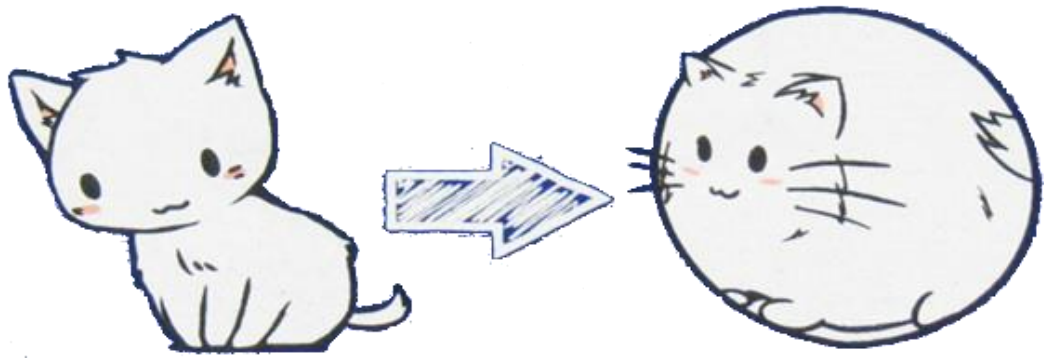
# 拓樸材料:
# 絕緣體、半金屬、超導體



Department of physics, National Cheng Kung University, Taiwan

（國立成功大學物理系）

Tay-Rong Chang (張泰榕)

2017/May./8

# Outline



1. **為什麼我們要關注材料物理...**

2. **要聽懂這場演講的基本知識**

   能帶理論
   計算方法

3. **所以,最近我們發現了什麼**

   拓樸材料

   i) 什麼是凝態物理中的拓樸
   ii) 拓樸絕緣體與可能的應用
   iii) 新類型拓樸相: 拓樸半金屬與拓樸超導體

# 為什麼材料重要



- 百萬年以前 ： 石頭，樹枝
- 石器時代 ： 製作石器工具
- 陶器時代 ： 辨識材料，以火製作陶器
- 青銅(鐵器)時代 ： 煉製金屬
- 19世紀 ： 煤礦，合金
- 20世紀 ： 半導體，石油
- 21世紀 ： ???

# 為什麼材料重要



- High Tc superconductors (Cuprates, Fe-based)
- Colossal magnetoresistance ($LaCaMnO_3$ )
- Half-metal ($CrO_2$ , $Fe_3O_4$, $SrRuO_3$)
- Nanotube, Graphene
- Multiferroic ($TbMnO_3$, $TbMn_2O_5$ )
- Large spin-orbital coupling materials : Rashba material (BiTeI), Iridate ($Sr_{n+1}Ir_nO_{3n+1}$), transition metal dichalcogenides (TMD), **Topological materials.**

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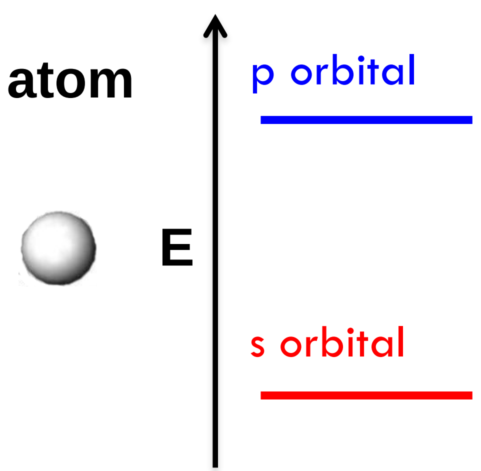
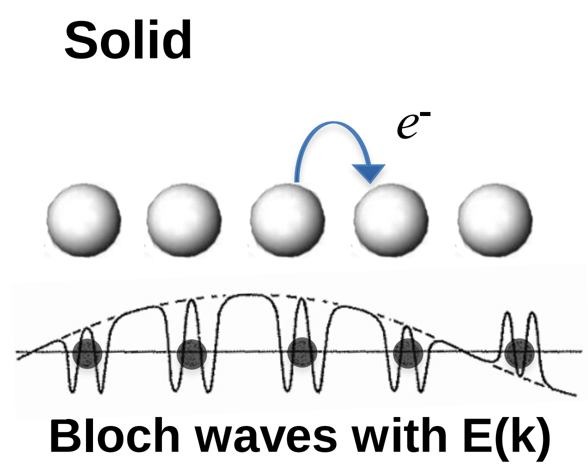
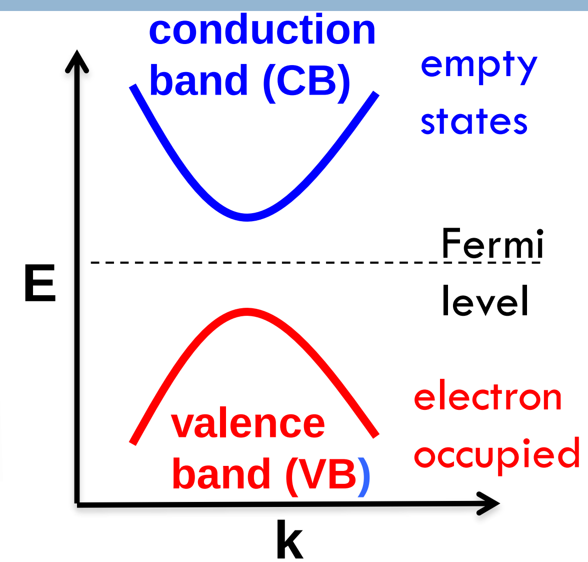
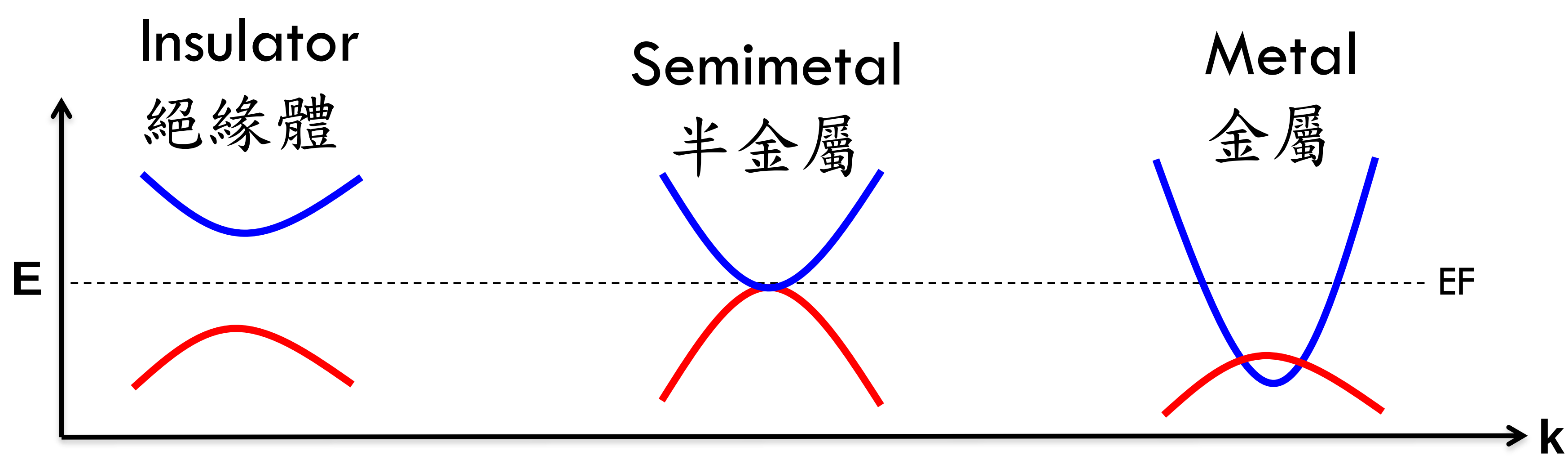
# 能帶理論




atom
E
p orbital
s orbital


Solid
$e^-$
Bloch waves with E(k)


conduction band (CB)
empty states
E
Fermi level
valence band (VB)
electron occupied
k


Insulator
絕緣體
Semimetal
半金屬
Metal
金屬
E
EF
k

# 計算方法

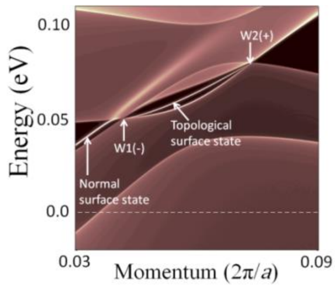


Step 1 Density functional theory (DFT)

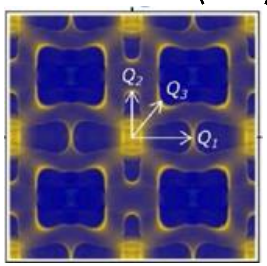
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_s(\vec{r})\right]\phi_i(\vec{r}) = \epsilon_i\phi_i(\vec{r}) \quad \text{where} \quad V_s(\vec{r}) = V(\vec{r}) + \int \frac{e^2 n_s(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\mathrm{d}^3r' + V_{\mathrm{XC}}[n_s(\vec{r})]$$

Step 2 Electronic structures

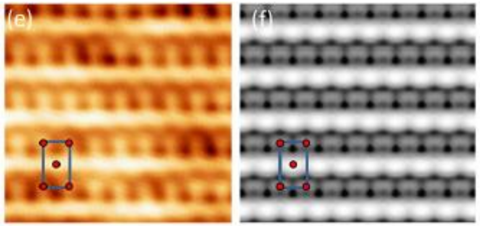
surface spectral weight simulation




quasiparticle interference (QPI)




STM imagine simulation




Step 3

原則上,只需給定元素種類與晶格位置,可求得所有物理量,
不須額外實驗參數,因此稱為ab-initio(from the beginning).

用電腦來做材料實驗...

我們像理論又像實驗,像物理又像化學

# 我們主要在幹嘛



馬後炮: 解釋實驗現象

煉金術: 預測新材料

↓

**理解自然,找有趣的物理!!**

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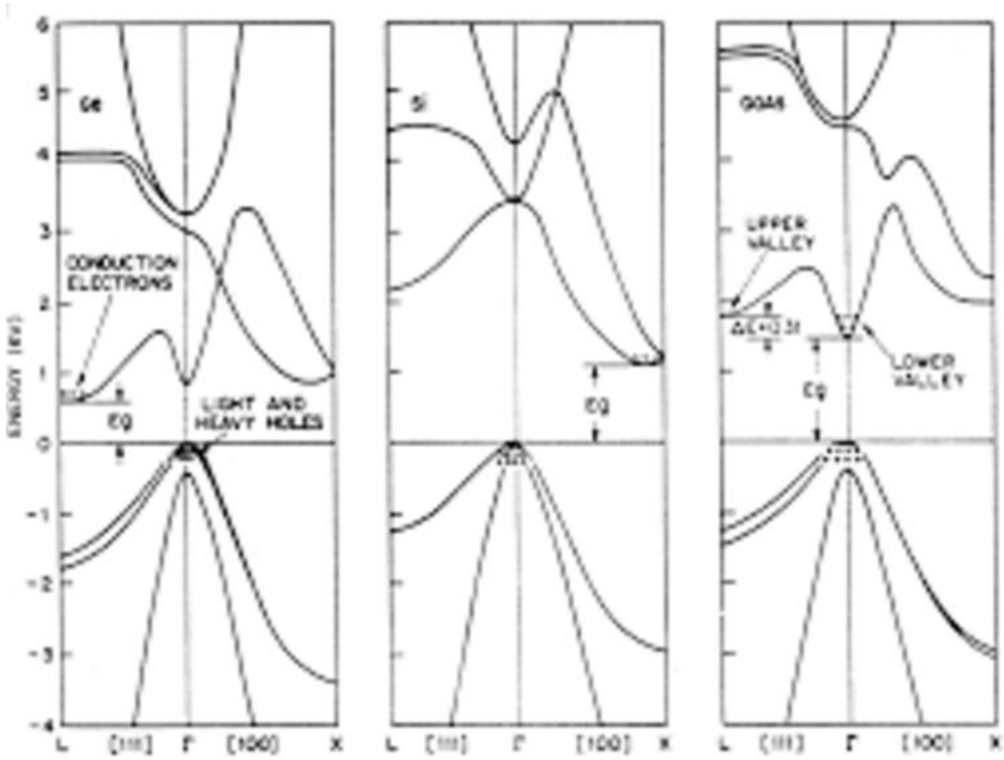
# 凝態物理的幾何



能帶幾何結構: 斜率, 能隙大小, 直接能隙或間接能隙…etc



# 凝態物理的拓樸



## Math => real space

**Gauss-Bonnet Theorem:**

≠

=

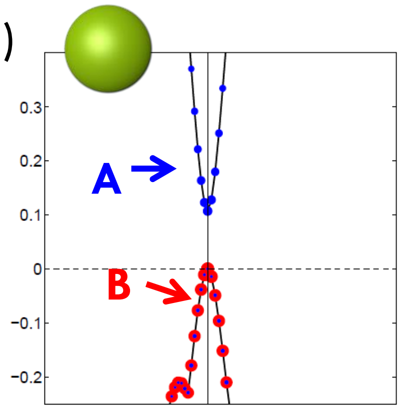
$$\oint_S K_{Gauss}\, ds = 2(1- g)$$

Gauss curvature    genus

genus    $g=0$    $g=1$    $g=1$

## Phys => momentum space

(1)

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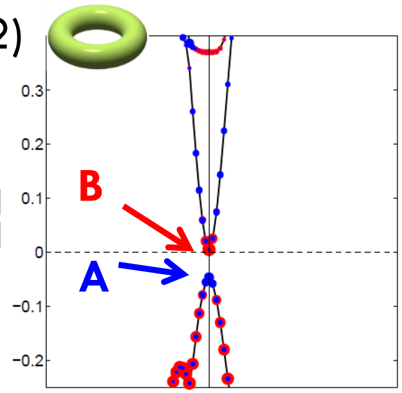
(2)

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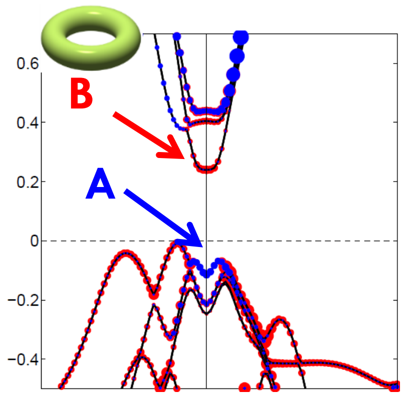
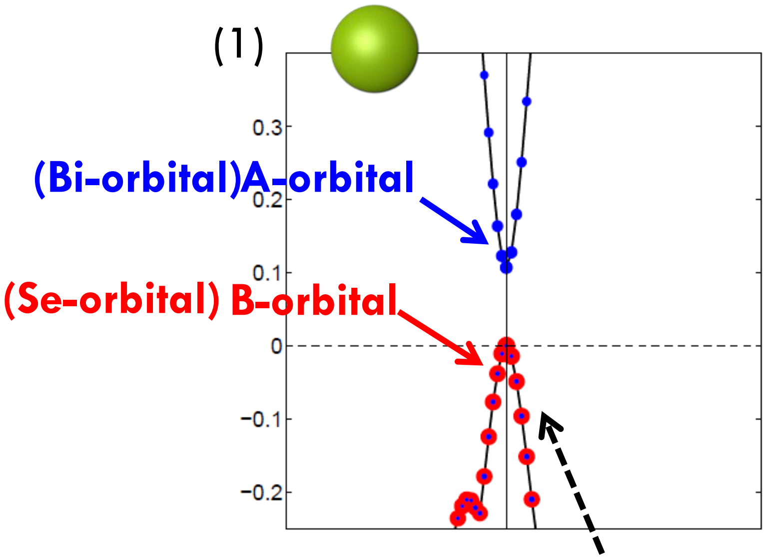
(3)

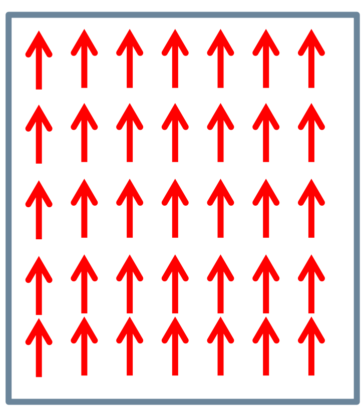


# 凝態物理的拓樸





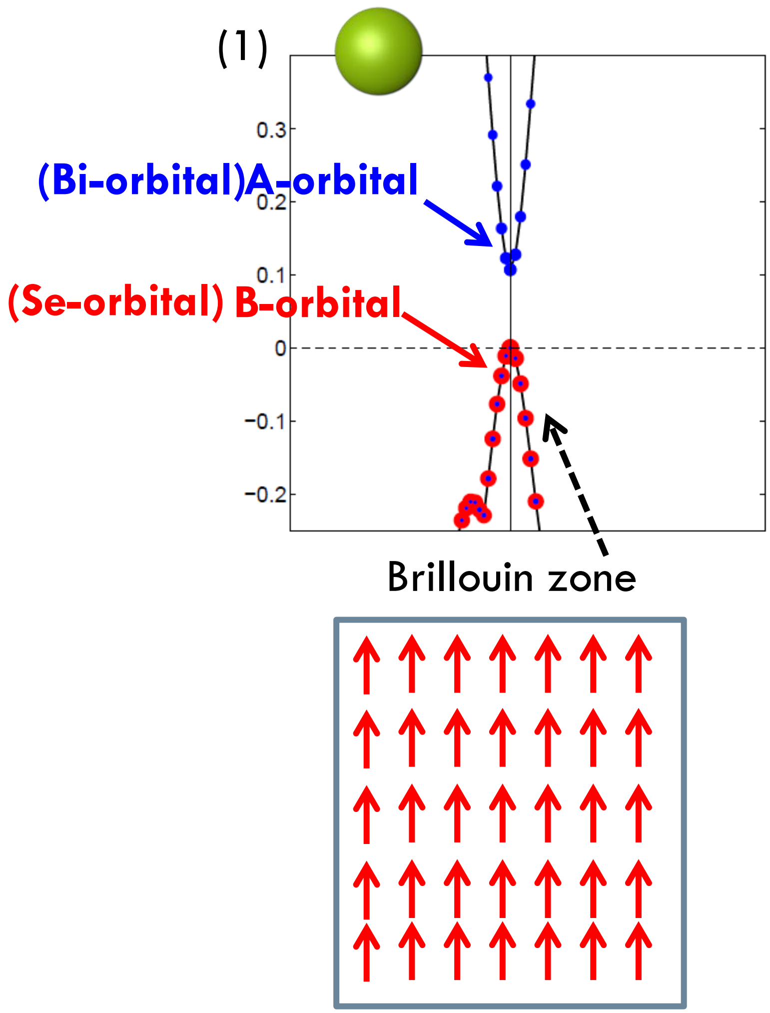

Brillouin zone



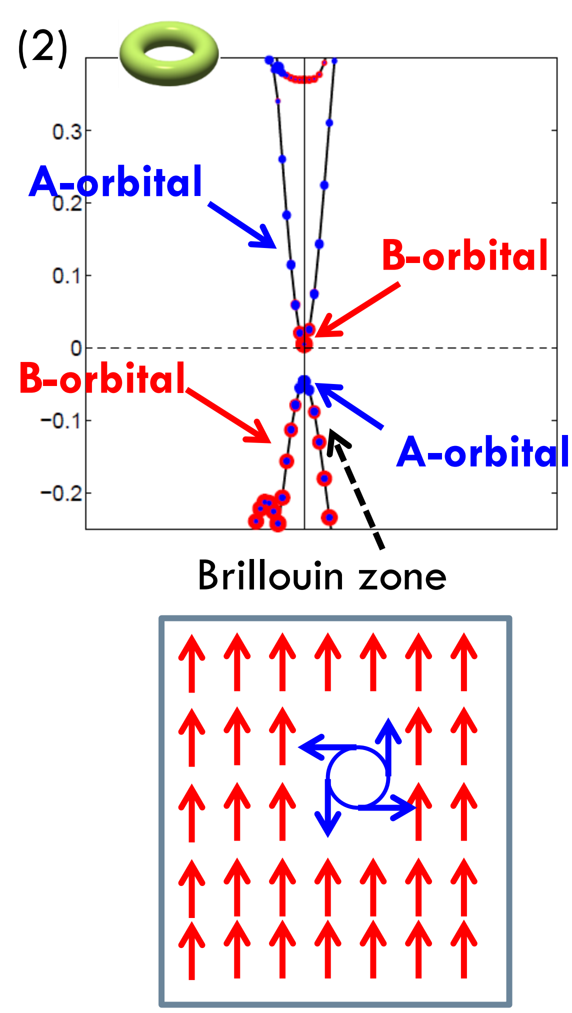
wavefunction is smoothly

# 凝態物理的拓樸





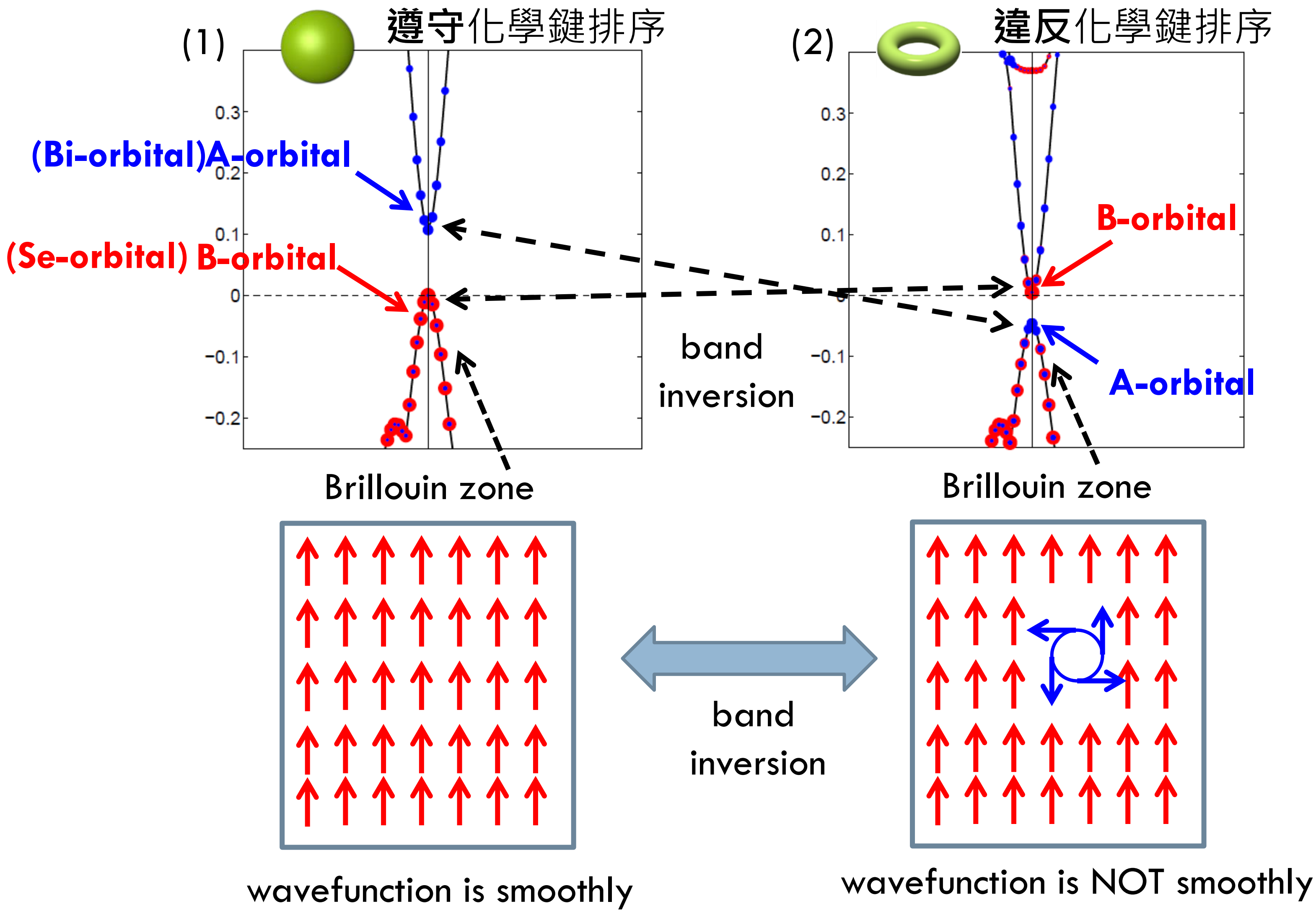

wavefunction is smoothly




wavefunction is NOT smoothly

# 凝態物理的拓樸

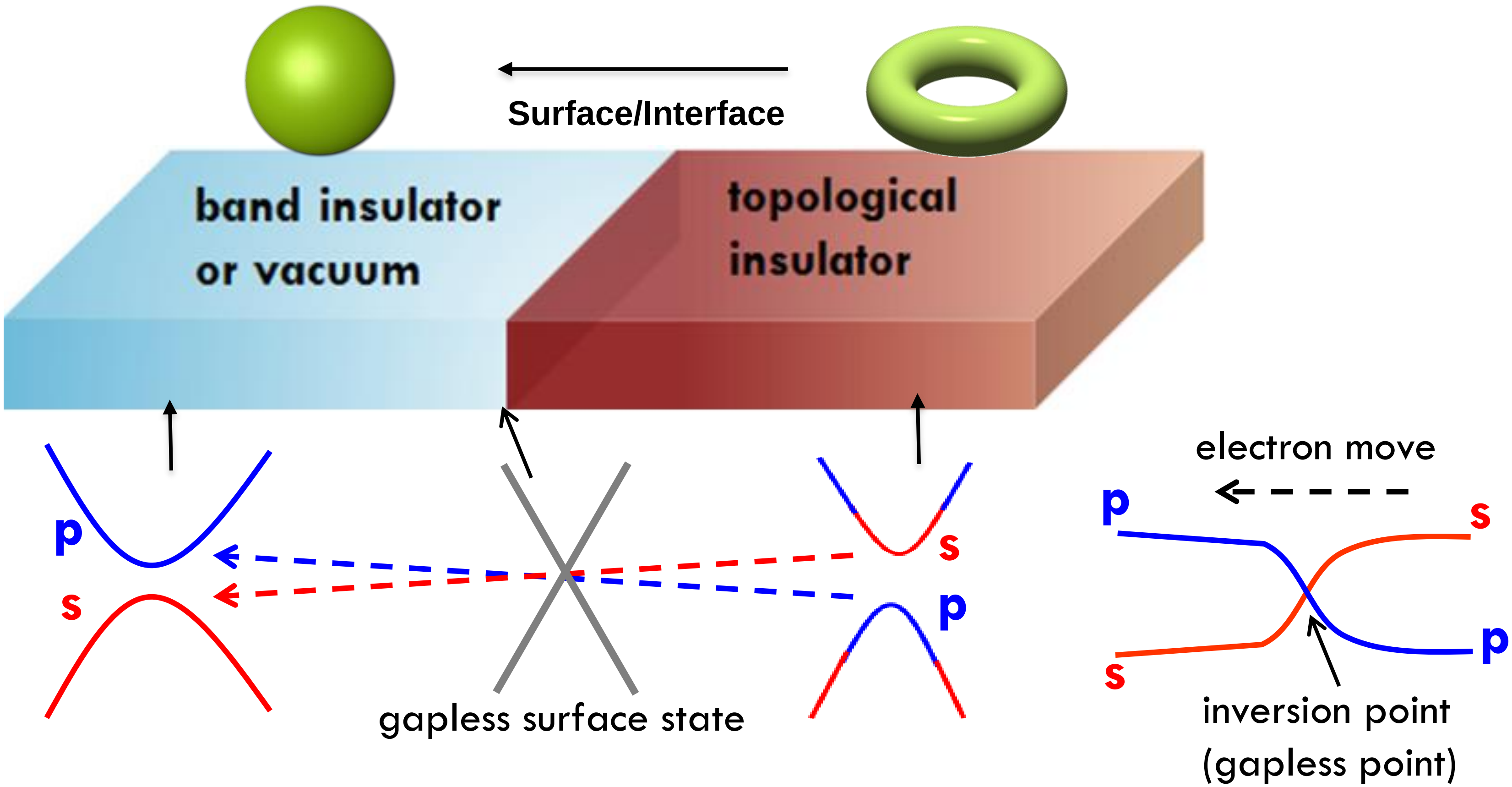




(1)
遵守化學鍵排序
(2)
違反化學鍵排序
(Bi-orbital)A-orbital
(Se-orbital) B-orbital
B-orbital
A-orbital
0.3
0.2
0.1
0
−0.1
−0.2
band
inversion
Brillouin zone
Brillouin zone
band
inversion
wavefunction is smoothly
wavefunction is NOT smoothly

# 拓樸材料的特徵



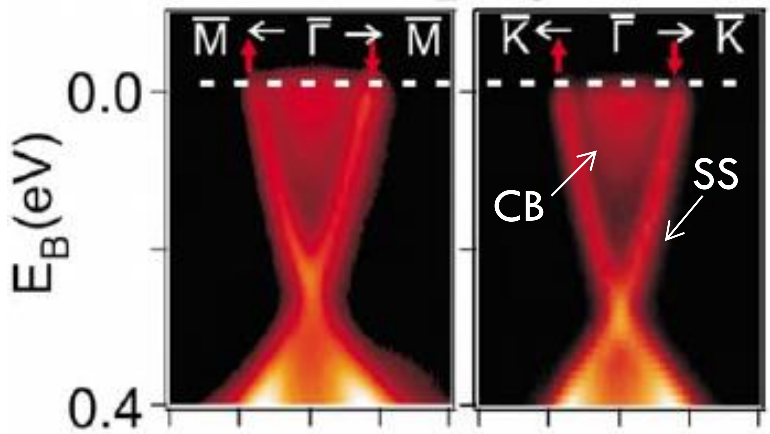



**The gapless surface state is the hallmark of topological phase.**

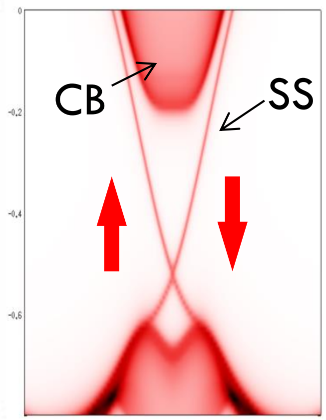
M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010)
X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011)

# 拓樸材料(絕緣體): $Bi_2Se_3$

**ARPES**




**Theory**




**Bulk**: insulating gap

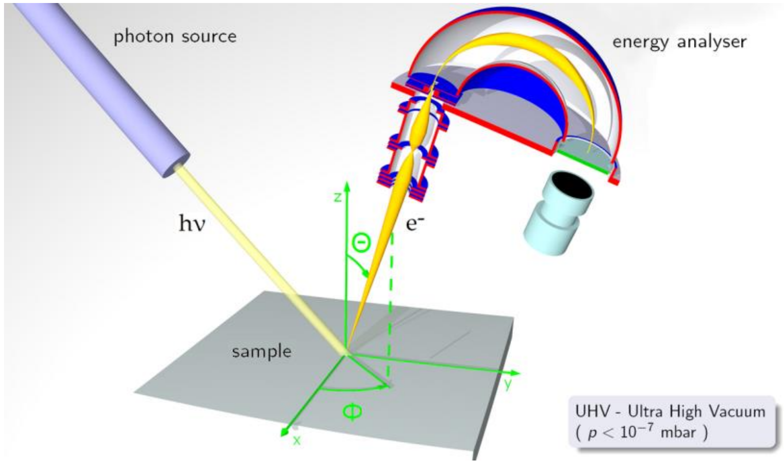
topological $Z_2$ invariant

odd/even number surface states

**Surface**: gapless surface states

spin-momentum locked

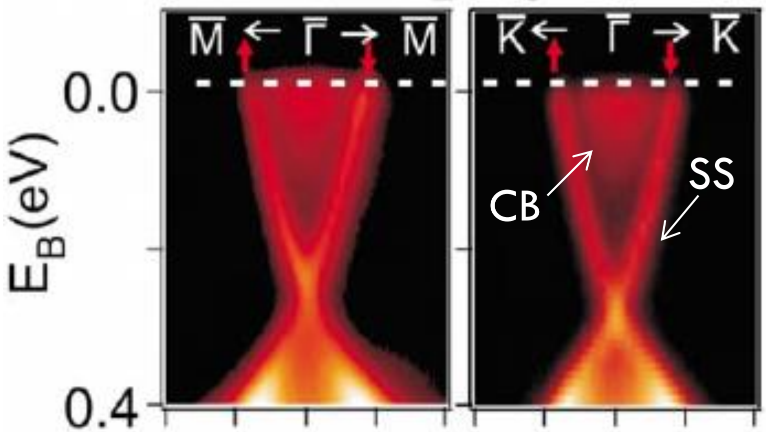
**Angle-Resolved Photoemission Spectroscopy (ARPES)**

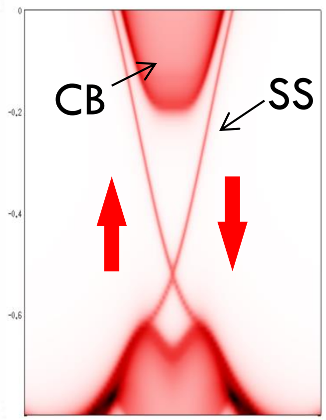


# 拓樸材料(絕緣體): $Bi_2Se_3$



**ARPES** **Theory**




Bulk: insulating gap

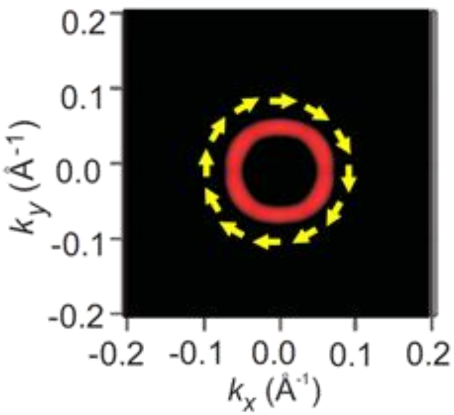
topological $Z_2$ invariant

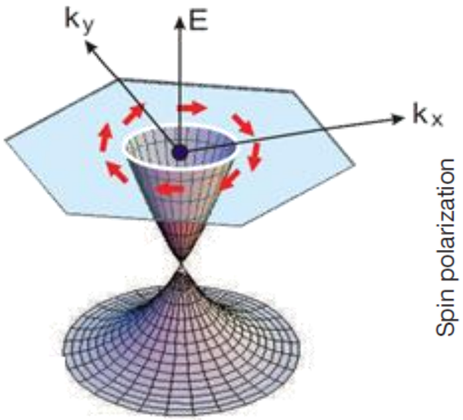
↓

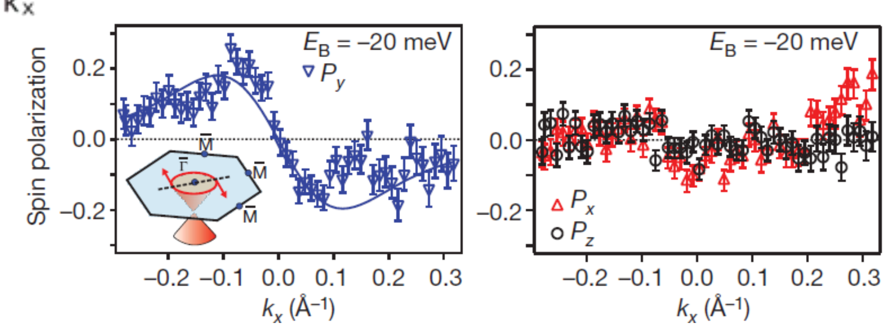
odd/even number
surface states

Surface: gapless surface states

spin-momentum locked



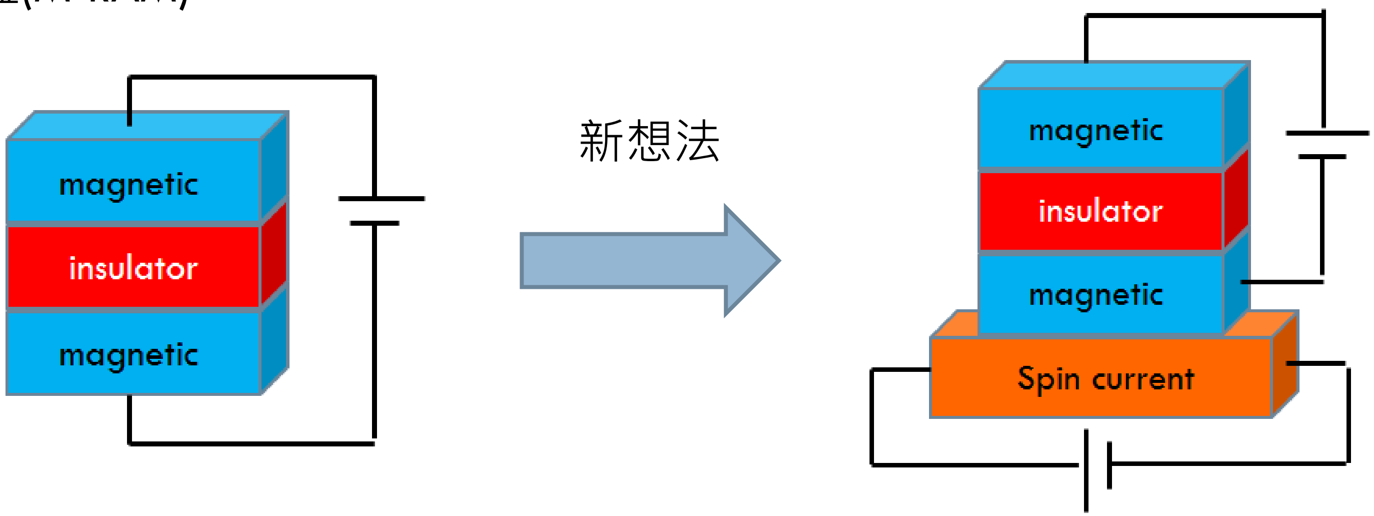

Y. Xia et al. Nature Physics **5**, 398 (2009)

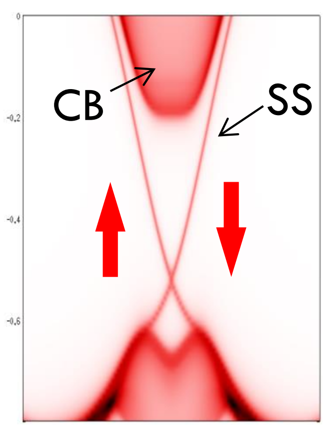
D. Hsieh et al. Nature **460**, 1101 (2009)

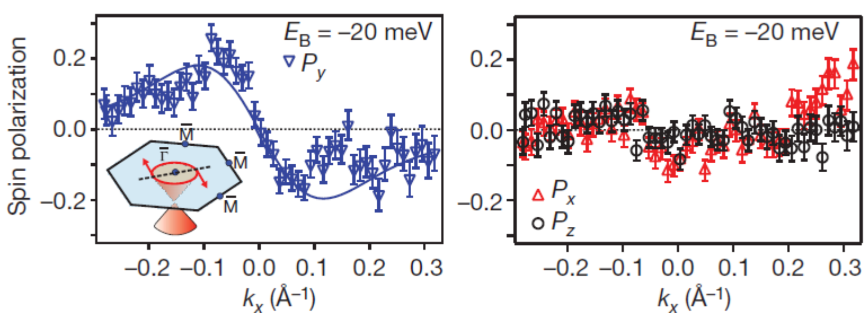
# 拓樸材料:可能的應用

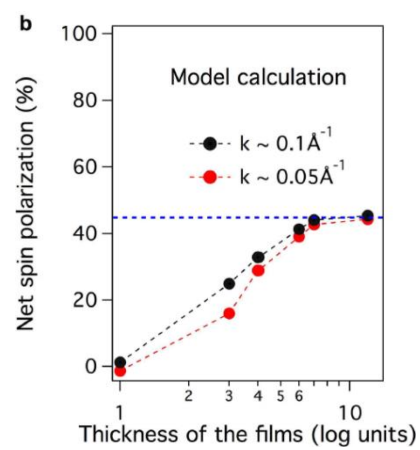


磁性記憶體(M-RAM)



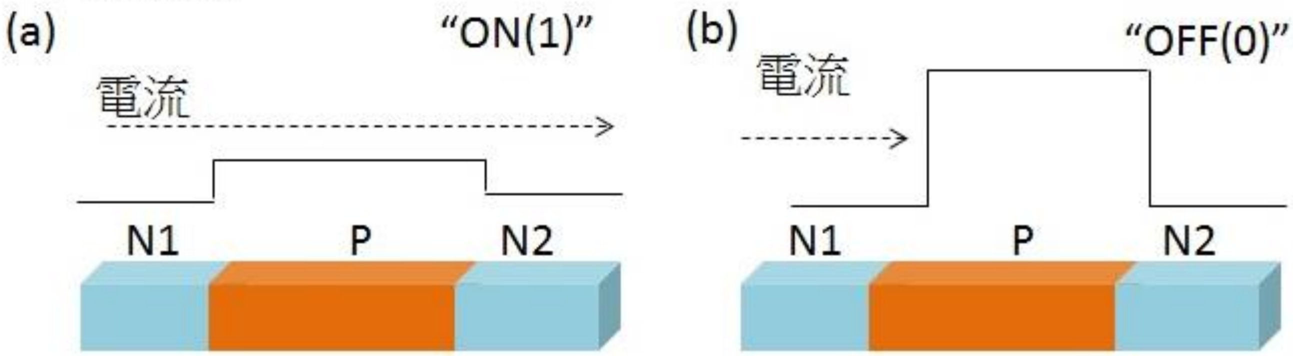



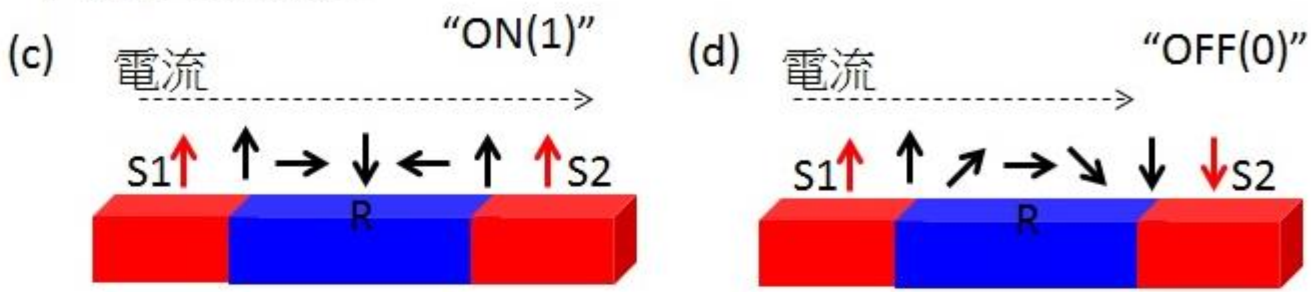
# 拓樸材料:可能的應用



## 電晶體




## 自旋電晶體



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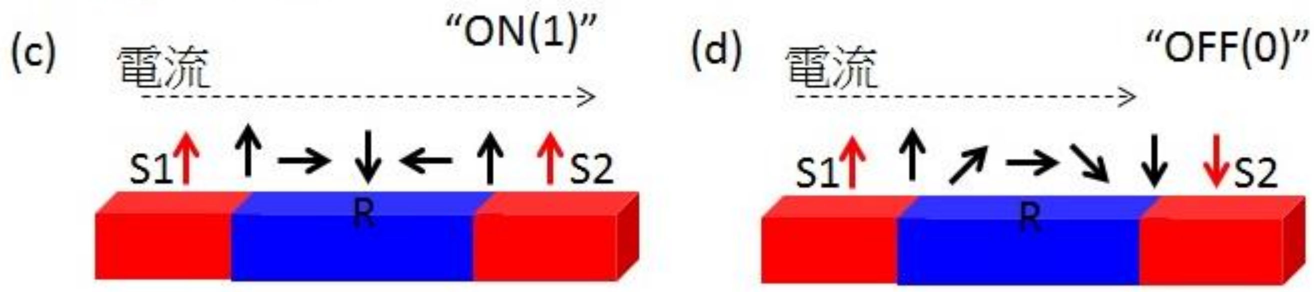
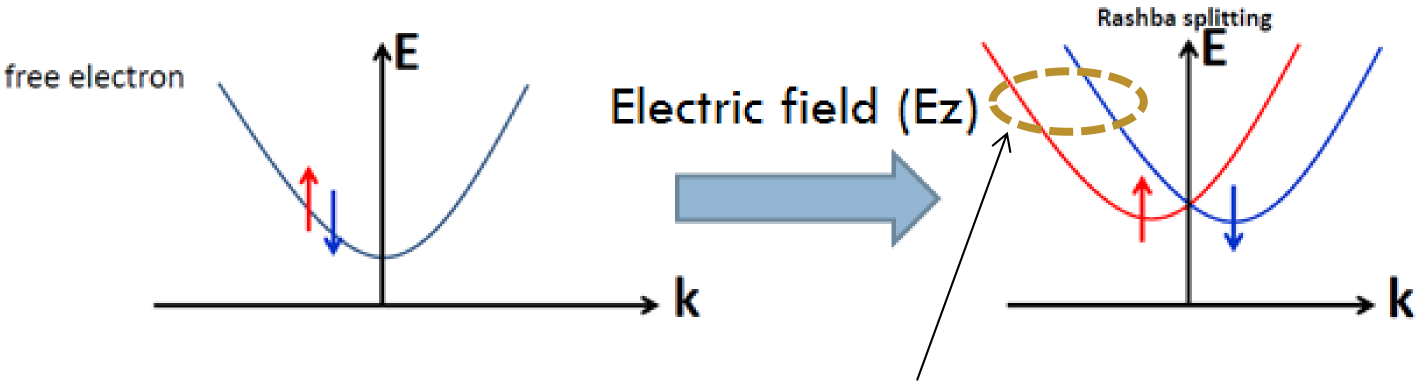
自旋電晶體




The crucial point is the value of the spin splitting.

# 拓樸材料:可能的應用



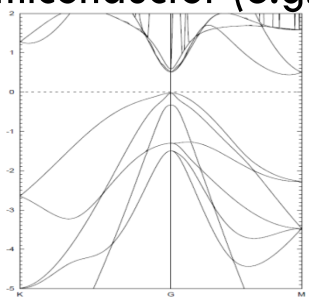
ORIGINAL ARTICLE

**Newtype large Rashba splitting in quantum well states induced by spin chirality in metal/topological insulator heterostructures**

*(Nature) NPG Asia Materials* ***8****, e332 (2016)*

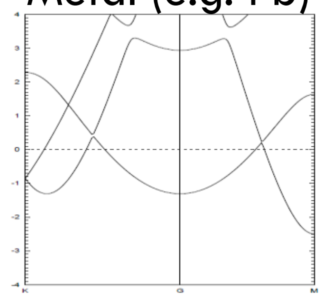
**Pb/Si**

Semiconductor (e.g. Si)



\+

Metal (e.g. Pb)



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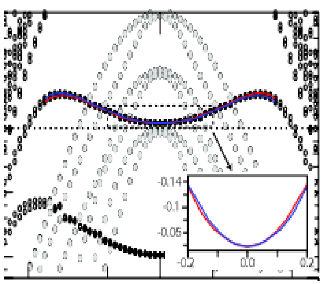
PRL**101**,266802

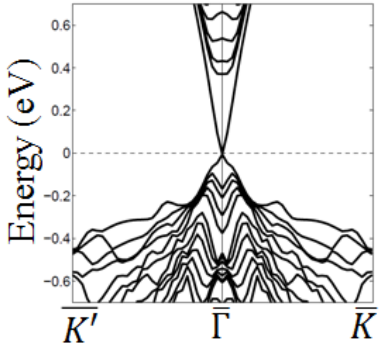


Rashba parameter

$\alpha_R = 0.04$

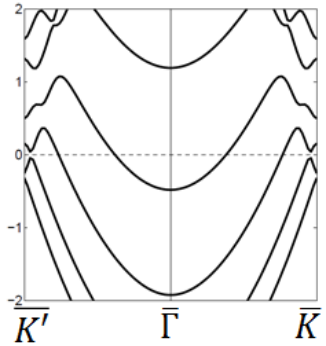
**$Ag/Bi_2Se_3$**

Topological insulator




\+

Normal metal

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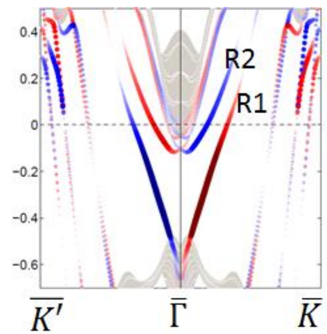
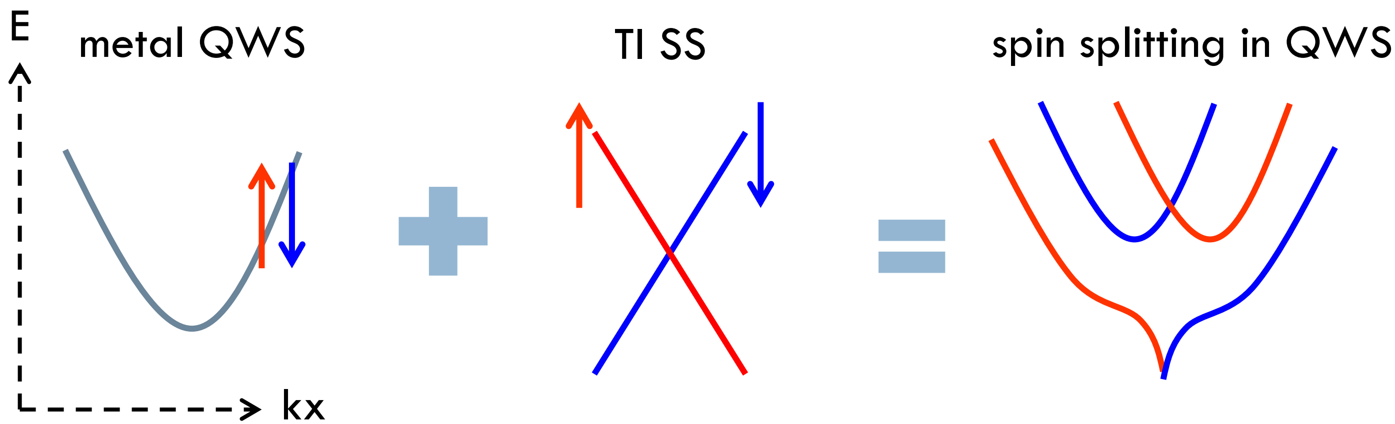



$\alpha_R = 1.75$

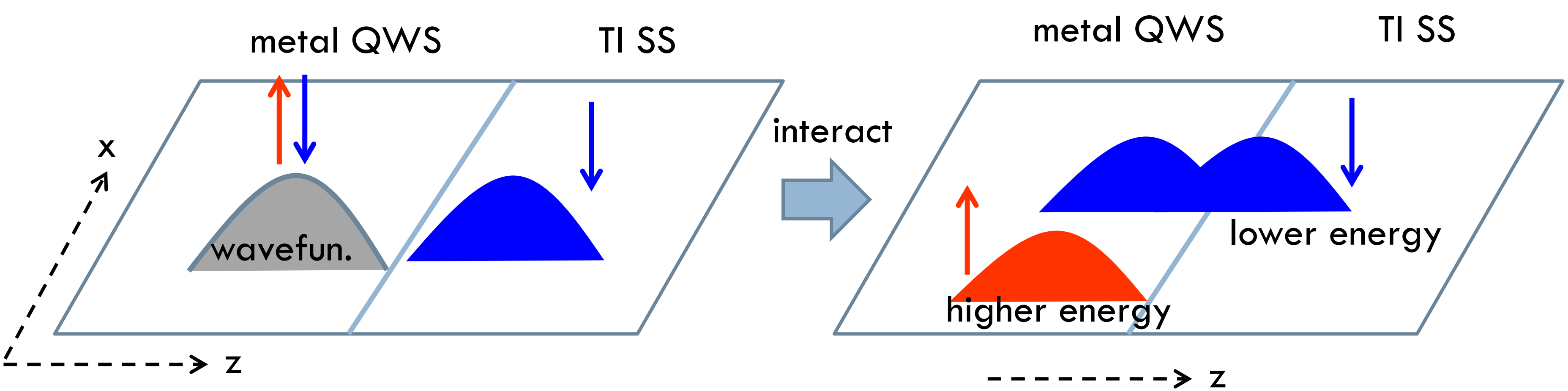
# 拓樸材料:可能的應用



The spin splitting in metal/TI is not due to potential gradient.




**The surface state of TI can be regraded as a spin filter.**



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# Topological phases



## Insulating phase

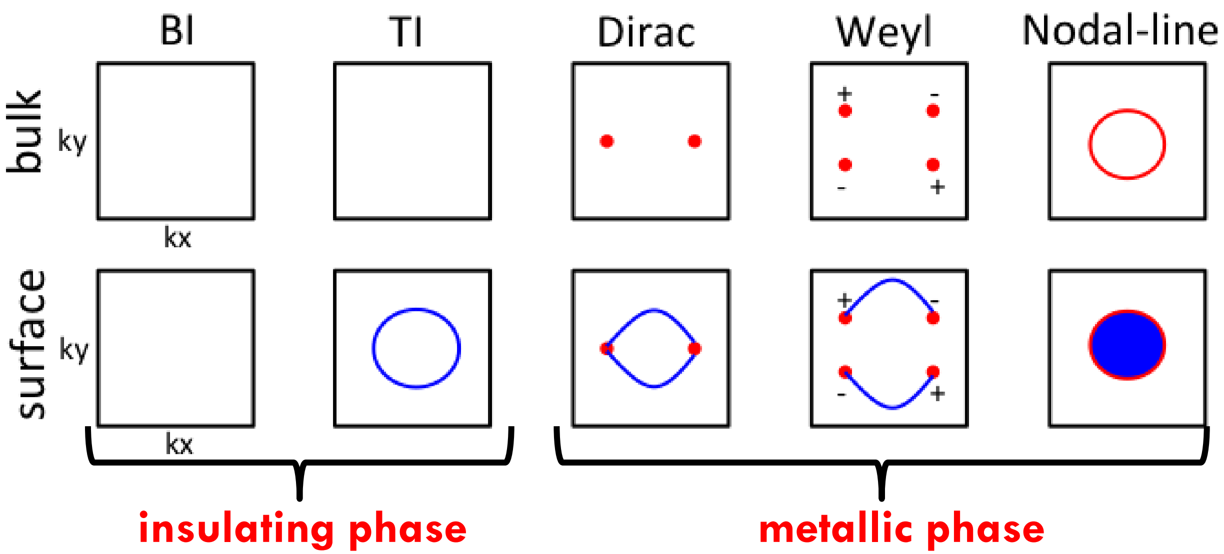
Topological insulator: $Bi_2Se_3$, $Bi_2Te_3$, LuPtBi …etc

Topological Kondo insulator: $SmB_6$, $YbB_6$ … etc

Weak topological insulator: KHgSb, $Bi_4Br_4$ … etc

topological crystalline insulator: SnTe

Topological superconductor: $Bi_2Se_3$/$NbSe_2$, $Cu_xBi_{1-x}Se_3$ …etc



# 拓樸材料(半金屬) vs 高能基本粒子



## High energy

Dirac Fermion

$$H = \begin{pmatrix} v\vec{\sigma}\cdot\vec{k} & m \\ m & -v\vec{\sigma}\cdot\vec{k} \end{pmatrix}$$

m=0

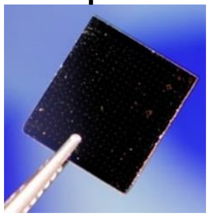
Weyl Fermion

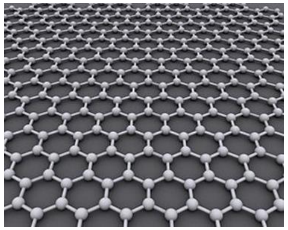
$$v\vec{\sigma}\cdot\vec{k} \qquad -v\vec{\sigma}\cdot\vec{k}$$

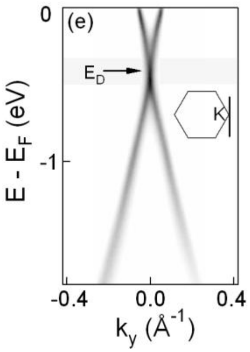
where $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

## Condensed matter

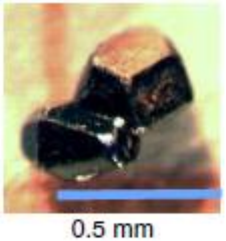
Graphene








Weyl semimetal (2015)




**TaAs: Theory**

S.-M. Huang et al, Nat. commun. **6**, 7373 (2015)

H. Weng et al, Phys. Rev. X **5**, 011029 (2015)

**TaAs: Experiment**

S.-Y. Xu et al, Science **349**, 613 (2015)

B. Q. Lv et al, Phys. Rev. X **5**, 031013 (2015)

L. X. Yang, Nat. phys. **11**, 724 (2015)

Nielsen-Ninomiya theorem: (Nuclear Physics B185 (1981) 20-40)

Equal numbers of $\chi$ =+1 and -1 WFs.

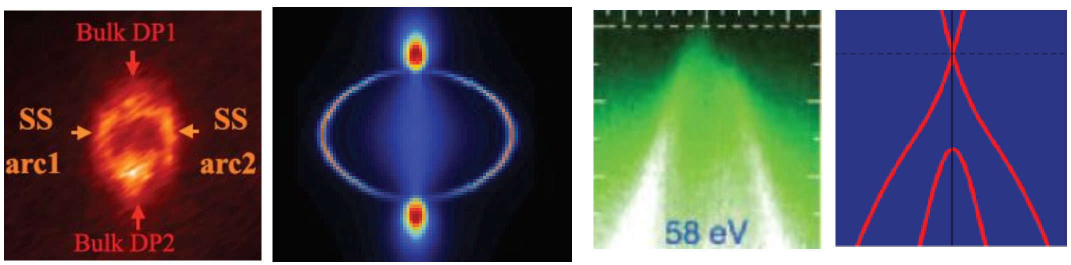
# 拓樸材料: Dirac and Weyl semimetal



Sciencexpress Reports

**Observation of Fermi arc surface states in a topological metal**

Publication date: December 18, 2014



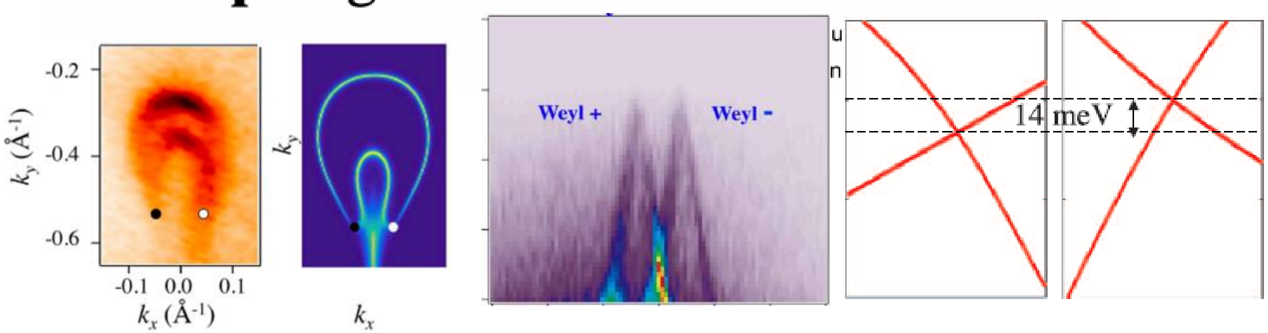

Dirac point (4重簡併)

$$H = \begin{pmatrix} v\vec{\sigma}\cdot\vec{k} & 0 \\ 0 & -v\vec{\sigma}\cdot\vec{k} \end{pmatrix}$$

無質量的電子

Sciencexpress Research Articles

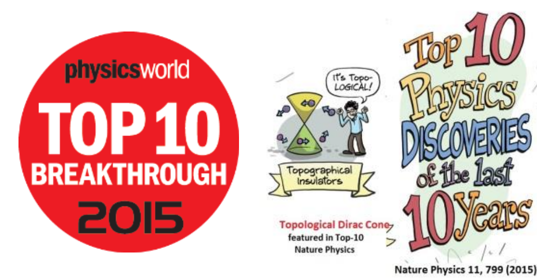
**Discovery of a Weyl Fermion semimetal and topological Fermi arcs**




Weyl point (2重簡併)

$$v\vec{\sigma}\cdot\vec{k} \qquad -v\vec{\sigma}\cdot\vec{k}$$

無質量的"半個"電子

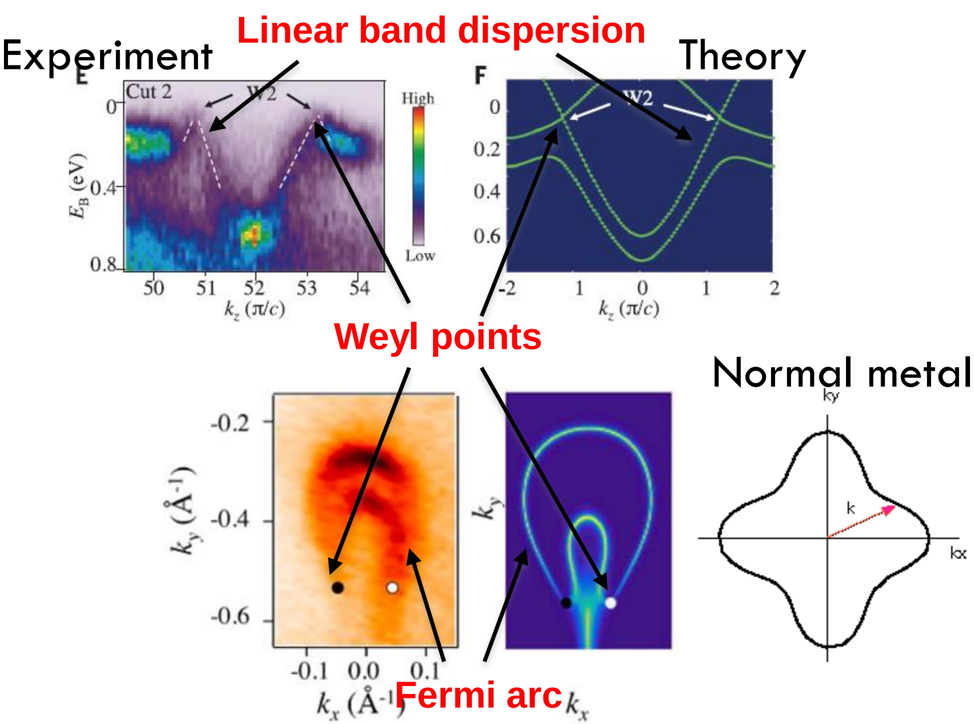


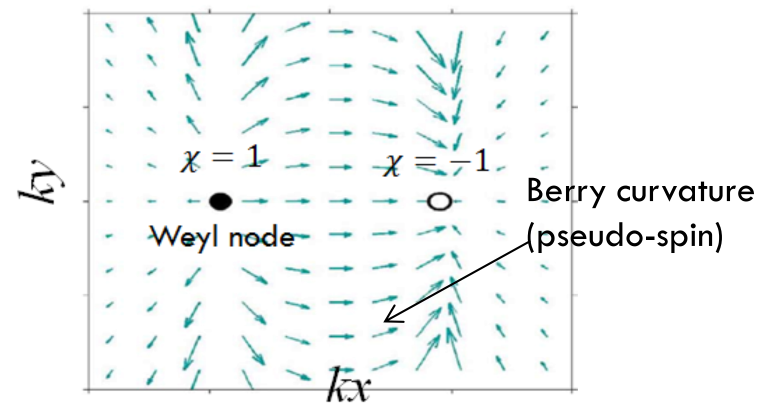
# Weyl semimetal (外爾半金屬)



**Weyl semimetals:**

1. Provide the realization of Weyl fermions (analogy with 3D graphene)
2. Extend the classification of topological phases of matter beyond insulators
3. Magnetic monopole in k-space (topological number called "chiral charge")
4. **Host exotic Fermi arc surface states**




**TaAs**
S.-Y. Xu et al,
Science **349**, 613 (2015)
**NbAs**
S.-Y. Xu… **T.-R. Chang** et al
Nat. Phys. **11**, 748 (2015)
**TaP**
S.-Y. Xu… **T.-R. Chang** et al
Sci. Adv. **1**, e1051092 (2015)

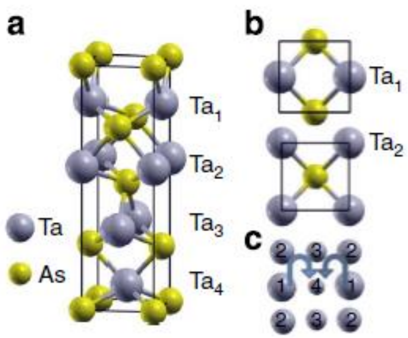
**NbP**
I. Belopolski … **T.-R. Chang** et al
PRL **116**, 066802 (2016)
**NbP (STM/STS)**
H. Zheng… **T.-R. Chang** et al
ACS nano **10**, 1378 (2016)
G. Chang… **T.-R. Chang** et al
PRL **116**, 066601 (2016)

# Weyl semimetal (外爾半金屬)

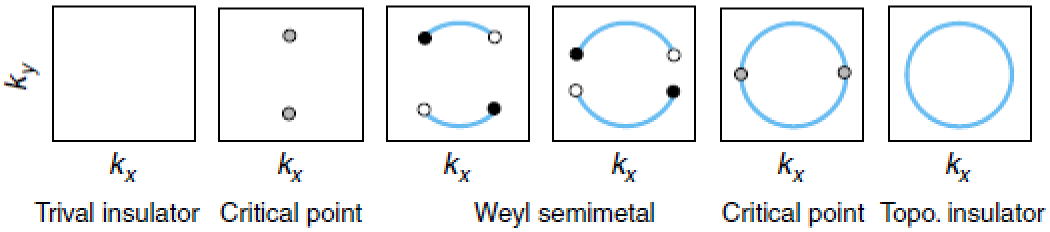


## Disadvantages of TaAs family

(1) 3D structure. Adversely to fabricate thin-film (e. g. MBE).




(2) Untunable Weyl points. Adversely to explore topological metal-insulator transition.




**Our goals**

(1) Searching Weyl semimetal with layer structure. (fabricating thin-film)

(2) Searching tunable Weyl semimetal. (exploring topological phase transition)

# Weyl semimetal (外爾半金屬)



ARTICLE
Received 23 Sep 2015 | Accepted 7 Jan 2016 | Published 15 Feb 2016
DOI: 10.1038/ncomms10639
OPEN

## Prediction of an arc-tunable Weyl Fermion metallic state in $Mo_xW_{1-x}Te_2$

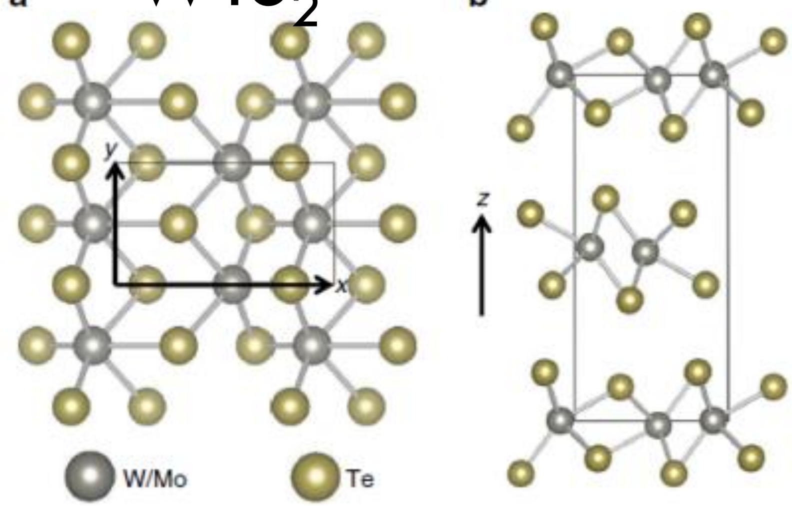
*Nature Commun.* ***7****, 10639 (2016)*

**Our goals**

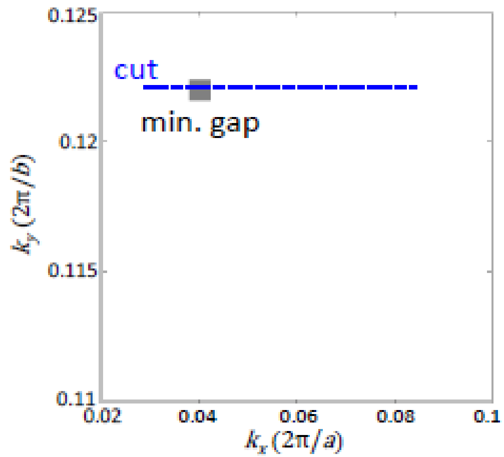
(1) Searching Weyl semimetal with layer structure. (fabricating thin-film)

(2) Searching tunable Weyl semimetal. (exploring topological phase transition)

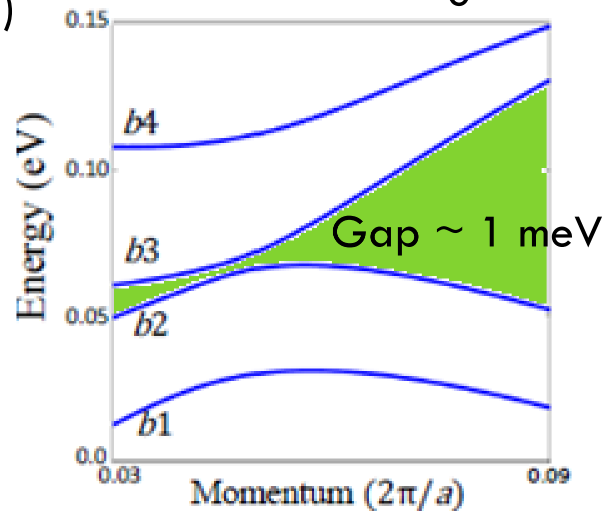
$WTe_2$




¼ BZ (location of gap min)




Band structure along cut



# Weyl semimetal (外爾半金屬)



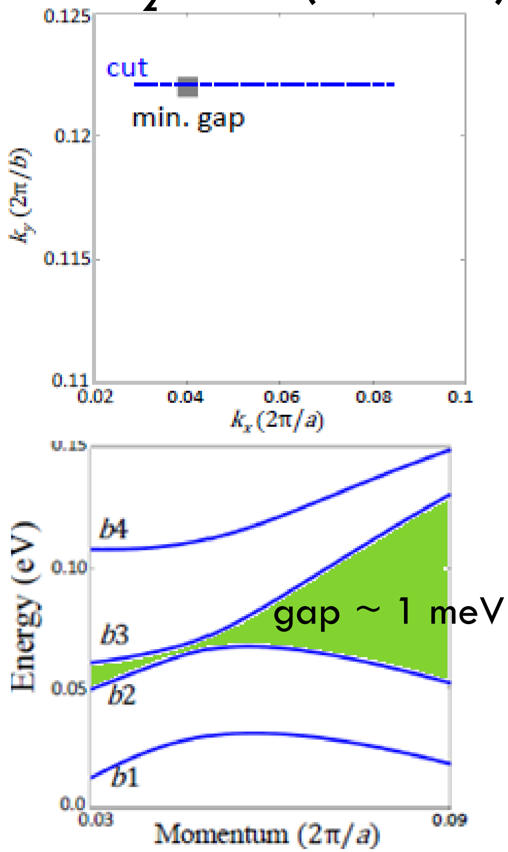
ARTICLE

Received 23 Sep 2015 | Accepted 7 Jan 2016 | Published 15 Feb 2016 DOI: 10.1038/ncomms10639 OPEN

*Nature Commun.* **7**, 10639 (2016)

Prediction of an arc-tunable Weyl Fermion metallic state in $Mo_xW_{1-x}Te_2$

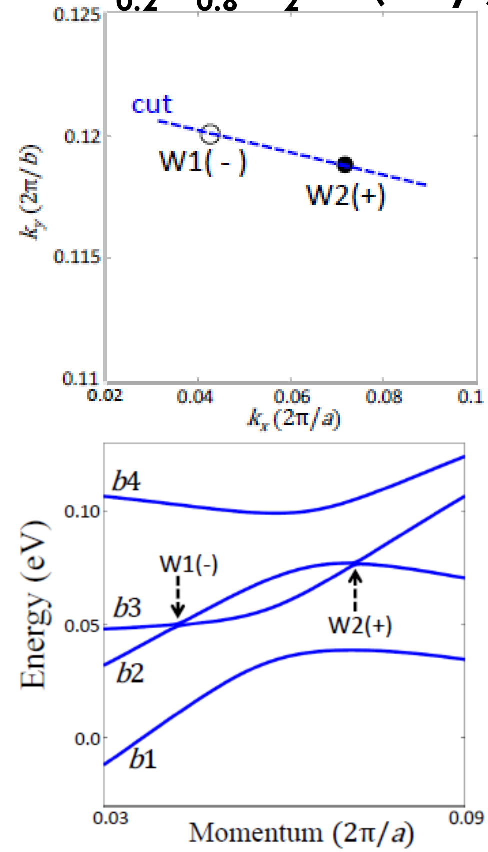
**$WTe_2$ (insulator)**




**We suggested: Mo doping**

reduce strength of SOC
as well as
lattice constants

**$Mo_{0.2}W_{0.8}Te_2$ (Weyl)**



# Weyl semimetal (外爾半金屬)

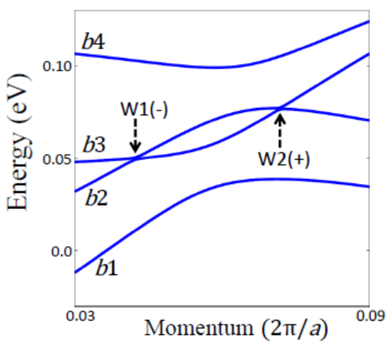


ARTICLE

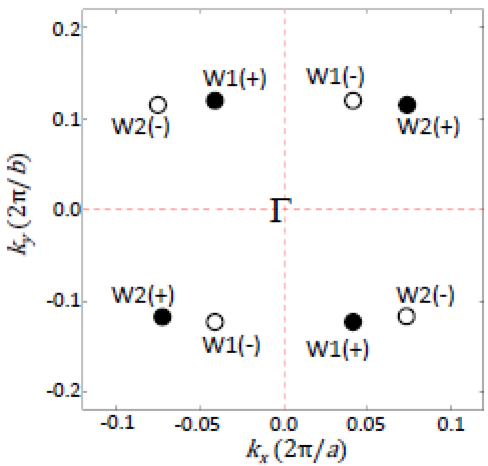
Received 23 Sep 2015 | Accepted 7 Jan 2016 | Published 15 Feb 2016 DOI: 10.1038/ncomms10639 OPEN

*Nature Commun.* **7**, 10639 (2016)

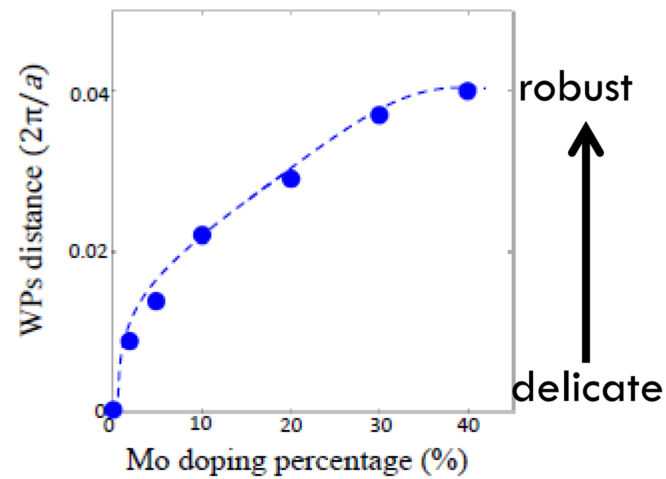
## Prediction of an arc-tunable Weyl Fermion metallic state in $Mo_xW_{1-x}Te_2$

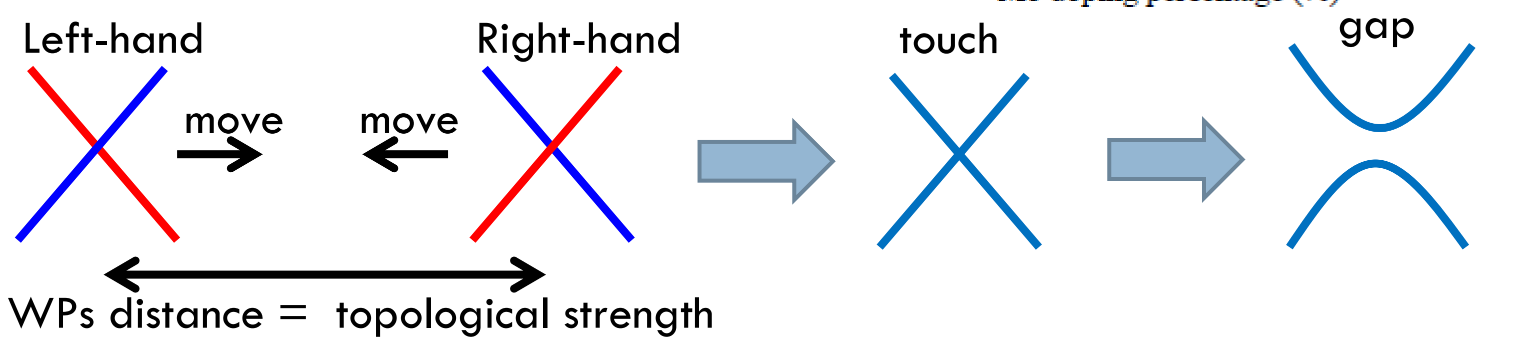



**Location of WPs (Mo 20%)**




**WPs distance (topological strength)**



# Weyl semimetal (外爾半金屬)



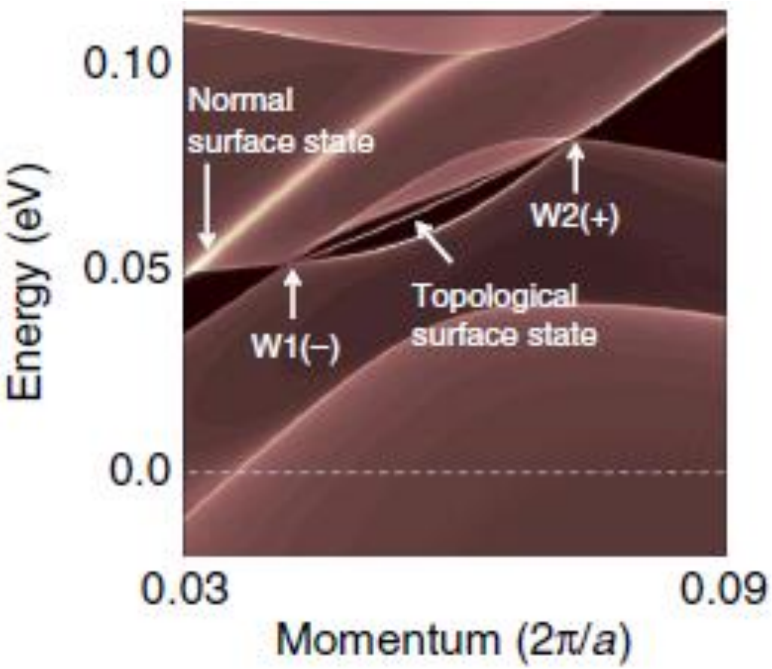
ARTICLE

Received 23 Sep 2015 | Accepted 7 Jan 2016 | Published 15 Feb 2016 DOI: 10.1038/ncomms10639 OPEN

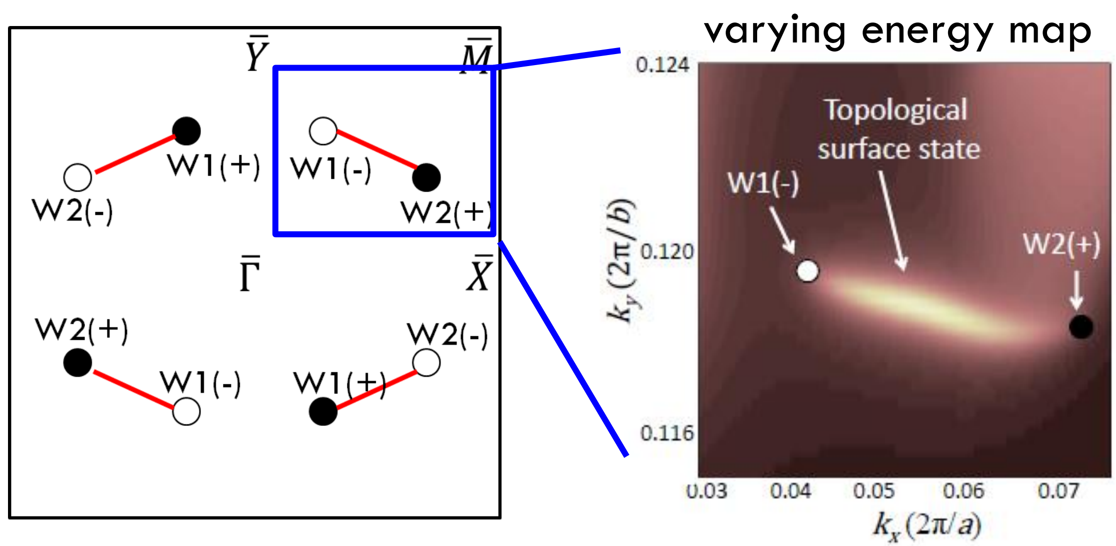
*Nature Commun.* ***7***, *10639 (2016)*

Prediction of an arc-tunable Weyl Fermion metallic state in $Mo_xW_{1-x}Te_2$

**Surface spectral weight simulation**




**Schematic of Fermi arc**




**Fermi arc surface state which connects the direct pair of Weyl nodes.**

# Weyl semimetal (外爾半金屬)



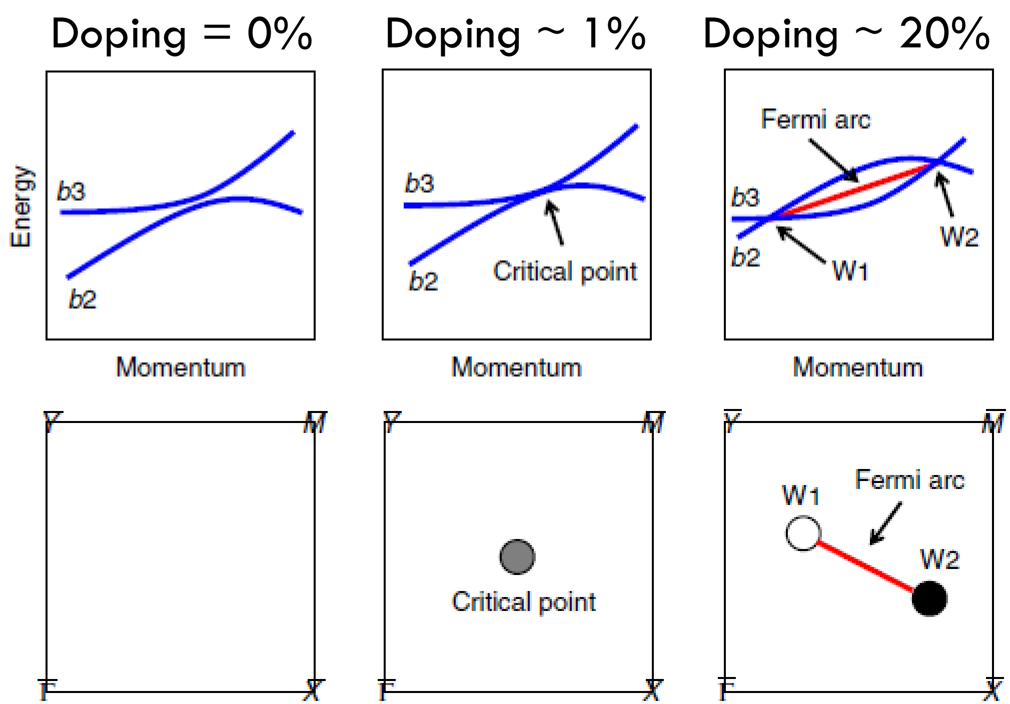
ARTICLE

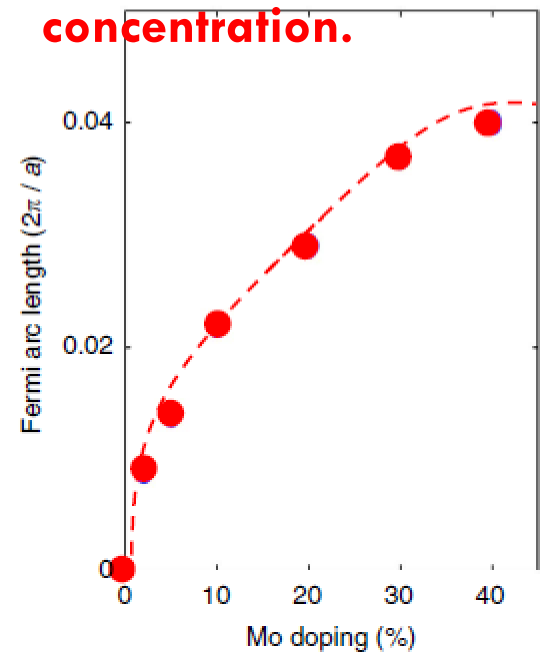
Received 23 Sep 2015 | Accepted 7 Jan 2016 | Published 15 Feb 2016 DOI: 10.1038/ncomms10639 OPEN

Prediction of an arc-tunable Weyl Fermion metallic state in $Mo_xW_{1-x}Te_2$

*Nature Commun.* ***7***, *10639 (2016)*

**topological strength can be tuned by varying Mo doping concentration.**




$Mo_xW_{1-x}Te_2$ is not only a Weyl semimetal with layer structure, but a tunable Weyl semimetal. This system is a good candidate for investigating topological metal-insulator phase transition.

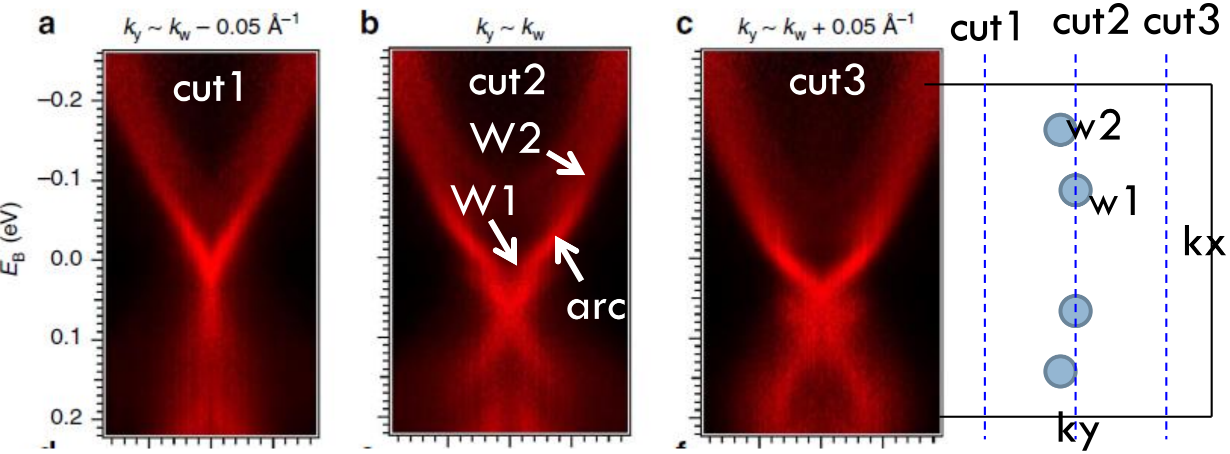
# Weyl semimetal: $Mo_xW_{1-x}Te_2$

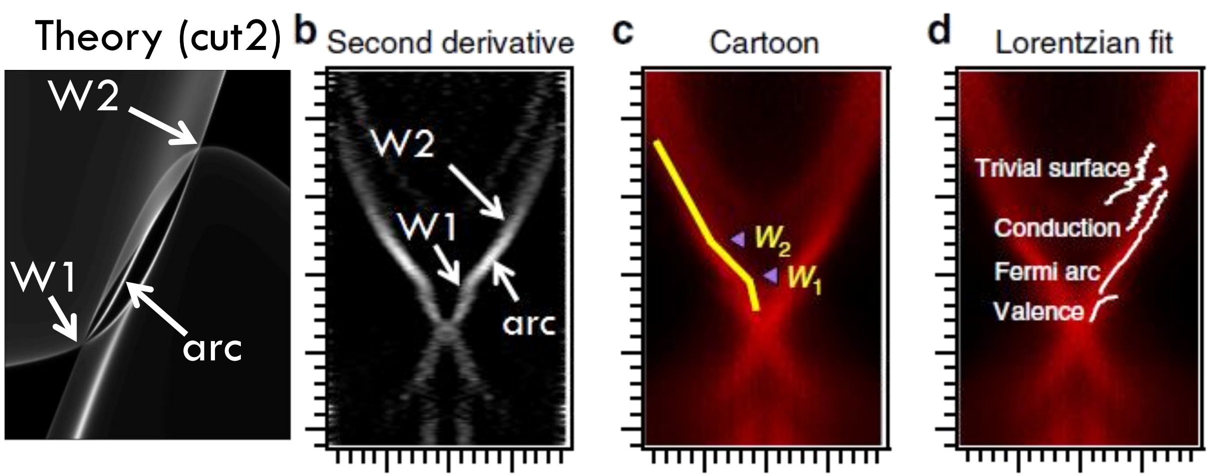


(1) *Nature Commun.* ***7****, 13643 (2016)*

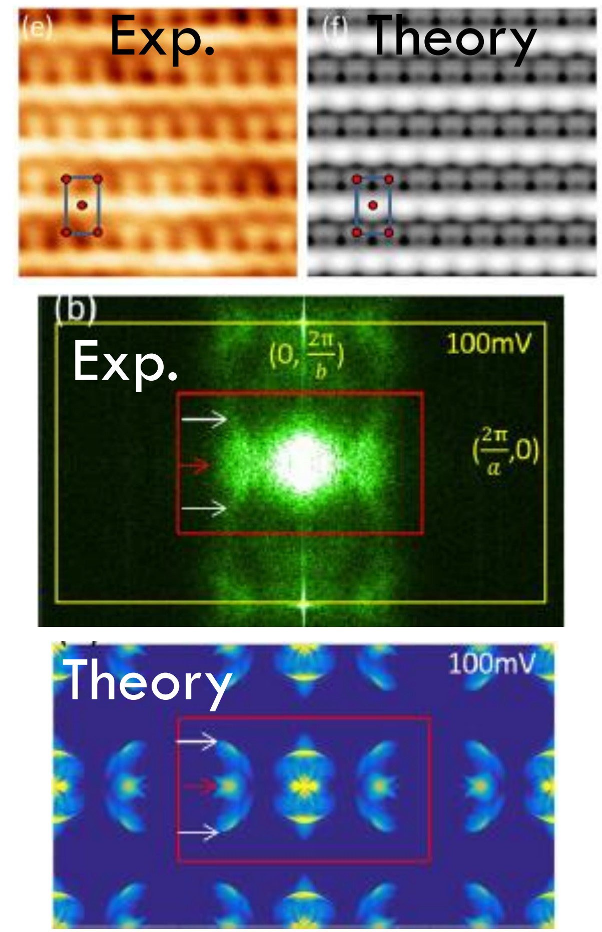
(2) *Phys. Rev. B* ***94****, 085127 (2016)*

**Experimental results**




(3)*Phys. Rev. Lett.* ***117****, 266804 (2016)*



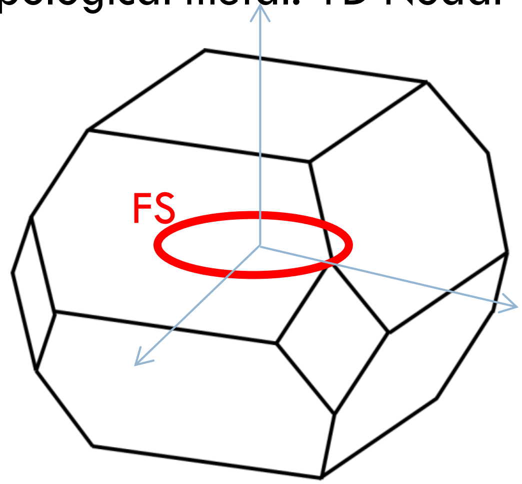
# Nodal-line semimetal (節線半金屬)



**Normal metal vs Topological metal**

Normal metal: 2D Fermi surface

Topological metal: 1D Nodal-line



# Nodal-line semimetal (節線半金屬)



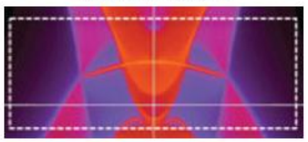
**Q:**

Nodal-line semimetals have yet to be found in real materials, even in DFT level.

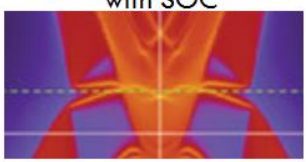
Previous works

$Cu_3PdN$
PRL **115**, 036807 (2015)

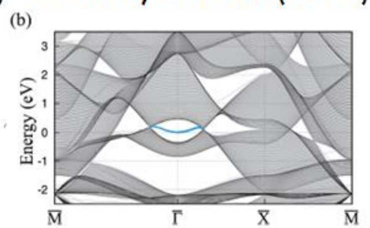
without SOC



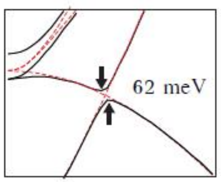
with SOC



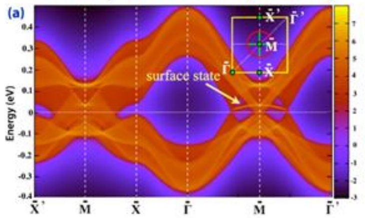
$Cu_3ZnN$
PRL **115**, 036806 (2015)



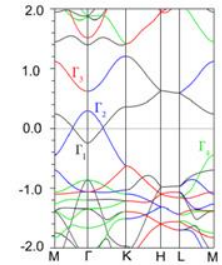

SOC gap



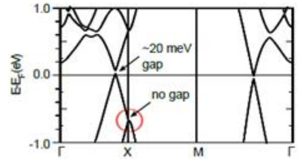

Graphene Networks
PRB **92**, 045108 (2015)




$Ca_3P_2$
APL Mat. **3**, 083602 (2015)



ZrSiS
Nat. commun. 7, 11696 (2016)




**Without SOC => Nodal-Line**
**With SOC => gap (or partially gapless)**

**Our goal:**

Searching Nodal-line Fermi surface in real materials.

# Nodal-line semimetal (節線半金屬)

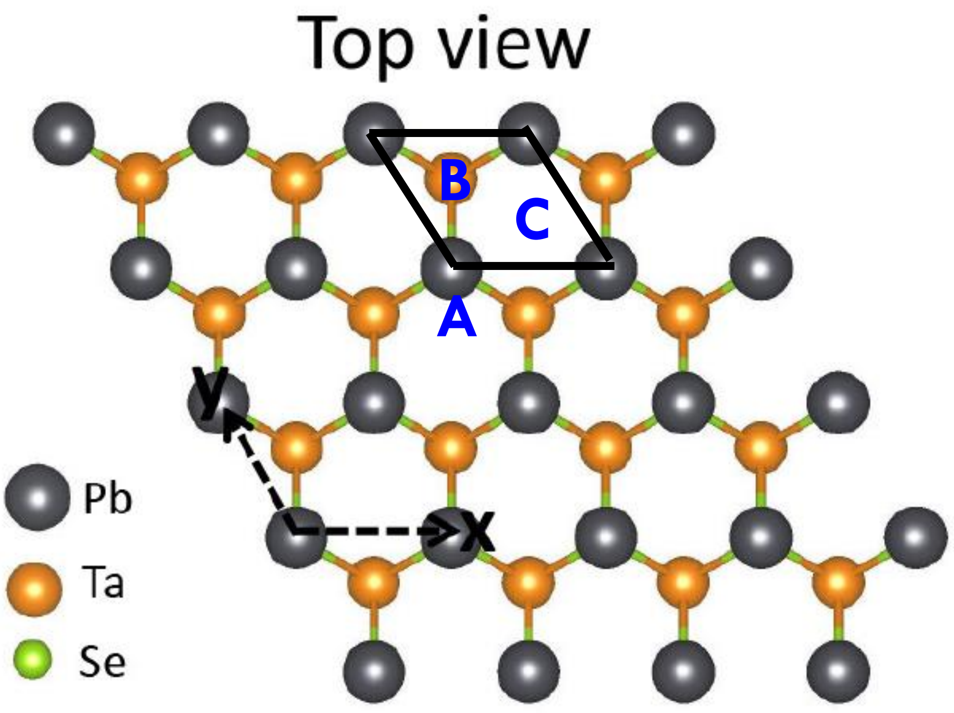


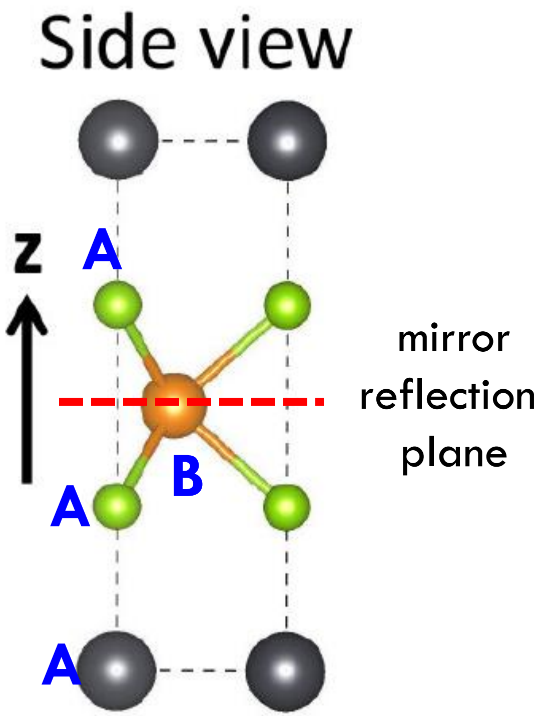
ARTICLE

Received 16 Nov 2015 | Accepted 28 Dec 2015 | Published 2 Feb 2016
DOI: 10.1038/ncomms10556 OPEN

Topological nodal-line fermions in spin-orbit metal $PbTaSe_2$

*Nature Commun.* **7**, 10556 (2016)



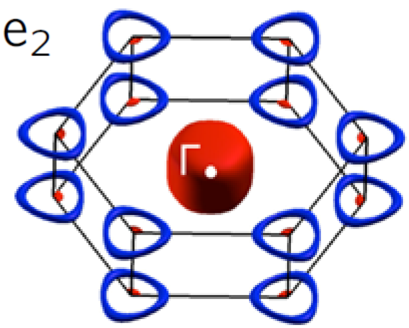
# Nodal-line semimetal (節線半金屬)



ARTICLE
Received 16 Nov 2015 | Accepted 28 Dec 2015 | Published 2 Feb 2016
DOI: 10.1038/ncomms10556
OPEN

*Nature Commun.* ***7****, 10556 (2016)*

Topological nodal-line fermions in spin-orbit metal $PbTaSe_2$

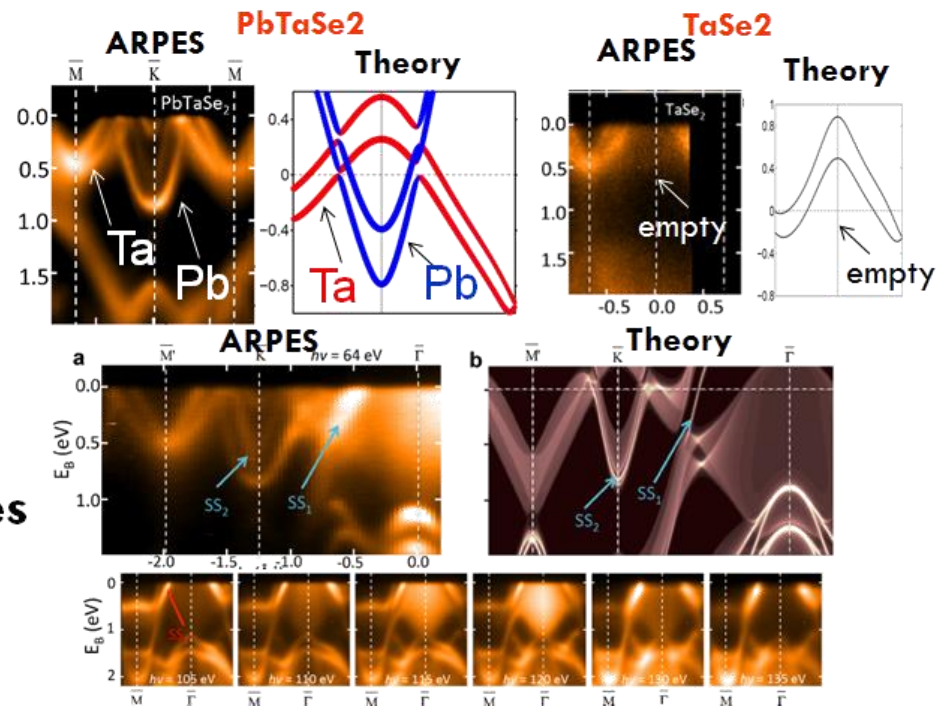



基本粒子物理完全無法描述的費米面.

Nodal-line Fermi surface (1維環).

**Bulk states**

**Surface states**

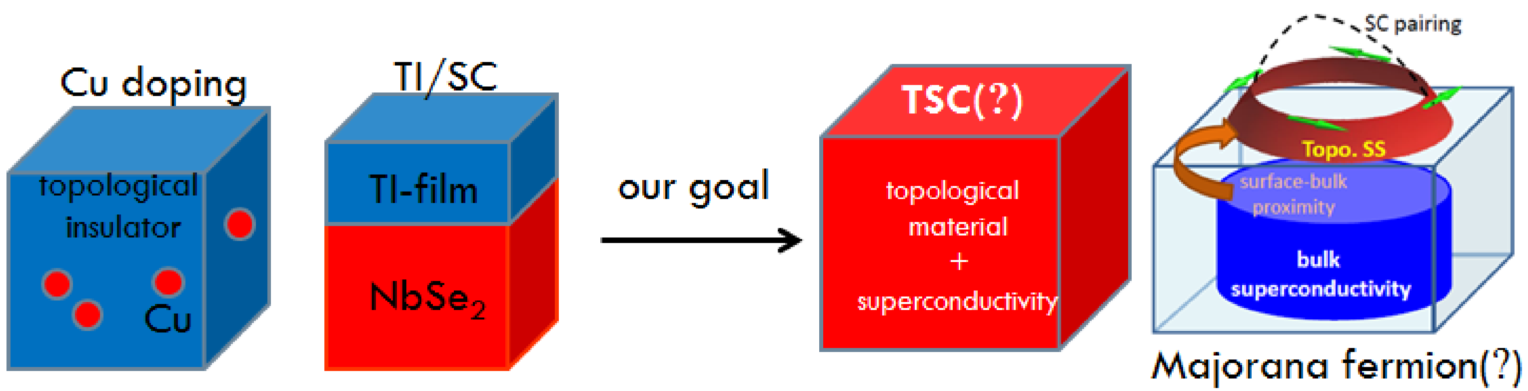


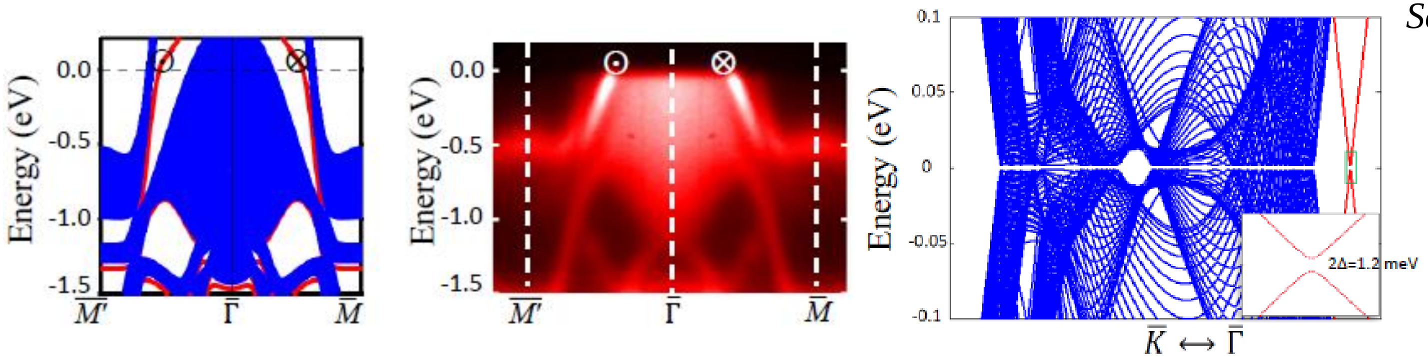
# Topological superconductor(拓樸超導體)



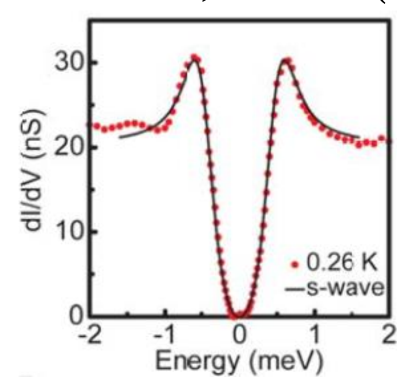
PHYSICAL REVIEW B 93, 245130 (2016)

**Topological Dirac surface states and superconducting pairing correlations in $PbTaSe_2$**

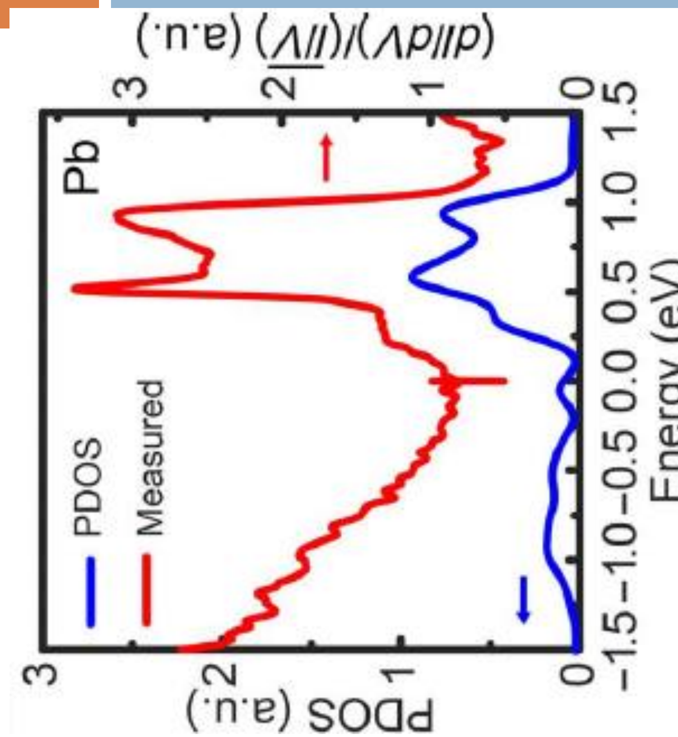



*Science Adv.* **2**, *e1600894 (2016)*

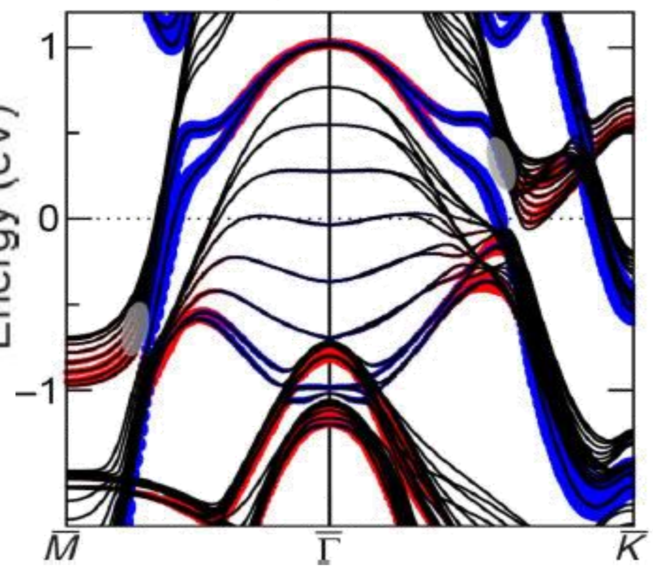


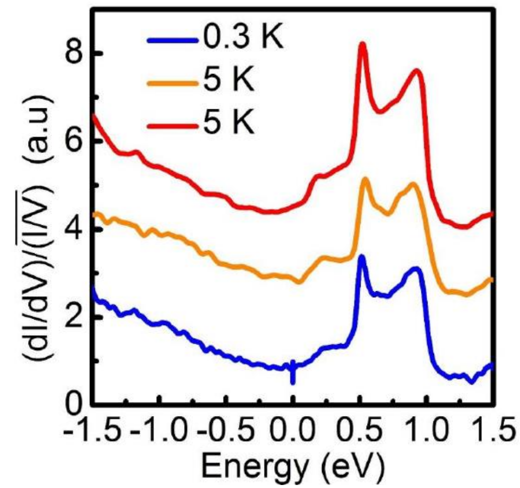
# Topological superconductor(拓樸超導體)

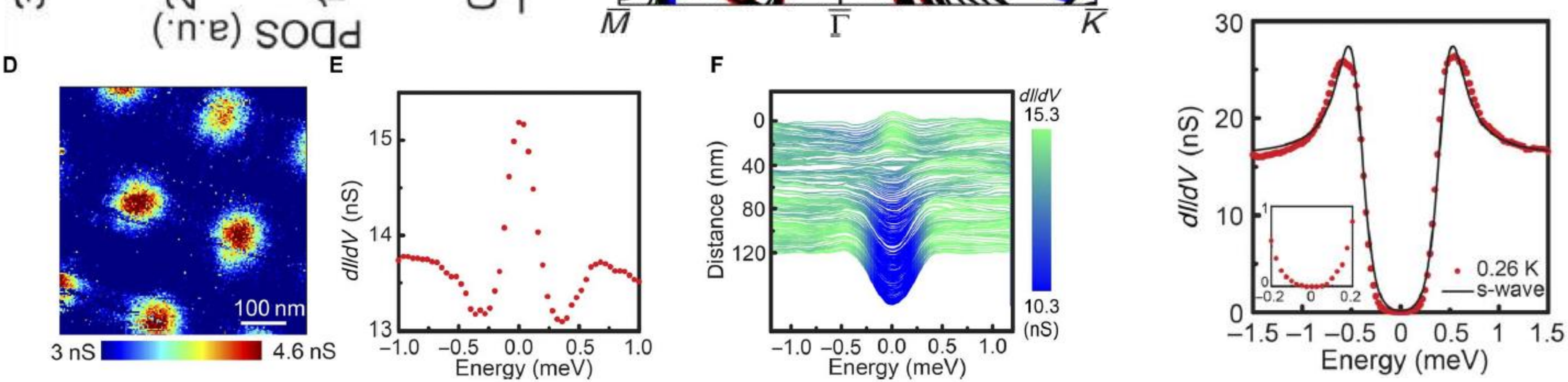



Science advances 2:e1600894 (2016)

**Superconducting topological surface states in the noncentrosymmetric bulk superconductor $PbTaSe_2$**



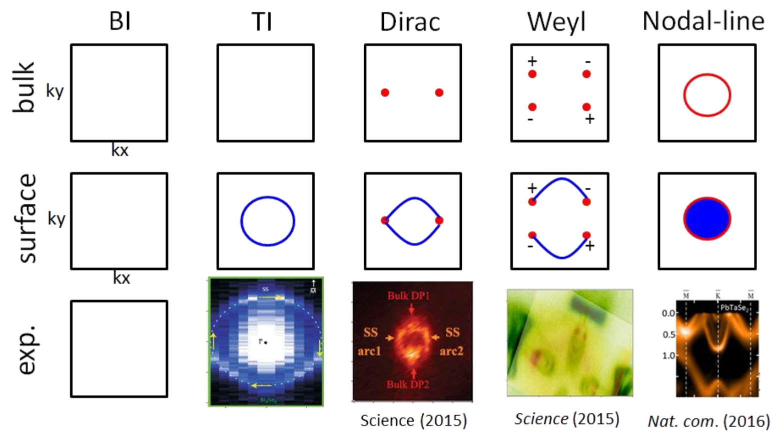



# Conclusion: Topological materials



**DFT + ab-initio tight-binding:**

- Comprehensively explore electronic structures of emerging materials
- Providing detailed theoretical interpretation for the experimental results.
- Prediction for new types of topological materials.




**Why topology is interesting in condensed matter physics?**

**Exotic states and potential applications**:

QAH, Magnetic monopole, Majorana fermion, Spintronics, Quantum computation…etc

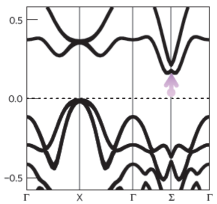
# 結論:馬後炮與煉金術還是可以做點東西



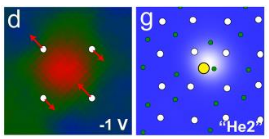
**Density functional theory (DFT) + ab-initio tight-binding model:**

## Transition metal oxides

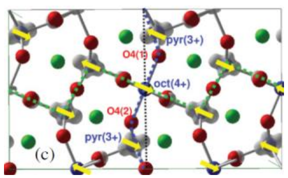
Iridate: $Sr_3Ir_2O_7$
Nat. Mat.




Cuprate: Bi2212
Nano Lett.

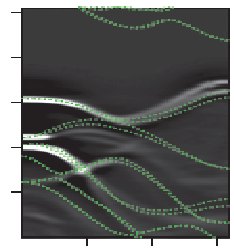



multiferroic: $TbMn_2O_5$
PRB

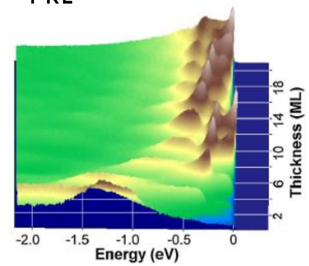



## 2D materials (TMDC and thin-film)

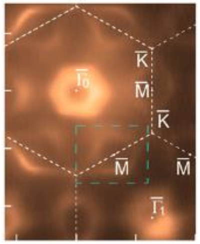
TMDC: $MoSe_2$
Nat. Nanotech.



Pb/Ge
PRL

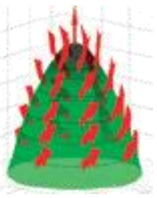


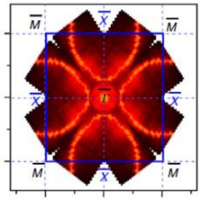

PbAu/Pb
NJP



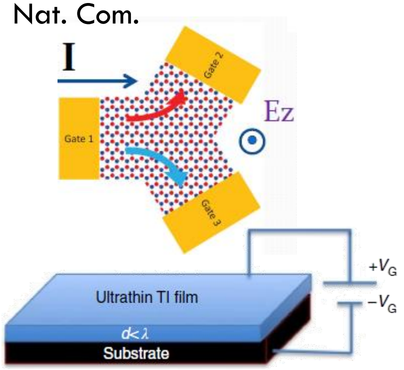
## Topological insulator

3D Topological insulator
Nat. Phys.
Nat. Com.
PRL



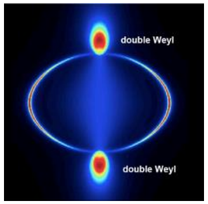


2D Topological insulator
Nat. Com.

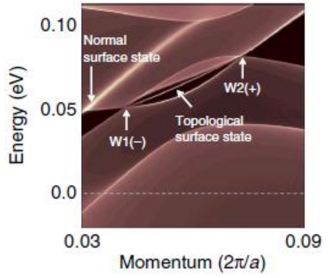



## Topological semimetals

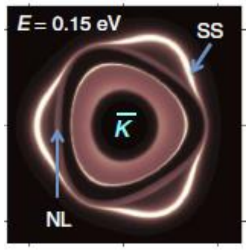
3D Dirac
Science
Nat. Com.




Weyl semimetals
Nat. Phys.
Nat. Com.
PRL




Nodal-line: $PbTaSe_2$
Nat. Com.



# Acknowledgements



**ARPES (topological)**

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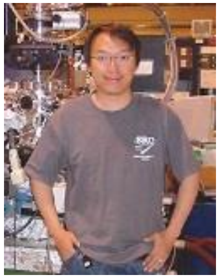

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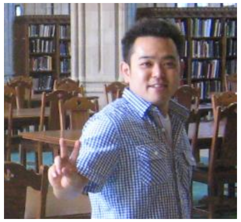

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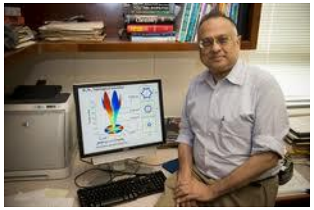

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**To see a world in a grain of sand …** —**William Blake**