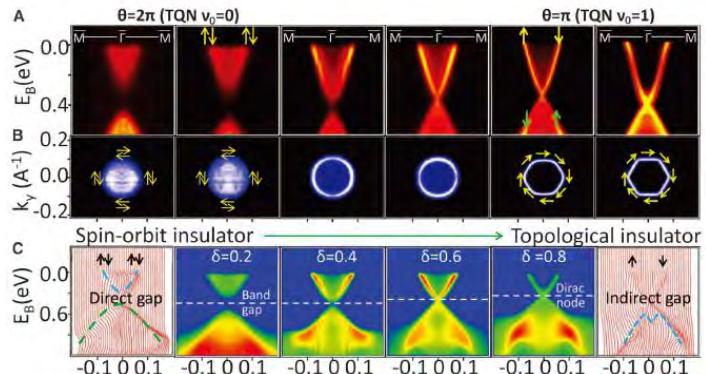
# Systems with inversion symmetry



- Gap closes at TRIM inversion of bands with opposite parities.
- Insulator-to-insulator transition

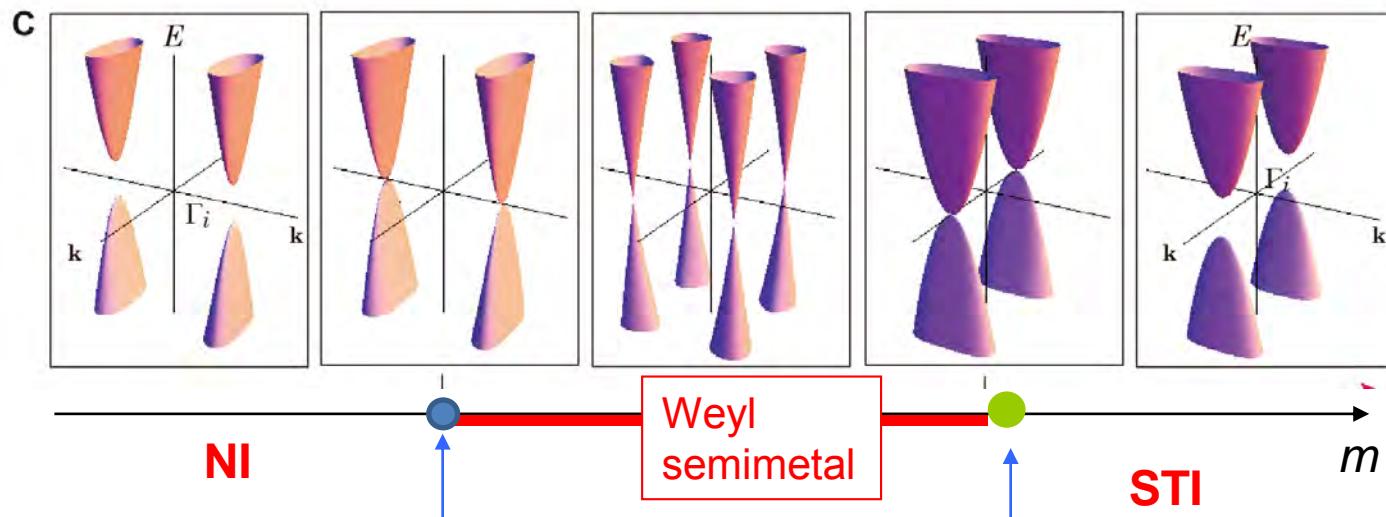
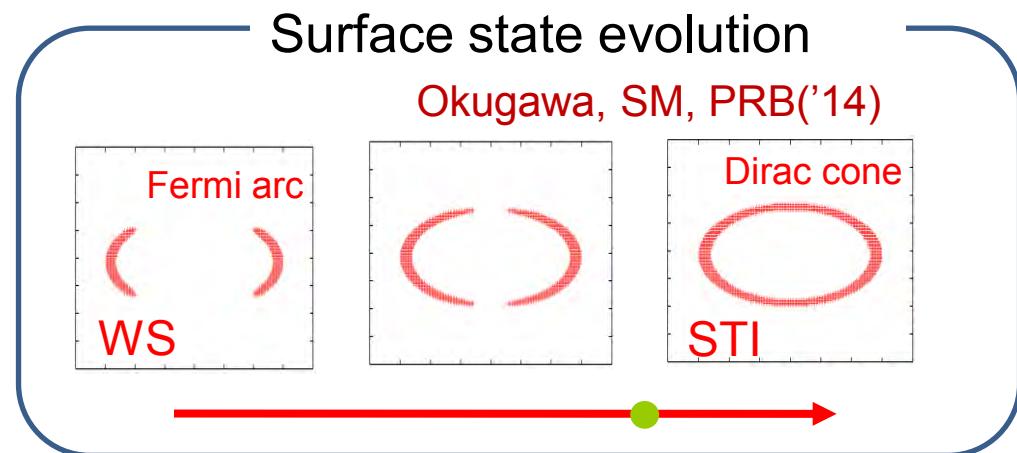
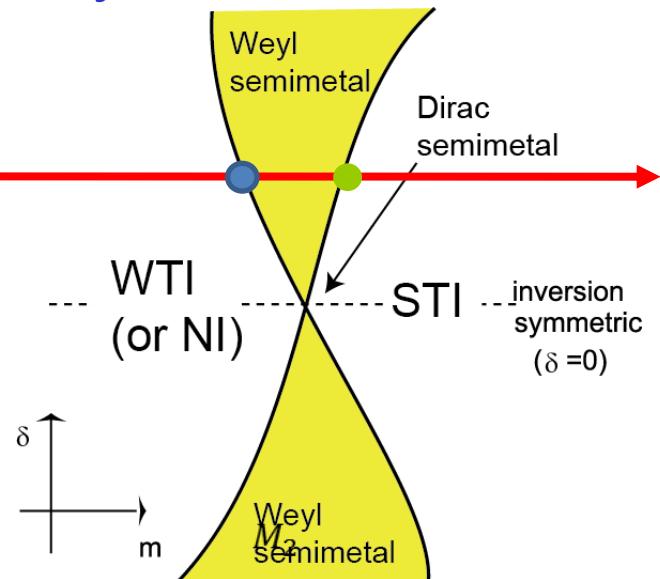


e.g. TlBi(S<sub>1-x</sub>Se<sub>x</sub>)<sub>2</sub>



Sato et al., Nature Phys.7, 840 ('11)

# Systems without inversion symmetry



pair creation of Weyl nodes  
(monopole+antimonopole)

Pair annihilation

SM, New J. Phys. ('07).  
SM. Kuga, PRB ('08)  
SM, Physica E('11)  
Okugawa, SM, PRB('14)

# $\mathbb{Z}_2$ topological number $v$

$v=0$ : normal insulator (NI)

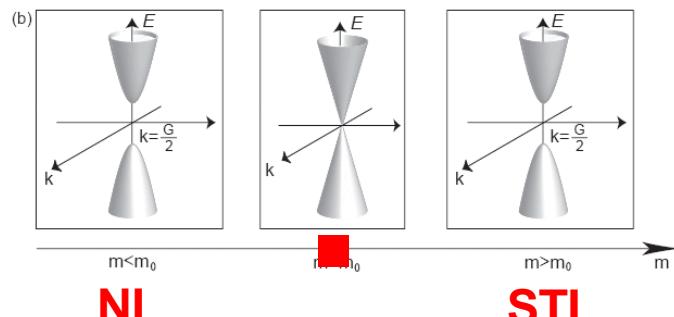
$v=1$ : topological insulator (TI)

## (A) systems with inversion symmetry

$$(-1)^v = \prod_i \prod_{m=1}^N \xi_{2m}(\Gamma_i) \text{ Parity eigenvalue } +1 \text{ or } -1$$

$\Gamma_i$ : TRIM

Fu,Kane, PRB(2007)



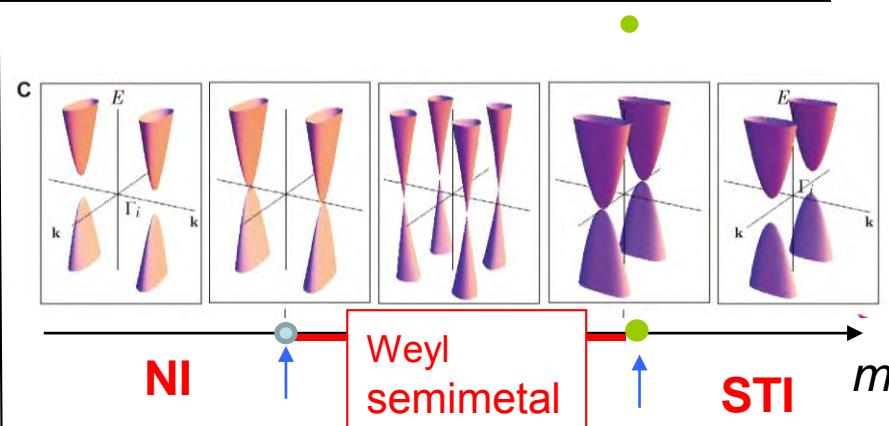
Gap closes at TRIM  
→parity eigenvalues are exchanged

## (B) systems without inversion symmetry

$$(-1)^v = \prod_i \frac{\sqrt{\det[w(\Gamma_i)]}}{\text{Pf}[w(\Gamma_i)]}$$

$$w_{mn}(\vec{k}) = \langle u_{-k,m} | \Theta | u_{k,n} \rangle$$

Fu,Kane, PRB(2006)



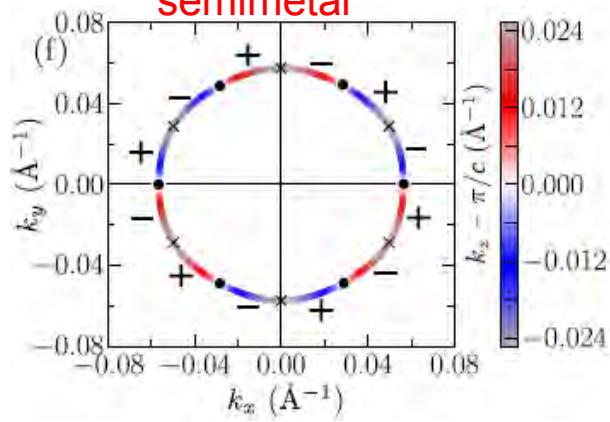
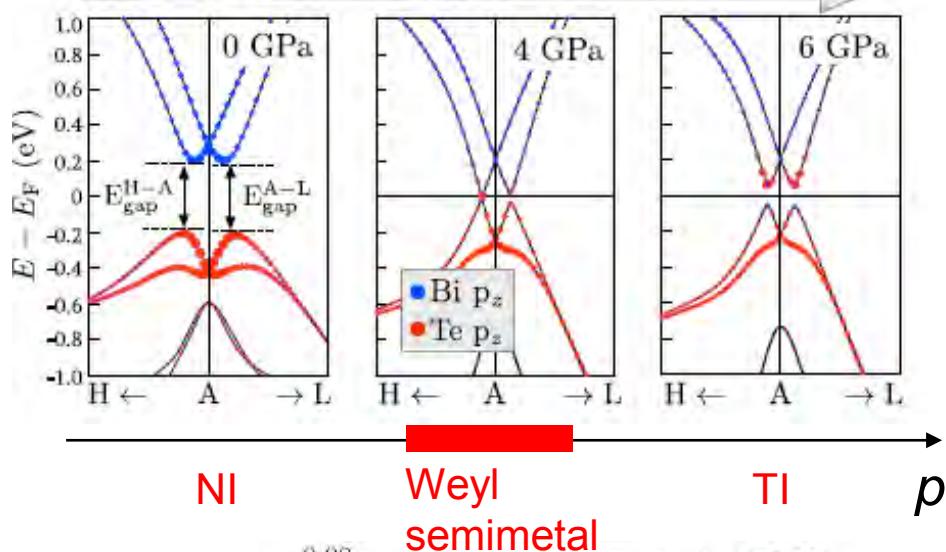
Gap closes at generic points  
→This gap closing should be a pair creation of Weyl nodes.

## BiTeI under pressure

Liu, Vanderbilt, PRB (2015)

Rusinov et al., NJP (2016)

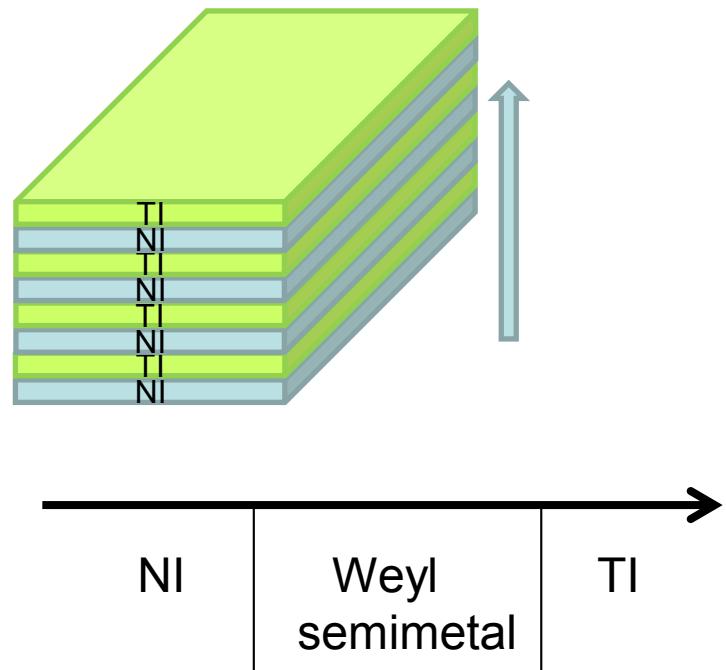
See also: Bahramy et al., Nat. Commun. (2012)



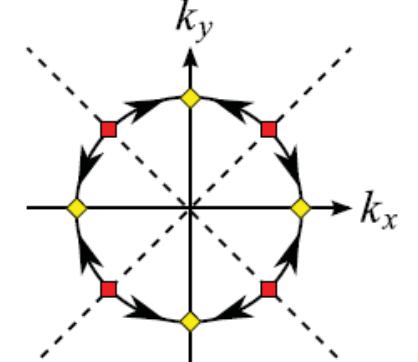
Trajectory of Weyl nodes

## TI//NI superlattice without inversion sym.

Halasz, Balents, PRB (2012)



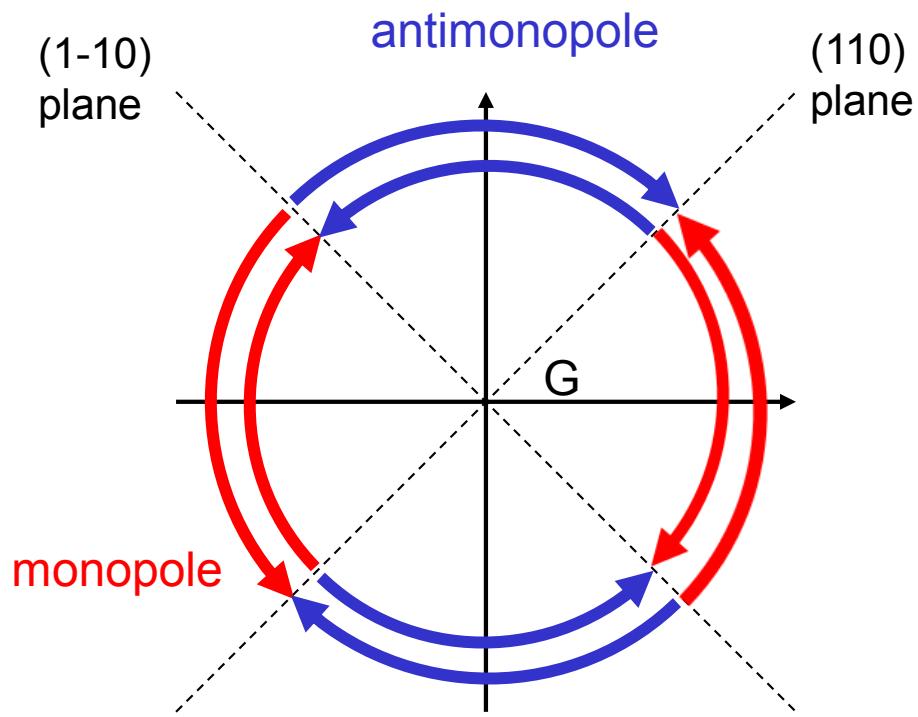
e.g.. Fourfold rotational symmetry



Trajectory of Weyl nodes

## HgTe<sub>x</sub>S<sub>1-x</sub> under [001] strain

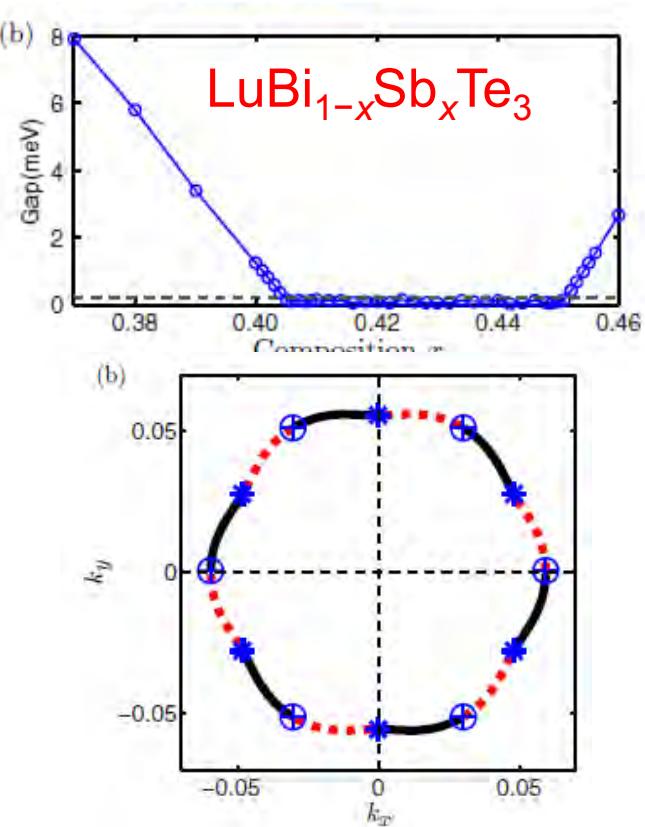
Rauch, Achilles, Henk, Mertig,,  
Phys. Rev. Lett. 114, 236805 (2015).



Trajectories of Weyl nodes in  $k_z=0$  plane

## LaBi<sub>1-x</sub>Sb<sub>x</sub>Te<sub>3</sub>, LuBi<sub>1-x</sub>Sb<sub>x</sub>Te<sub>3s</sub>

Liu, Vanderbilt,  
Phys. Rev. B 90, 155316 (2014).



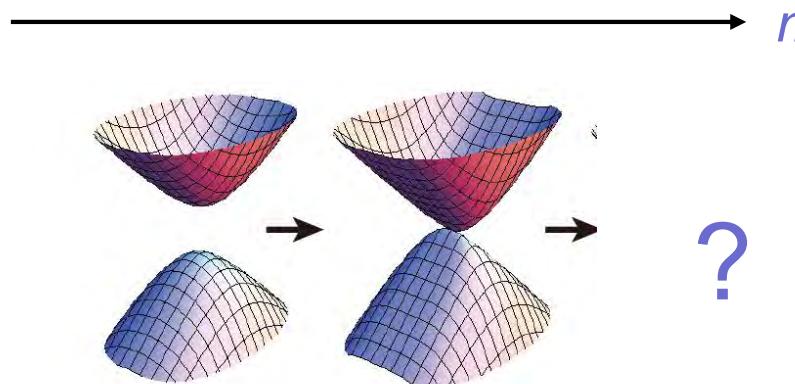
Trajectories of Weyl nodes  
(within  $k_x$ - $k_y$  plane)

## Problem:

Start from any band insulator **without inversion symmetry**  
(spinful + time-reversal symm.)

→ suppose a gap closes by changing a parameter  $m$

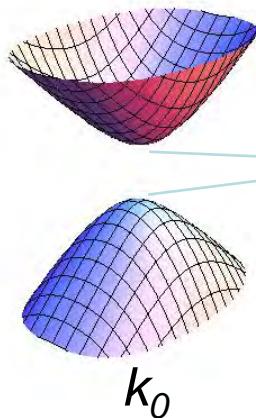
*What phase appears next?*



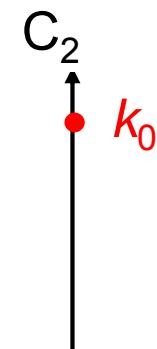
Classification  
by space groups &  $k$ -points.

138 space groups  
without inversion symm.

(Example #1):  $C_2$  symmetry (i.e.  $k$  : invariant under  $C_2$ )

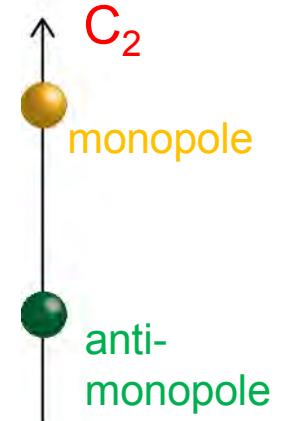
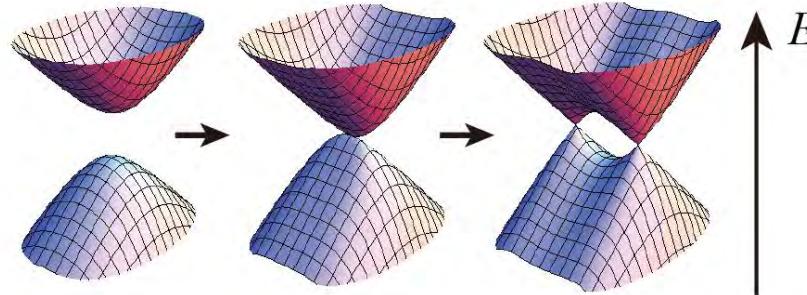


$C_2$  eigenvalue =  $+i$  or  $-i$

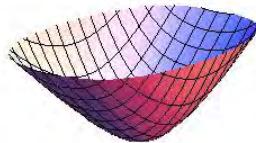


(i) Same signs of  $C_2$   
gap **cannot** close at  $k$  – level repulsion

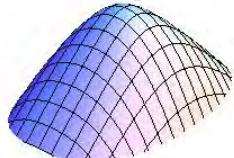
(ii) Different signs of  $C_2$   
Weyl semimetal  
Weyl nodes along  $C_2$  line



(Example #2): mirror symmetry (i.e.  $k$  : invariant under  $M$ )



$M$  eigenvalue =  $+i$  or  $-i$

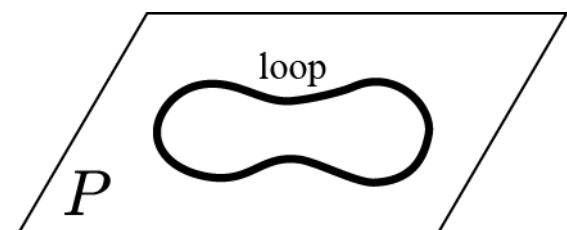
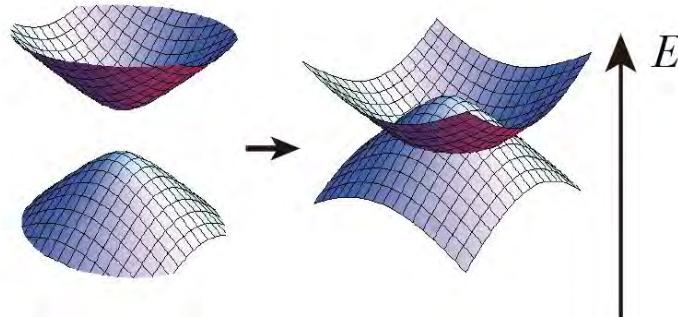
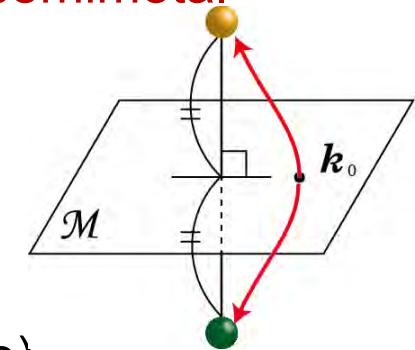


$k_0$

(i) Same signs of  $M$

gap closes at  $k$  on the mirror plane  $\rightarrow$  Weyl semimetal

(ii) Different signs of  $M$   
nodal-line semimetal  
(gap closing along a loop on a mirror plane)

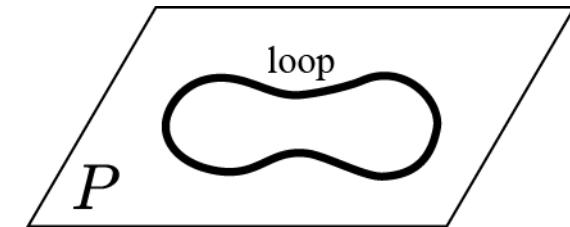
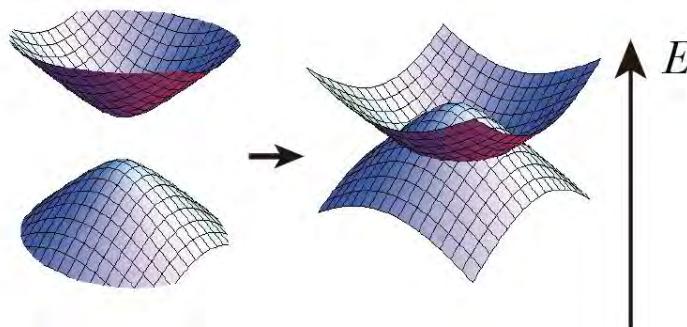


## Semiconductors without inversion symmetry

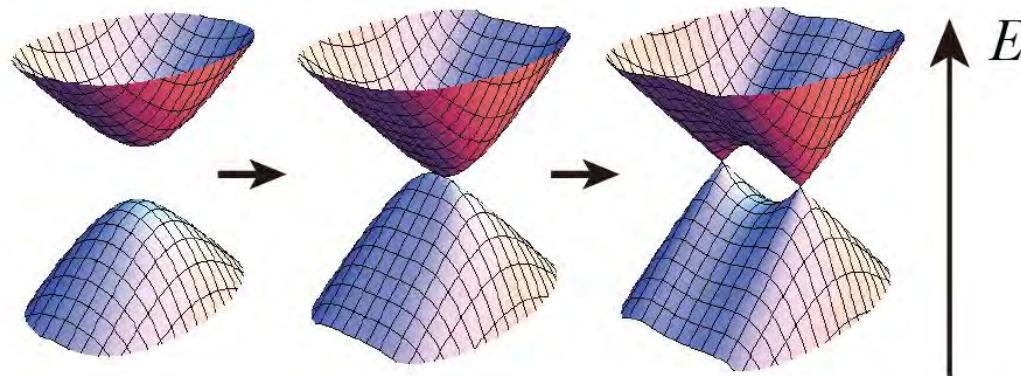
→ Gap-closing always leads to topological semimetals

Murakami, Hirayama, Okugawa, Miyake,

(a) Nodal-line semimetal ( $\leftarrow$  mirror plane) Sci. Adv. 3, e1602680 (2017)

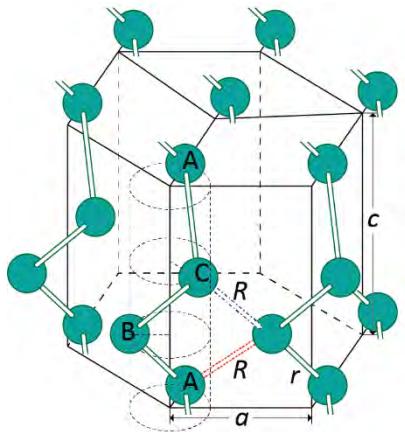


(b) Weyl semimetal

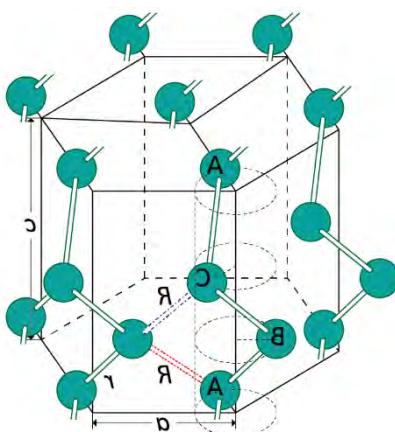


Only two possibilities. No insulator-to-insulator transition happens.  
(in contrast to inversion symmetric systems)

## Te : lattice with helical chains

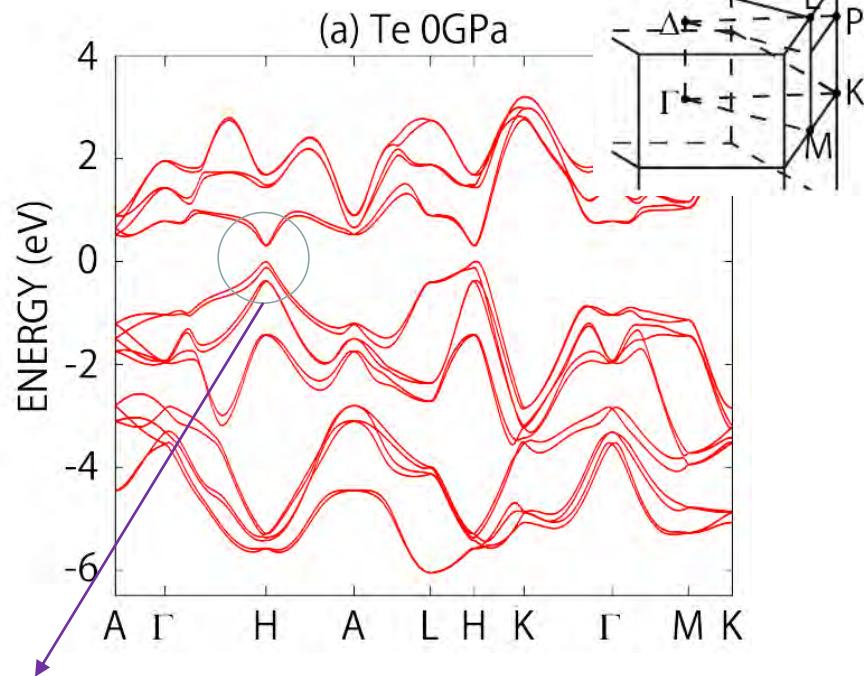


$P3_121$

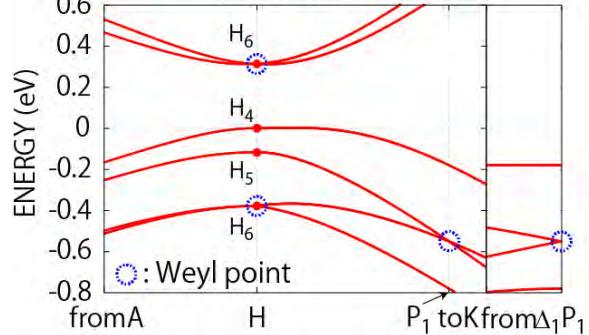


$P3_221$

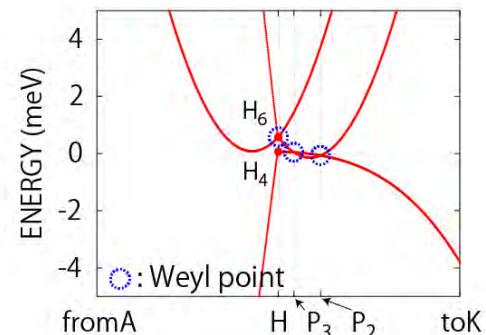
M. Hirayama, R. Okugawa, S. Ishibashi,  
S. Murakami, T. Miyake,  
PRL (2015)



- Chiral lattice with helical chains
- No inversion symmetry
- No mirror symmetry
- Allow Weyl nodes



Insulator: gap=0.3eV



Weyl semimetal

# Conclusions

- Weyl semimetals (in inversion asymmetric systems)
  - Appear in TI-NI phase transition  
e.g. Tellurium: Weyl semimetal at high pressure

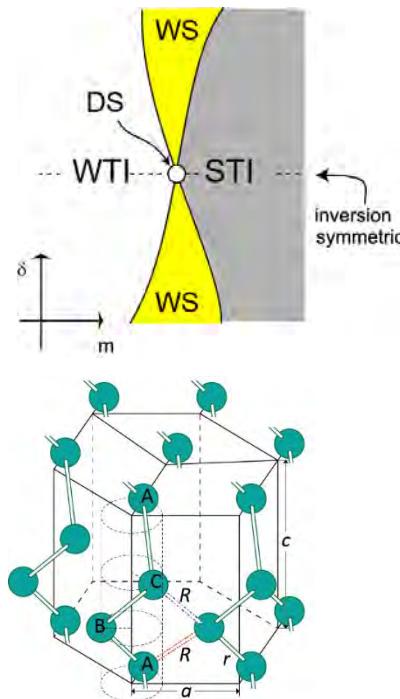
Murakami, NJP 9, 356 (2007)

Murakami, Kuga, PRB78, 165313 (2008)

Okugawa, Murakami, PRB 89, 235315 (2014)

Hirayama et al., PRL 114, 206401 (2015)

Murakami, Hirayama, Okugawa, Miyake,  
Sci. Adv. 3, e1602680 (2017)



- Nodal lines in alkaline earth metals Ca, Sr, Yb
  - nodal lines if spin-orbit coupling is neglected
  - large “polarization” for  $k_{\parallel}$  inside the nodal line
  - surface Rashba SOC is enhanced e.g. Bi/Sr(111), Bi/Ag(111)

Hirayama et al., Nat. Commun. 8, 14022 (2017)

