Towards ideal topological materials: Comprehensive database searches using symmetry indicators

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2019年10月10日@北京大学

Cooperation

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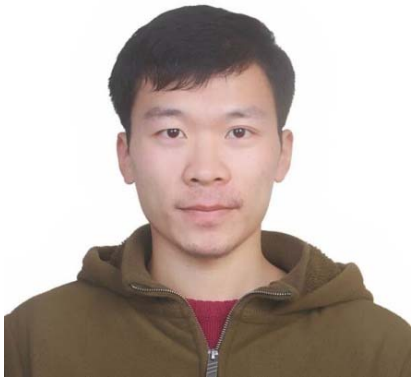



Hoi Chun Po & Ashvin Vishvanath； ***Harvard University***


Tang, Po, Vishwanath, ***Wan****, Nature Physics* ***15****, 470 (2019)*
Tang, Po, Vishwanath, ***Wan****, Science Advances* ***5****, eaau8725 (2019)*
Tang, Po, Vishwanath, ***Wan****, Nature* ***566****, 486 (2019)*
Wang, Tang, Ji, Zhang, Vishwanath, Po, ***Wan****, arXiv:1906.01283 (2019)*

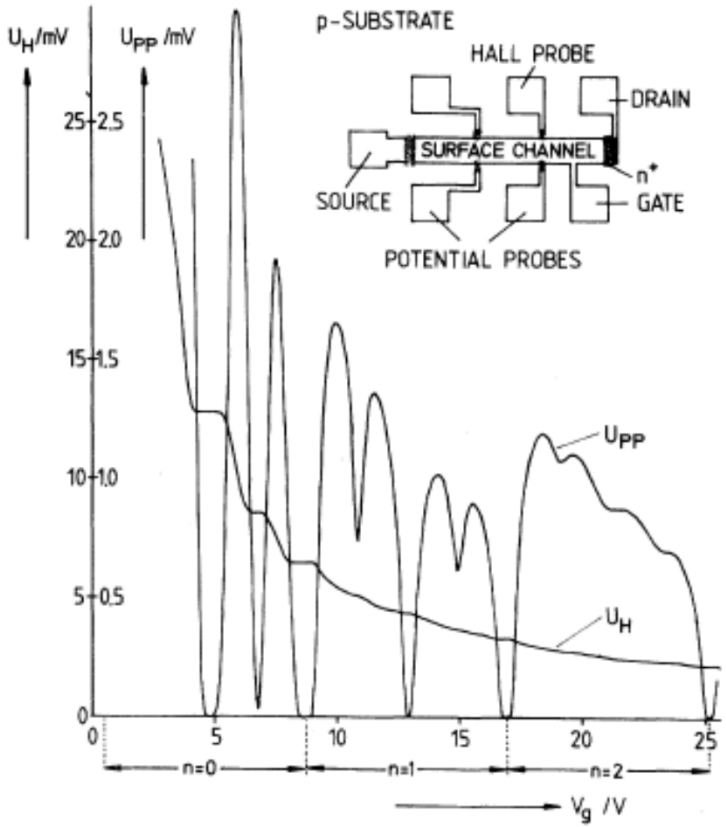
Content

- Symmetry Indicators
- Topological Materials

拓扑

- 朗道相变理论→对称性、序参量

- 1980



Quantized Hall Conductance in a Two-Dimensional Periodic Potential

D. J. Thouless, M. Kohmoto,[a] M. P. Nightingale, and M. den Nijs
Department of Physics, University of Washington, Seattle, Washington 98195
(Received 30 April 1982)

The Hall conductance of a two-dimensional electron gas has been studied in a uniform magnetic field and a periodic substrate potential U. The Kubo formula is written in a form that makes apparent the quantization when the Fermi energy lies in a gap. Explicit expressions have been obtained for the Hall conductance for both large and small $U/\hbar\omega_c$.

$$\sigma_H = \frac{ie^2}{A_0\hbar} \sum_{\epsilon_\alpha < E_F} \sum_{\epsilon_\beta > E_F} \frac{(\partial\hat{H}/\partial k_1)_{\alpha\beta}(\partial\hat{H}/\partial k_2)_{\beta\alpha} - (\partial\hat{H}/\partial k_2)_{\alpha\beta}(\partial\hat{H}/\partial k_1)_{\beta\alpha}}{(\epsilon_\alpha - \epsilon_\beta)^2},$$

Chern Number

- 2D BZ是一个torus，它组成的曲面包含的monopole的个数只能是整数

$$\sigma_{\mathrm{H}}=\frac{ie^2}{A_0\hbar}\sum_{\epsilon_\alpha<E_{\mathrm{F}}}\sum_{\epsilon_\beta>E_{\mathrm{F}}}\frac{(\partial\hat{H}/\partial k_1)_{\alpha\beta}(\partial\hat{H}/\partial k_2)_{\beta\alpha}-(\partial\hat{H}/\partial k_2)_{\alpha\beta}(\partial\hat{H}/\partial k_1)_{\beta\alpha}}{(\epsilon_\alpha-\epsilon_\beta)^2}$$

$$\Omega_{\mu\nu}^{n}(\boldsymbol{R})=i\sum_{n'\neq n}\frac{\langle n|\partial H/\partial R^{\mu}|n'\rangle\langle n'|\partial H/\partial R^{\nu}|n\rangle-(\nu\leftrightarrow\mu)}{(\varepsilon_n-\varepsilon_{n'})^2}.$$

$$\sigma_{xy}=\frac{e^2}{\hbar}\int_{\mathrm{BZ}}\frac{d^2k}{(2\pi)^2}\Omega_{k_xk_y}=n\frac{e^2}{h}.$$

Chern Number

Z2 Topological insulator

PRL 95, 226801 (2005) PHYSICAL REVIEW LETTERS week ending 25 NOVEMBER 2005

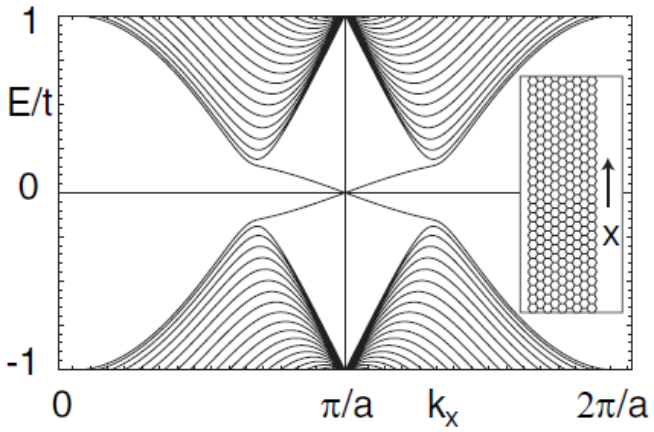
Quantum Spin Hall Effect in Graphene

C. L. Kane and E. J. Mele

PRL 95, 146802 (2005) PHYSICAL REVIEW LETTERS 30

Z_2 Topological Order and the Quantum Spin Hall Effect

C. L. Kane and E. J. Mele



Z2拓扑不变量

时间反演对称

SOC

Topological invariants in energy band

- **Chern number** in *T*-symmetry breaking system

- **Z_2 topological invariant** in *T*-symmetry invariant system

Relativistic Quantum Mechanics

- Klein-Gordon equation 1926

相对论+量子化

$$\mathbf{k} \to -i\nabla \qquad E \to i\partial_t \quad \text{+} \quad E^2=m^2+p^2 \quad \Rightarrow \quad (\Box - \mu^2)\phi(\mathbf{x}, t) = 0, \quad \Box = \nabla^2 - \partial_t^2$$

$$\textit{Negative Energies} \quad e^{(i\mathbf{k}\cdot\mathbf{x} - iEt)} \Rightarrow E = \pm(\mathbf{k}^2 + \mu^2)^{1/2}$$

$$\phi^*(\Box - \mu^2)\phi = 0 \qquad \phi(\Box - \mu^2)\phi^* = 0 \Rightarrow \partial_\mu j_\mu(x) = 0 \qquad \rho(x) = 2E\phi^*(x)\phi(x)$$

non-positive-definite

$$j_\mu(x) = i[(\partial_\mu\phi^*(x))\phi(x) - \phi^*(x)\partial_\mu\phi(x)]$$

Relativistic Quantum Mechanics

- Dirac equation 1928

$$(\gamma_\mu \partial_\mu + m)\psi = 0$$

$$\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2\delta_{\mu\nu}$$

$$(\mu, \nu = 1 \ldots 4)$$

- Dirac representation

Euclidian vector $x_\mu = (\mathbf{x}, it)$

Greek letters $\mu, \nu, \ldots$ take values from 1 to $d+1$

$A \cdot B \quad \sum_\mu A_\mu B_\mu$

$c = \hbar = 1$

Relativistic Quantum Mechanics

- Dirac equation 1928

$$(\gamma_\mu \partial_\mu + m)\psi = 0$$

$$\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2\delta_{\mu\nu}$$

$$(\mu, \nu = 1 \ldots 4)$$

- Dirac representation

在静止系，Dirac方程对角化

spinor index as $(\xi\sigma)$ where $\xi = \pm$ and $\sigma = \uparrow, \downarrow$

- Weyl representation

the representation of the Lorentz group is $(\frac{1}{2}, 0) \oplus (0, \frac{1}{2})$

spinor index $(\zeta\sigma)$ where $\zeta = L, R$ and $\sigma = \uparrow, \downarrow$

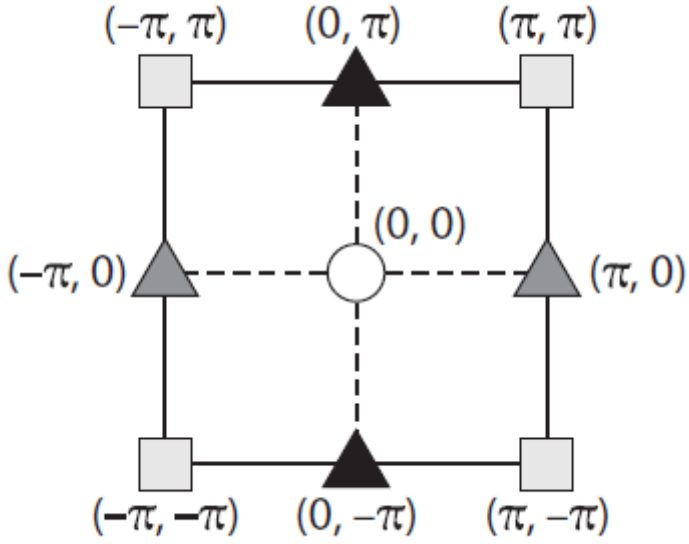
$$\psi_{+,\sigma} = \frac{1}{\sqrt{2}}(\psi_{L,\sigma} - \psi_{R,\sigma}),\ \psi_{-,\sigma} = \frac{1}{\sqrt{2}}(\psi_{L,\sigma} + \psi_{R,\sigma})$$

Topological Insulator

- Bulk insulator
- Topological protected surface state

- Mass term in Dirac Equation change Sign

$$H_t = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m$$



Bulk-boundary correspondence

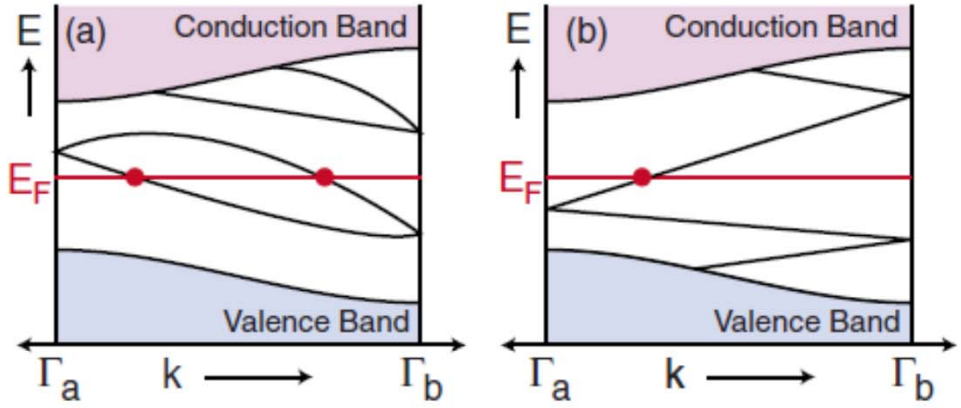


FIG. 3. (Color online) Electronic dispersion between two boundary Kramers degenerate points $\Gamma_a=0$ and $\Gamma_b=\pi/a$. In (a) the number of surface states crossing the Fermi energy E_F is even, whereas in (b) it is odd. An odd number of crossings leads to topologically protected metallic boundary states.

Weak topological insulator

Z_2 invariants (γ0; γ1,γ2,γ3)

Strong topological insulator

$$\mathcal{H}_{\text{surface}} = -i\hbar v_F \vec{\sigma} \cdot \vec{\nabla},$$

Justify 3D TI

① Surface State Electron Structure

② Adiabatic Continue Band Transformation

③ Band inversion

④ Calculate Z_2

Calculate Z_2

➢ **With inversion symmetry**

Fu-Kane theorem (*Fu & Kane, 2007*)

➢ **Without inversion symmetry**

directly calculate Z_2

(*Feng, Wen, Zhou, Xiao & Yao (2012)*)

$$Z_2 = \frac{1}{2\pi}\left[\oint_{\partial \mathcal{B}^+} d\boldsymbol{k}\cdot\mathcal{A}(\boldsymbol{k}) - \int_{\mathcal{B}^+} d^2k\,\mathcal{F}(\boldsymbol{k})\right] \bmod 2,$$

where $\mathcal{A}(\boldsymbol{k})$ and $\mathcal{F}(\boldsymbol{k})$ are the Berry connection and Berry curvature, respectively,

$$\mathcal{A}(\boldsymbol{k}) = i\sum_n \langle u_n(\boldsymbol{k}) \mid \nabla_{\boldsymbol{k}} u_n(\boldsymbol{k})\rangle \qquad \mathcal{F}(\boldsymbol{k}) = \nabla_{\boldsymbol{k}} \times \mathcal{A}(\boldsymbol{k})\mid_z .$$

周期表

PHYSICAL REVIEW B **78**, 195125 (2008)

Classification of topological insulators and superconductors in three spatial dimensions

Andreas P. Schnyder,[1] Shinsei Ryu,[1] Akira Furusaki,[2] and Andreas W. W. Ludwig[3]

		TRS	PHS	SLS	$d=1$	$d=2$	$d=3$
Standard	A (unitary)	0	0	0	-	Z	-
(Wigner-Dyson)	AI (orthogonal)	+1	0	0	-	-	-
	AII (symplectic)	−1	0	0	-	Z_2	Z_2
Chiral	AIII (chiral unitary)	0	0	1	Z	-	Z
(sublattice)	BDI (chiral orthogonal)	+1	+1	1	Z	-	-
	CII (chiral symplectic)	−1	−1	1	Z	-	Z_2
BdG	D	0	+1	0	Z_2	Z	-
	C	0	−1	0	-	Z	-
	DIII	−1	+1	1	Z_2	Z_2	Z
	CI	+1	−1	1	-	-	Z

TABLE I. Ten symmetry classes of single-particle Hamiltonians classified in terms of the presence or absence of time-reversal symmetry (TRS) and particle-hole symmetry (PHS), as well as "sublattice" (or "chiral") symmetry (SLS) (Refs. 37 and 38). In the table, the absence of symmetries is denoted by "0." The presence of these symmetries is denoted by either "+1" or "−1," depending on whether the (antiunitary) operator implementing the symmetry at the level of the single-particle Hamiltonian squares to "+1" or "−1" (see text). [The index ± 1 equals η_c in Eq. (1b); here $\epsilon_c = +1$ and -1 for TRS and PHS, respectively.] For the first six entries of the table (which can be realized in nonsuperconducting systems), TRS$=+1$ when the SU(2) spin is an integer [called TRS (even) in the text] and TRS$=-1$ when it is a half-integer [called TRS (odd) in the text]. For the last four entries, the superconductor "Bogoliubov–de Gennes" (BdG) symmetry classes D, C, DIII, and CI, the Hamiltonian preserves SU(2) spin-1/2 rotation symmetry when PHS$=-1$ [called PHS (singlet) in the text], while it does not preserve SU(2) when PHS$=+1$ [called PHS (triplet) in the text]. The last three columns list all topologically non-trivial quantum ground states as a function of symmetry class and spatial dimension. The symbols Z and Z_2 indicate whether the space of quantum ground states is partitioned into topological sectors labeled by an integer or a Z_2 quantity, respectively.

Topological Crystalline Insulators

Spatial Symmetries

PRL **106,** 106802 (2011) PHYSICAL REVIEW LETTERS

Topological Crystalline Insulators

Liang Fu

ARTICLES
PUBLISHED ONLINE:16 DECEMBER 2012 | DOI:10.1038/NPHYS2513
nature physics

The space group classification of topological band-insulators

Robert-Jan Slager[1], Andrej Mesaros[2], Vladimir Juričić[1]* and Jan Zaanen[1]

Y. Ando and L. Fu, Annual Review of Condensed Matter Physics **6**, 361 (2015).

Topological Crystalline Insulators

- Mirror Chern Insulator

Ando and Fu, Annu. Rev. Condens. Matter Phys. ***6****, 361 (2015)*

- Hourglass Fermions

Wang, Alexandradinata, Cava, Bernevig, Nature ***532****, 189 (2016).*

- Wallpaper Fermions

Wieder et al., Science ***361****, 246 (2018)*

- Higher-order topological insulators

Fang&Fu; Schindler et al., Langbehn et al., Song, Fang&Fang; Benalcazar et al., (2017)

…

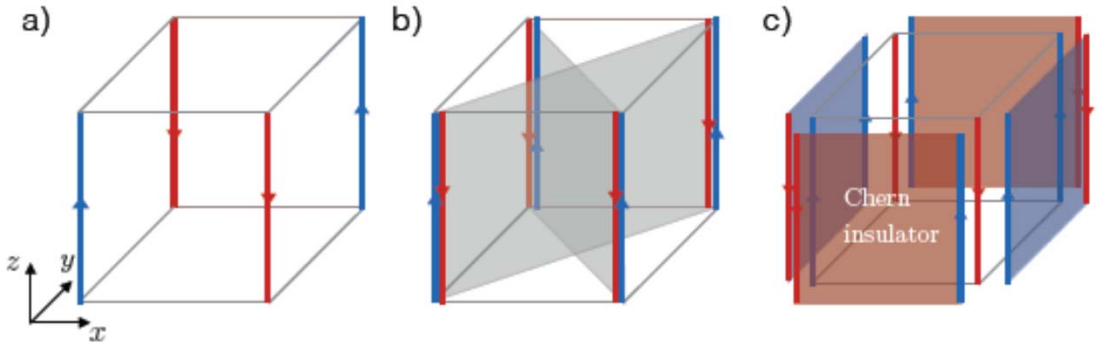
Higher-Order Topological Insulators

arXiv:1708.03636

Frank Schindler,[1] Ashley M. Cook,[1] Maia G. Vergniory,[2,3] Zhijun Wang,[4]
Stuart S. P. Parkin,[5] B. Andrei Bernevig,[4,2,6] and Titus Neupert[1]

bulk (d)→d-1, d-2, d-3

Second order



Topological Insulators Turn a Corner

Theorists have discovered topological insulators that are insulating in their interior and on their surfaces but have conducting channels at corners or along edges.

by Siddharth A. Parameswaran* and Yuan Wan†

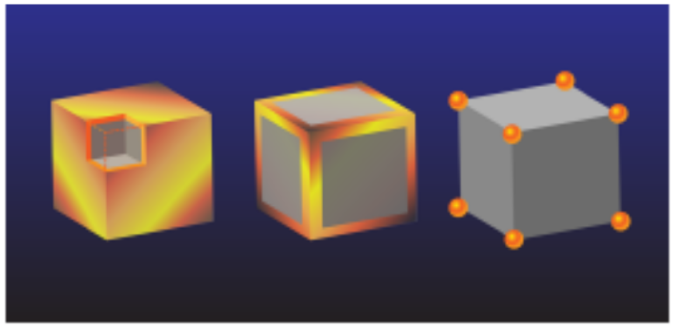


Figure 1: Usually, 3D topological insulators conduct via gapless states on their 2D surfaces but are insulating in their bulk (left). Recently proposed second- and third-order 3D TIs have gapless states on their 1D hinges (middle) or 0D corners (right), respectively, and they constitute a new class of topological phases of matter. (APS/Alan Stonebraker)

[2] W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, "Quantized Electric Multipole Insulators," Science **357**, 61 (2017).
[3] W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, "Electric Multipole Moments, Topological Multipole Moment Pumping, and Chiral Hinge States in Crystalline Insulators," Phys. Rev. B. **96**, 245115 (2017).
[4] Z. Song, Z. Fang, and C. Fang, "$(d-2)$-dimensional edge states of rotation symmetry protected topological states," Phys. Rev. Lett. **119**, 246402 (2017).
[5] J. Langbehn, Y. Peng, L. Trifunovic, F. von Oppen, and P. W. Brouwer, "Reflection-symmetric second-order topological insulators and superconductors," Phys. Rev. Lett. **119**, 246401 (2017).

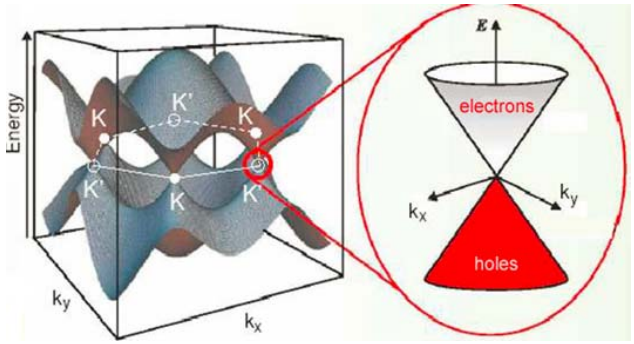
11 December 2017 Physics 10, 132

Dirac Fermion in Condensed Matter

Massless Dirac Fermion

K-point at BZ of Graphene (1947)

2004, 2005



Two-dimensional gas of massless Dirac fermions in graphene

Vol 438|10 November 2005|doi:10.1038/nature04233

K. S. Novoselov[1], A. K. Geim[1], S. V. Morozov[2], D. Jiang[1], M. I. Katsnelson[3], I. V. Grigorieva[1], S. V. Dubonos[2] & A. A. Firsov[2]

Vol 438|10 November 2005|doi:10.1038/nature04235

Experimental observation of the quantum Hall effect and Berry's phase in graphene

Yuanbo Zhang[1], Yan-Wen Tan[1], Horst L. Stormer[1,2] & Philip Kim[1]

Dirac Fermion in CM

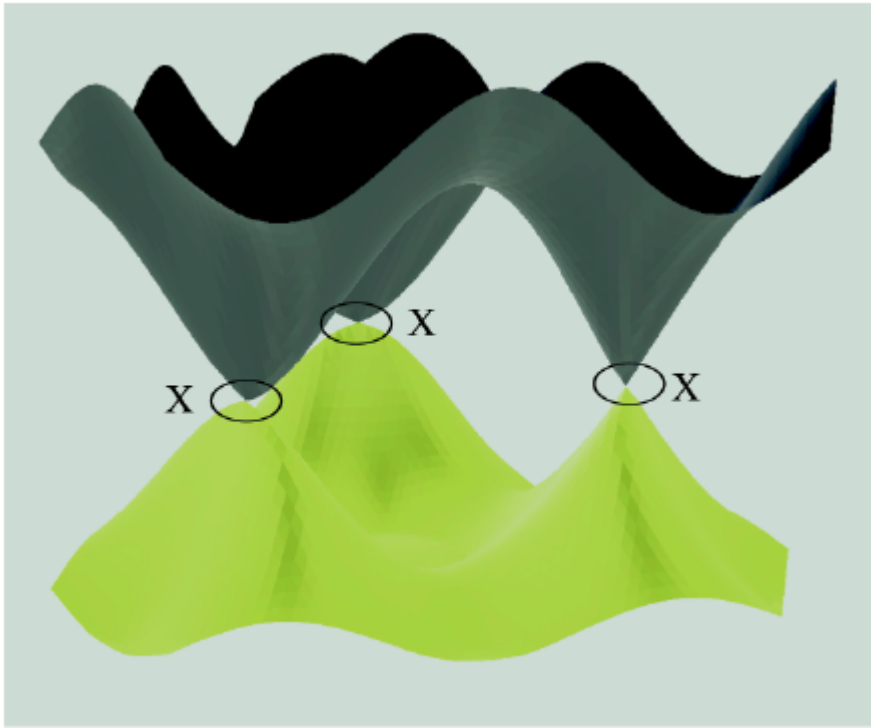
Massless Dirac Fermion 3D

symmetry protected degeneracies

Dirac Semimetal in Three Dimensions

S. M. Young,[1] S. Zaheer,[2] J. C. Y. Teo,[2,*] C. L. Kane,[2] E. J. Mele,[2] and A. M. Rappe[1]

PRL **108,** 140405 (2012)



- **Four dimensional irreducible representations at high symmetry points of BZ**
- **Linearly in all directions around these points**

Dirac Fermion in CM

Dirac semimetal and topological phase transitions in A_3Bi (A = Na, K, Rb)

Zhijun Wang,[1] Yan Sun,[2] Xing-Qiu Chen,[2] Cesare Franchini,[2] Gang Xu,[1] Hongming Weng,[1,*] Xi Dai,[1] and Zhong Fang[1,†]

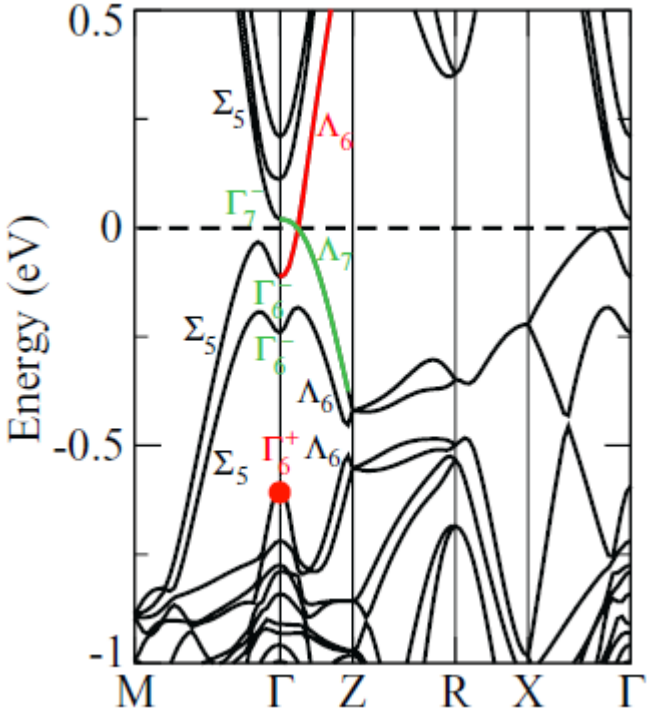
PHYSICAL REVIEW B **85**, 195320 (2012)

Three-dimensional Dirac semimetal and quantum transport in Cd_3As_2

Zhijun Wang, Hongming Weng,* Quansheng Wu, Xi Dai, and Zhong Fang†

PHYSICAL REVIEW B **88**, 125427 (2013)

- **Two bands along high symmetry lines of BZ belong to different two dimensional irreducible representations→**

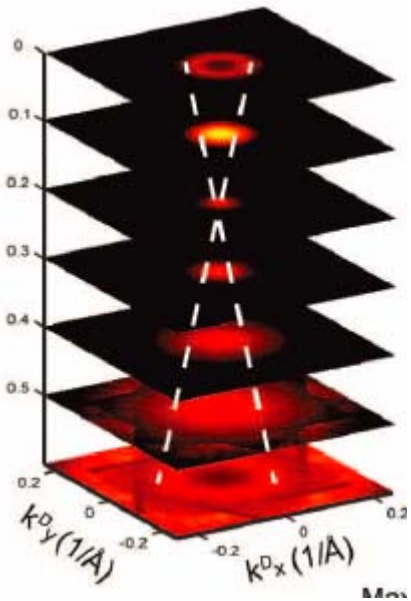


Dirac Fermion in CM

Discovery of a Three-Dimensional Topological Dirac Semimetal, Na_3Bi

Z. K. Liu,[1*] B. Zhou,[2,3*] Y. Zhang,[3] Z. J. Wang,[4] H. M. Weng,[4,5] D. Prabhakaran,[2] S.-K. Mo,[3] Z. X. Shen,[1] Z. Fang,[4,5] X. Dai,[4,5] Z. Hussain,[3] Y. L. Chen[2,6]†

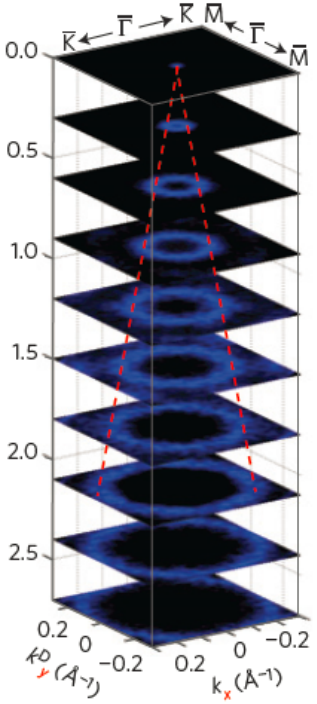
21 FEBRUARY 2014 VOL 343 SCIENCE



A stable three-dimensional topological Dirac semimetal Cd_3As_2

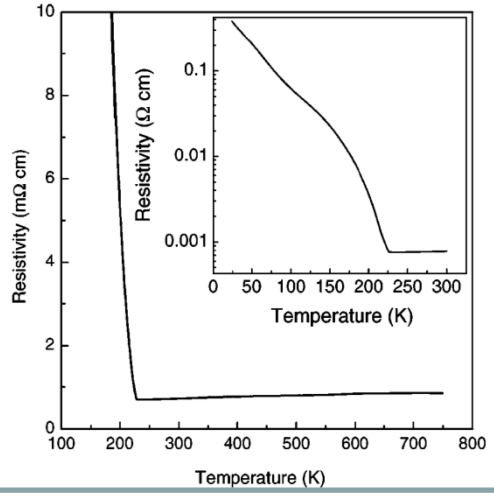
Z. K. Liu[1†], J. Jiang[2,3†], B. Zhou[2,4†], Z. J. Wang[5†], Y. Zhang[1,4], H. M. Weng[5], D. Prabhakaran[2], S-K. Mo[4], H. Peng[2], P. Dudin[6], T. Kim[6], M. Hoesch[6], Z. Fang[5], X. Dai[5], Z. X. Shen[1], D. L. Feng[3], Z. Hussain[4] and Y. L. Chen[1,2,4,6*]

PUBLISHED ONLINE: 25 MAY 2014 | DOI: 10.1038/NMAT3990



磁性体系工作—大难题

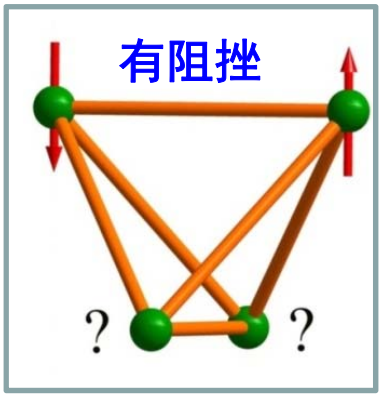
烧绿石晶格结构$A_2B_2O_7$有磁阻挫，定其磁结构是一大难题



有磁结构导致的金属绝缘体转变

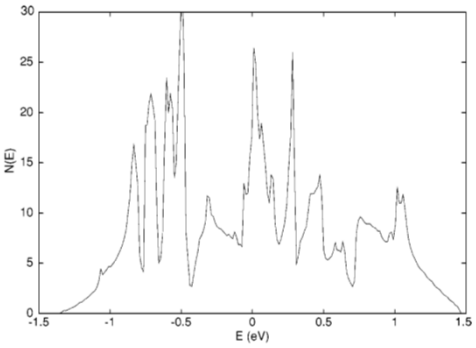
$Cd_2Os_2O_7$

Mandrus *et al.*, PRB 63, 195104 (2001)



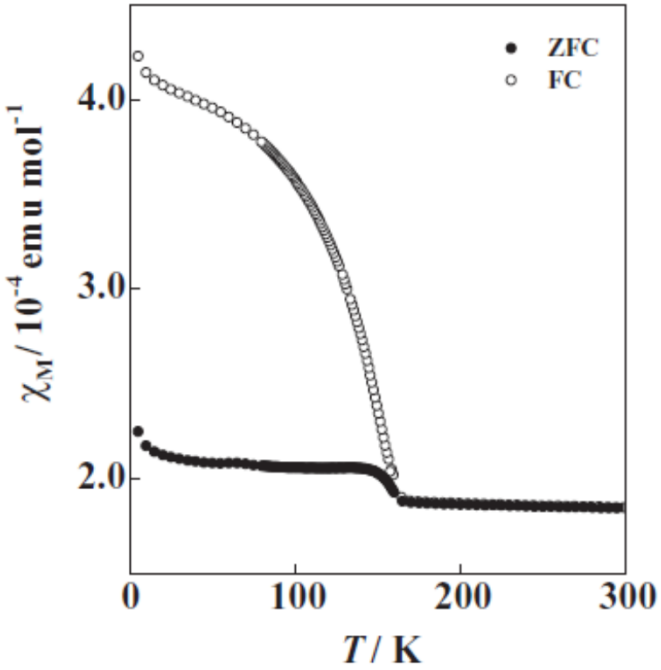
The Os sublattice consists of corner sharing tetrahedra, with the Os atoms at the corners. As a result it is not possible to find a structure in which all nearest-neighbor Os bonds are antiferromagnetic, and additionally, the lattice is strongly geometrically frustrated for nearest-neighbor spin Hamiltonians. However, based on our band-structure results, the proximity of $Cd_2Os_2O_7$ to magnetism is itinerant in nature,

Os原子在子晶格通过四面体共顶点连接。当最近邻Os反铁磁排列时，有强大的几何阻挫因此不可能发现磁结构

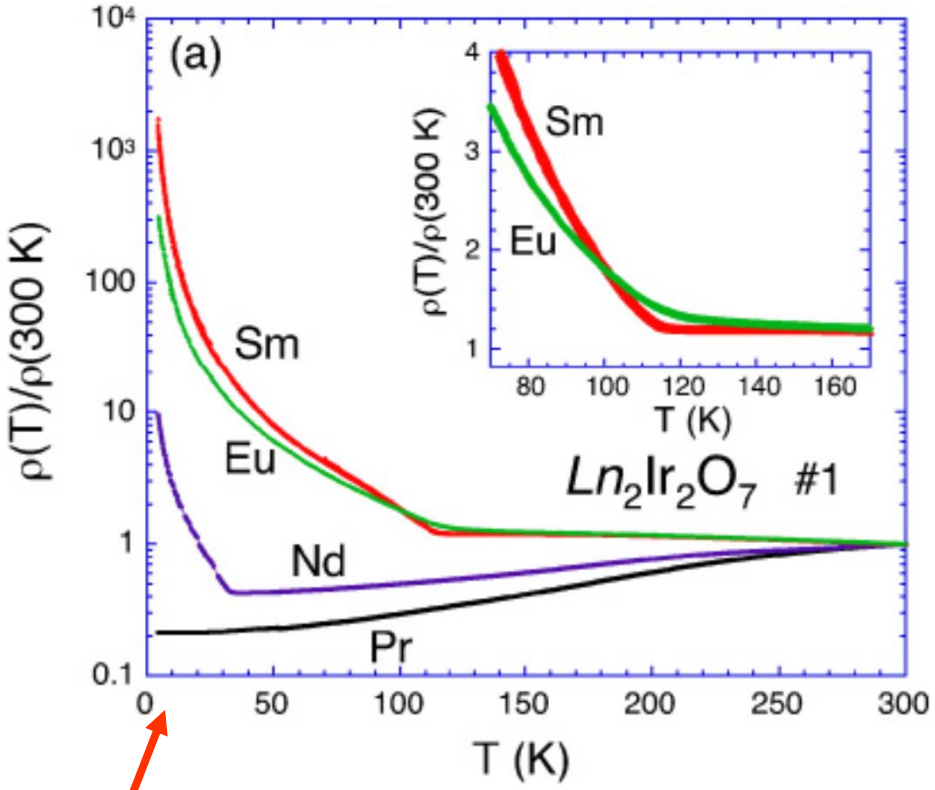


Singh, Blaha, Schvwarz, Sofo, PRB 65, 155109 (2002)

烧绿石结构铱氧化物$A_2Ir_2O_7$(A=Y,稀土元素)
实验事实



N. Taira, et al., (2001)



MATSUHIRA et al., (2007)

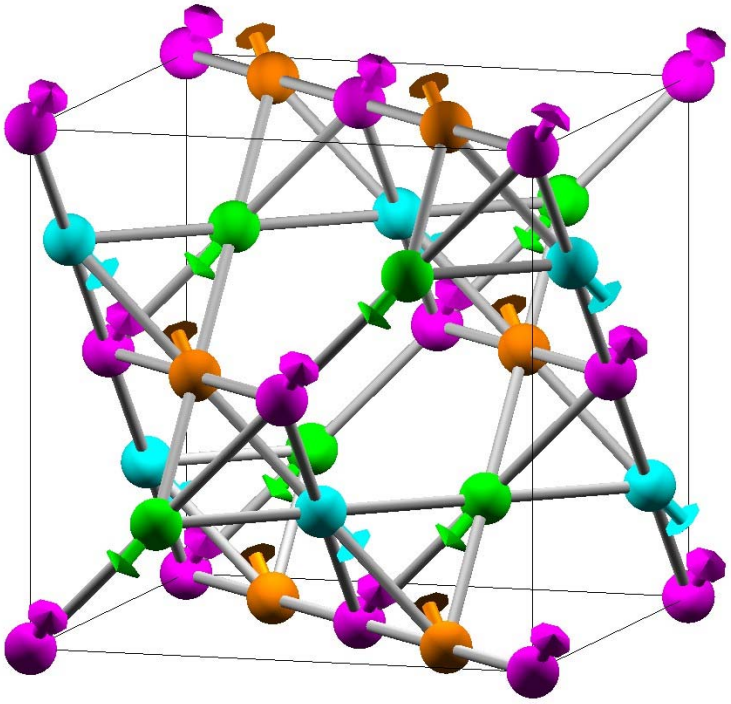
这些材料表现强的磁响应

实验定磁结构不容易

基本没有能带计算的工作

U !!!

磁性基态构型



All-in/all-out非共线磁结构

- 根据:

- 1) 有转过去的趋势
- 2) 此构型是我们计算的唯一稳定的磁构型
- 3) J(q)在q=0是极大
- 4) 没有Fermi surface nesting

实验证实

Magnetic transition, long-range order, and moment fluctuations in the pyrochlore iridate $Eu_2Ir_2O_7$

Songrui Zhao,[1,*] J. M. Mackie,[1] D. E. MacLaughlin,[1] O. O. Bernal,[2] J. J. Ishikawa,[3] Y. Ohta,[3] and S. Nakatsuji[3]

Magnetic order in the pyrochlore iridates $A_2Ir_2O_7$ (A = Y, Yb)

S. M. Disseler,[1] Chetan Dhital,[1] A. Amato,[2] S. R. Giblin,[3] Clarina de la Cruz,[4] Stephen D. Wilson,[1] and M. J. Graf[1,*]

Continuous transition between antiferromagnetic insulator and paramagnetic metal in the pyrochlore iridate $Eu_2Ir_2O_7$

Jun J. Ishikawa,[*] Eoin C. T. O'Farrell, and Satoru Nakatsuji[†]

Magnetic order and the electronic ground state in the pyrochlore iridate $Nd_2Ir_2O_7$

S. M. Disseler,[1] Chetan Dhital,[1] T. C. Hogan,[1] A. Amato,[2] S. R. Giblin,[3] Clarina de la Cruz,[4] A. Daoud-Aladine,[3] Stephen D. Wilson,[1] and M. J. Graf[1]

Emergence of Magnetic Long-range Order in Frustrated Pyrochlore $Nd_2Ir_2O_7$ with Metal-insulator Transition

K. Tomiyasu,[1,*] K. Matsuhira,[2] K. Iwasa,[1] M. Watahiki,[1] S. Takagi,[2] M. Wakeshima,[3] Y. Hinatsu,[3] M. Yokoyama,[4] K. Ohoyama,[5] and K. Yamada[6]

All-in/all-out非共线磁结构

Noncollinear Magnetism and Spin-Orbit Coupling in 5*d* Pyrochlore Oxide $Cd_2Os_2O_7$

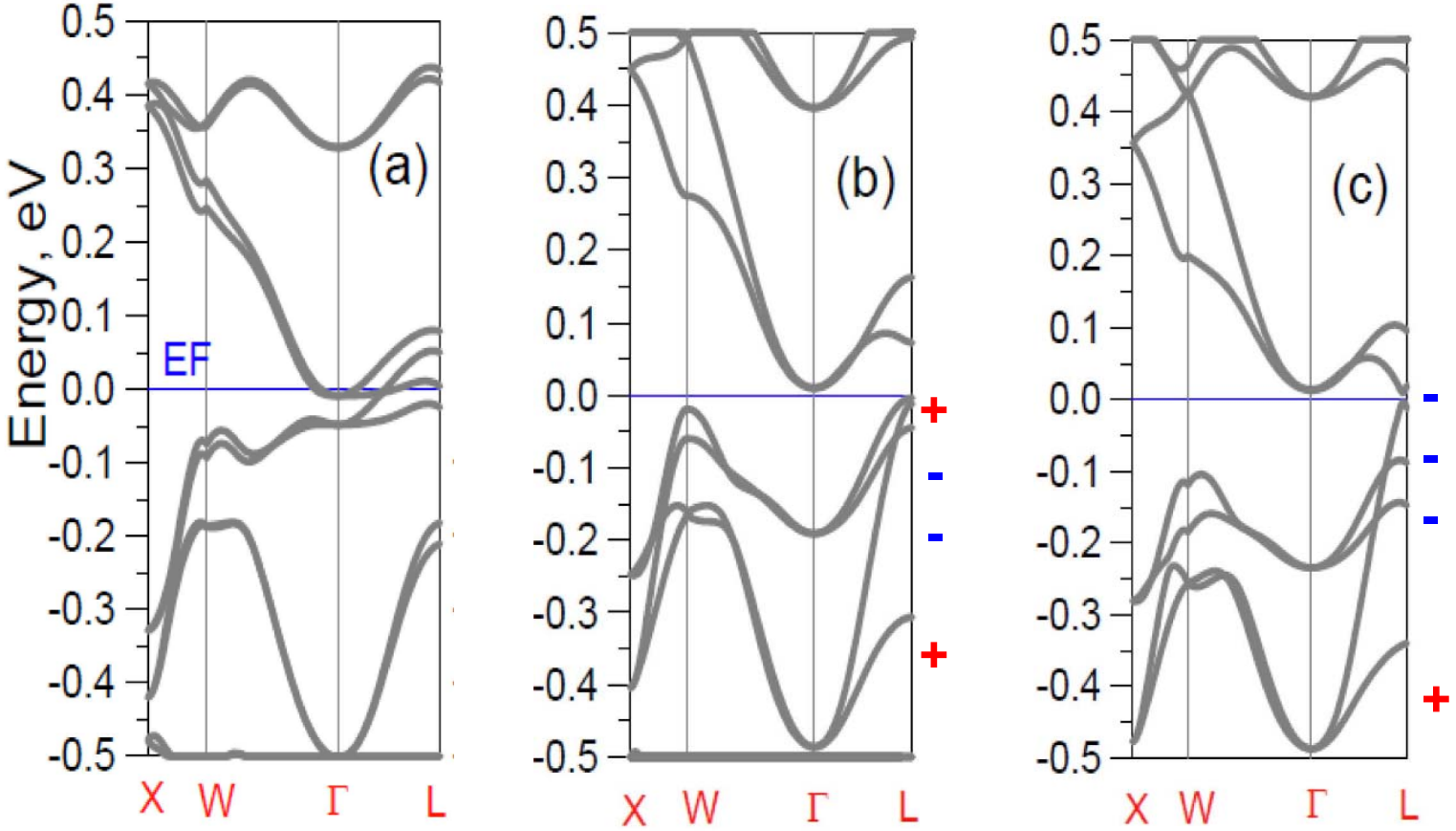
We investigate the electronic and magnetic properties of the pyrochlore oxide $Cd_2Os_2O_7$ using the density-functional theory plus on-site repulsion (U) method, and depict the ground-state phase diagram with respect to U. We conclude that the all-in–all-out noncollinear magnetic order is stable in a wide range of U. We also show that the easy-axis anisotropy arising from the spin-orbit coupling plays a significant role in stabilizing the all-in–all-out magnetic order. A *pseudogap* was observed near the transition between

Tetrahedral Magnetic Order and the Metal-Insulator Transition in the Pyrochlore Lattice of $Cd_2Os_2O_7$

accompanied with any spatial symmetry breaking. We propose a noncollinear all-in–all-out spin arrangement on the tetrahedral network made of Os atoms. Based on this we suggest that the transition is not caused by the Slater mechanism as believed earlier but by an alternative mechanism related to the

Correlation→band structure evolution

$Y_2Ir_2O_7$ **LDA+U method** All-in/All-out magnetic order



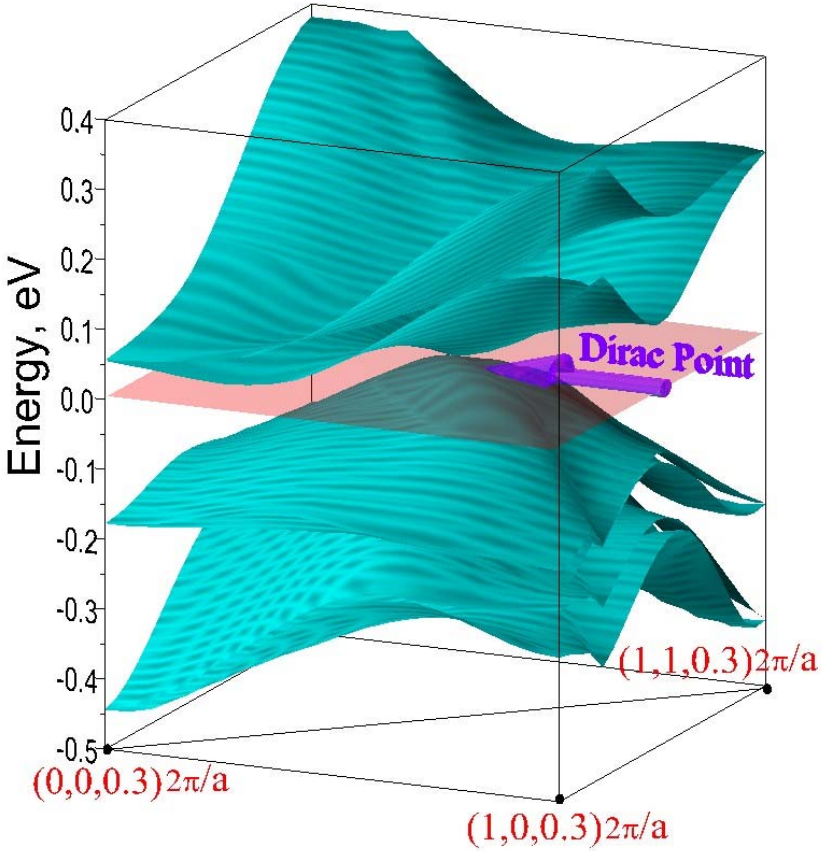
U=0 **U=1.5 eV** **U=2.0 eV**

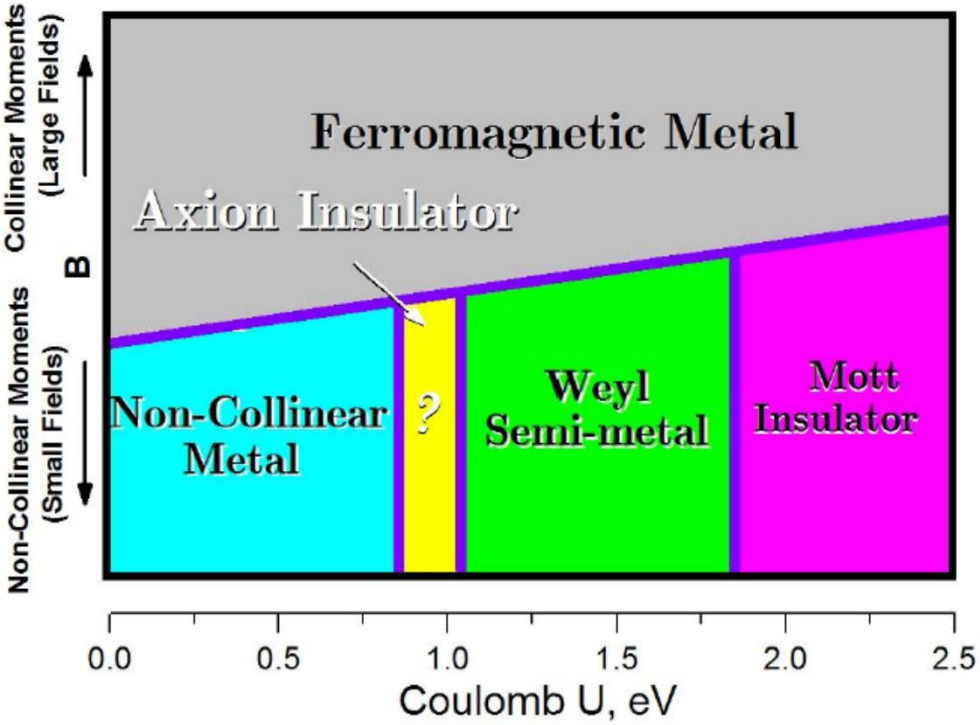
enlarge

Wan et al., (2011) **U** → **+U calculation**

Weyl Semimetal

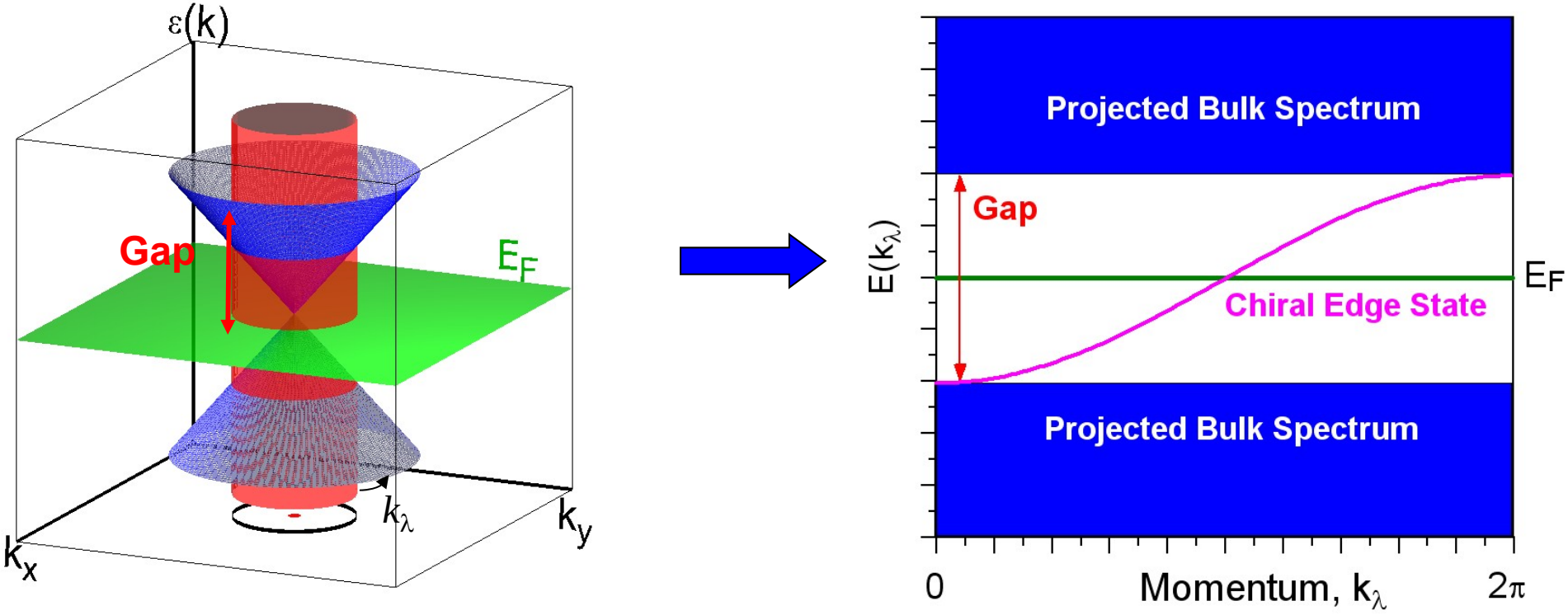
$Y_2Ir_2O_7$





Wan, Turner, Vishwanath, Savrasov, Phys. Rev. B **83**, 205101 (2011)

Fermi Arc (费米面是不连续的线段)



Weyl Semimetal

TaAs:

Theory:
Weng et al., PRX (2015)
Huang et al., Nature Commum. (2015)

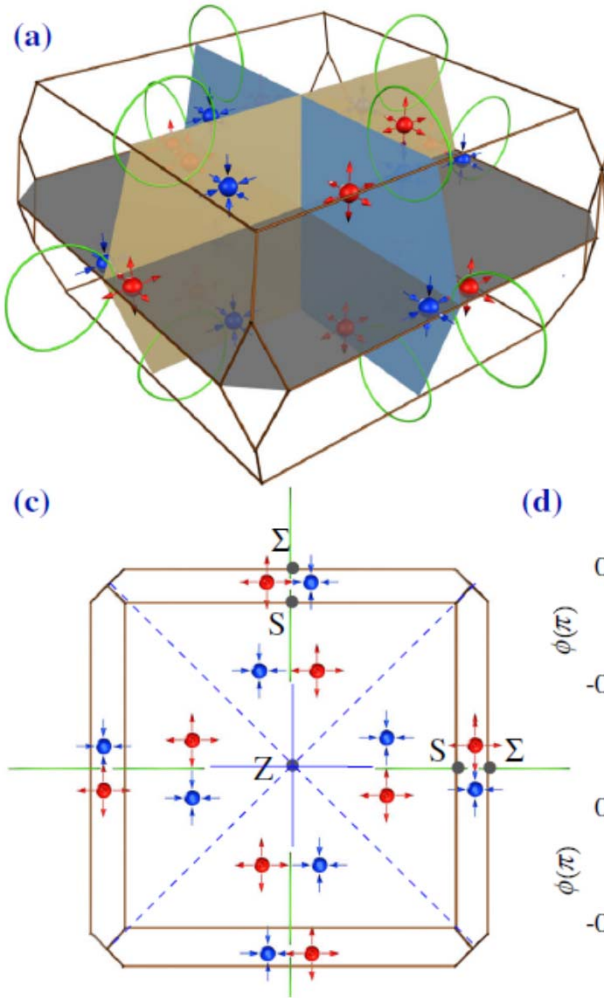
Exp:
Lv et al., PRX (2015), Nature Phys. (2015);
Xu et al., Science (2015);

…….. …….

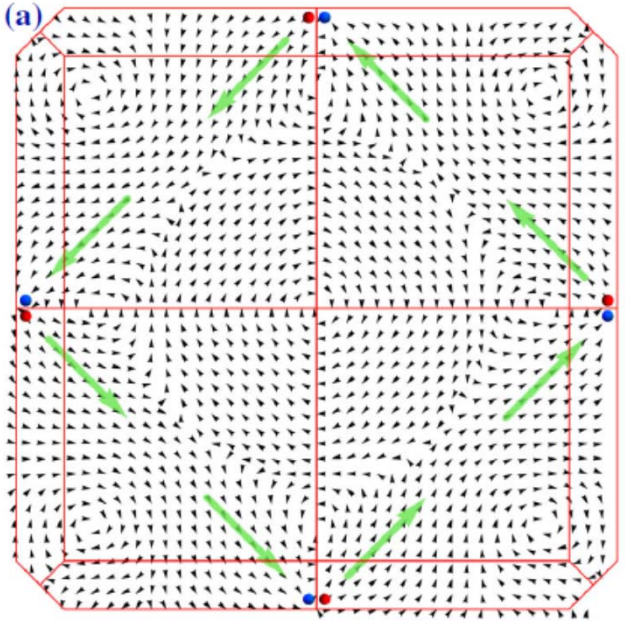
PHYSICAL REVIEW X 5, 011029 (2015)

Weyl Semimetal Phase in Noncentrosymmetric Transition-Metal Monophosphides

Hongming Weng,[1,2,*] Chen Fang,[3] Zhong Fang,[1,2] B. Andrei Bernevig,[4] and Xi Dai[1,2]



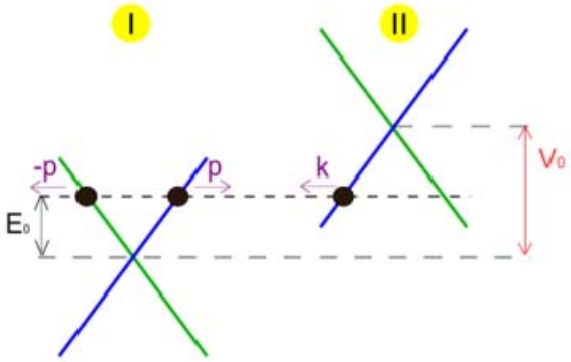
3D view of the nodal rings (in the absence of SOC) and Weyl points (with SOC) in the BZ. Once the SOC is turned on, the nodal rings are gapped and give rise to Weyl points off the mirror planes



Berry curvature distribution

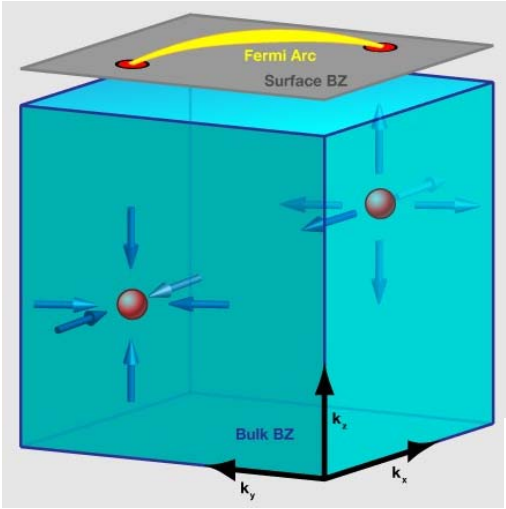
Novel Properties of Quasiparticle

➢ **Klein tunneling** (Katsnelson et al., 2006)



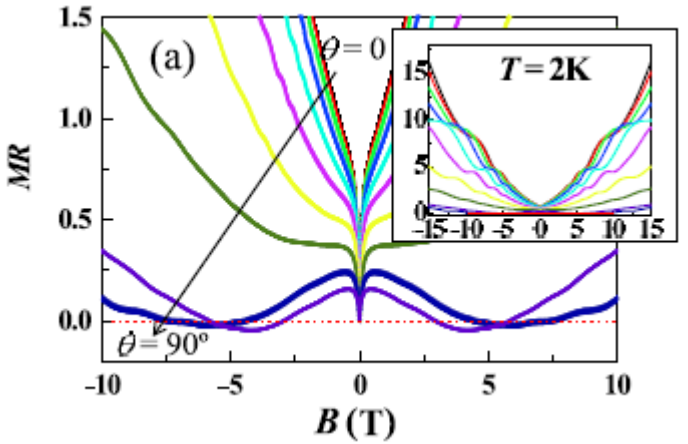
➢ **Fermi Arc**

(Wan, Turner, Vishwanath, Savrasov, (2011))



➢ **Chiral Anomaly**

(Aji (2011), Son & Spivak (2013))



Topological (Crystalline) Insulators

- Z2 topological insulator (*Kane&Mele PRL 2005*)
- Mirror Chern Insulator

Ando and Fu, Annu. Rev. Condens. Matter Phys. ***6****, 361 (2015)*

- Hourglass Fermions

Wang, Alexandradinata, Cava, Bernevig, Nature ***532****, 189 (2016).*

- Higher-order topological insulators

Fang&Fu;Schindler et al., Langbehn et al.,Song, Fang&Fang;Benalcazar et al., (2017)

- Quantized electric multipole insulators

Benalcazar, Bernevig, Hughes, Science 357, 61 (2017)

- Nodal-chain metals

Bzdušek, Wu, Rüegg, Sigrist & Soluyanov, Nature ***538****, 75 (2016).*

- Three-fold (or higher) band degeneracies Semimetal

Bradlyn et al., Science (2016)

Semimetal

- Dirac Semimetal
- Weyl Semimetal
- Multi-degeneracy points
- Nodal-line semimetal
- Hopf-line Semimetal

……..

How to find Topo Mater

There are so much topological blablabla

Many topological invariants

- **Wave function?!!!**
- **Need calculate all** topological invariants for one material

Thus find any new topo-mater is a big success

Crystal Symmetry

- Analyzing various crystallographic symmetries

Fu & Kane (2007); parity →Z2 Topological insulator

Fang, Gilbert & Bernevig, (2012); Slager et al., (2012);
Fang & Fu (2015); Fang & Fu (2017); Zhou et al., (2018)……

Do not use wave-function

- Exploiting the mismatch between the real and momentum-space descriptions of the band structure

Kruthoff et al., PRX (2017); Bradlyn et al., Nature (2017);

Po, Vishwanath & Watanabe, Nature Communications (2017)

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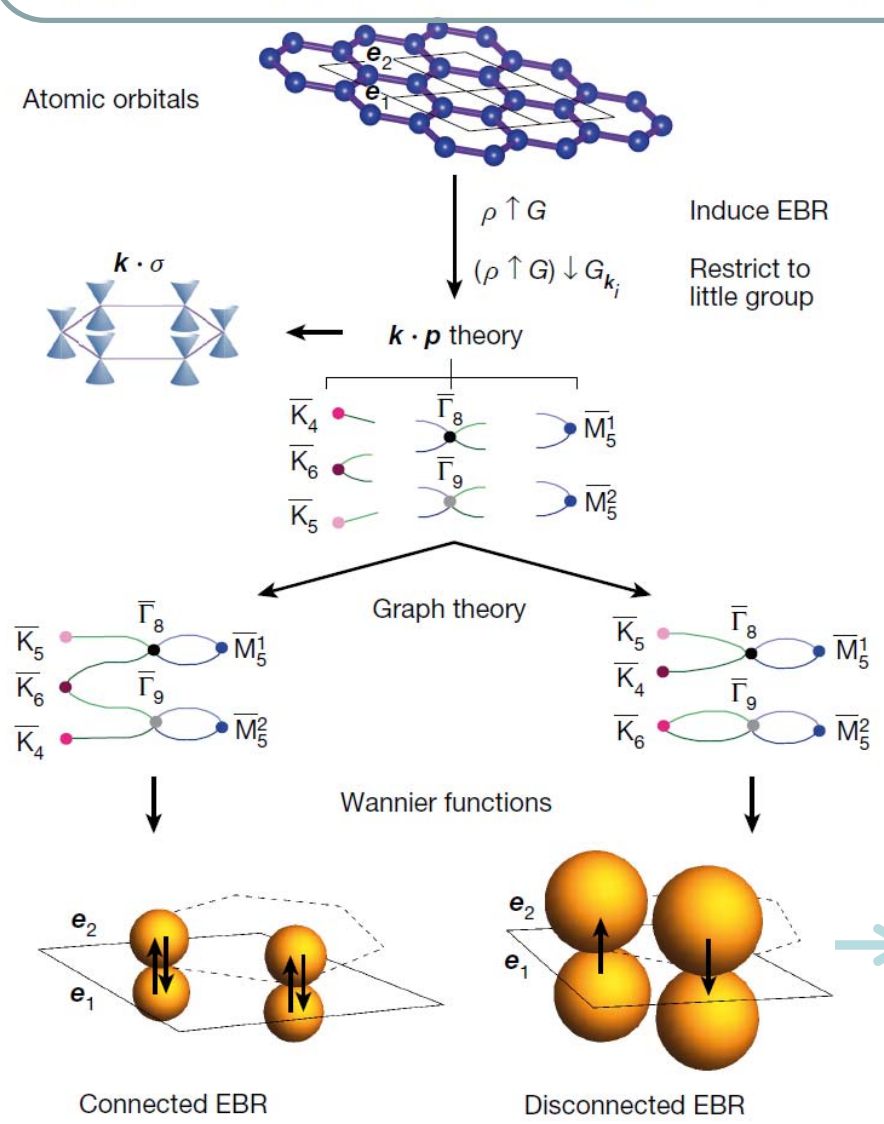
Topological quantum chemistry

Barry Bradlyn[1]*, L. Elcoro[2]*, Jennifer Cano[1]*, M. G. Vergniory[3,4,5]*, Zhijun Wang[6]*, C. Felser[7], M. I. Aroyo[2] & B. Andrei Bernevig[3,6,8,9]

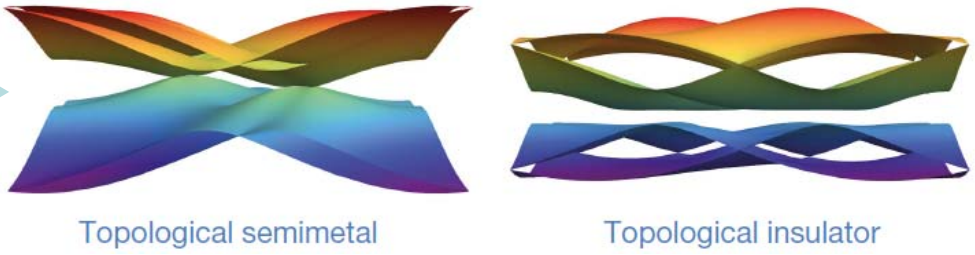


Atomic limit
Representation + Compatibility

Graph theory and band structure

Connected bands (EBR) → Semimetal
Disonnected bands (EBR)→ topo insulator

In total 10403 different EBRs



Symmetry-based Indicators of Band Topology in the 230 Space Groups

Hoi Chun Po,[1,2] Ashvin Vishwanath,[1,2,*] and Haruki Watanabe[3]

Band structure (has direct band gap at high symmetry points)

$$\{\mathrm{BS}\} \equiv \ker \mathcal{C} \cap \mathbb{Z}^D \simeq \mathbb{Z}^{d_{\mathrm{BS}}} \quad \mathrm{BS} = \sum_{i=1}^{d_{\mathrm{BS}}} m_i \mathbf{b}_i$$

$$\{\mathrm{AI}\} \simeq \mathbb{Z}^{d_{\mathrm{AI}}} \equiv \left\{ \sum_{i=1}^{d_{\mathrm{AI}}} m_i \mathbf{a}_i \ : \ m_i \in \mathbb{Z} \right\}$$

Quotient Group

商群

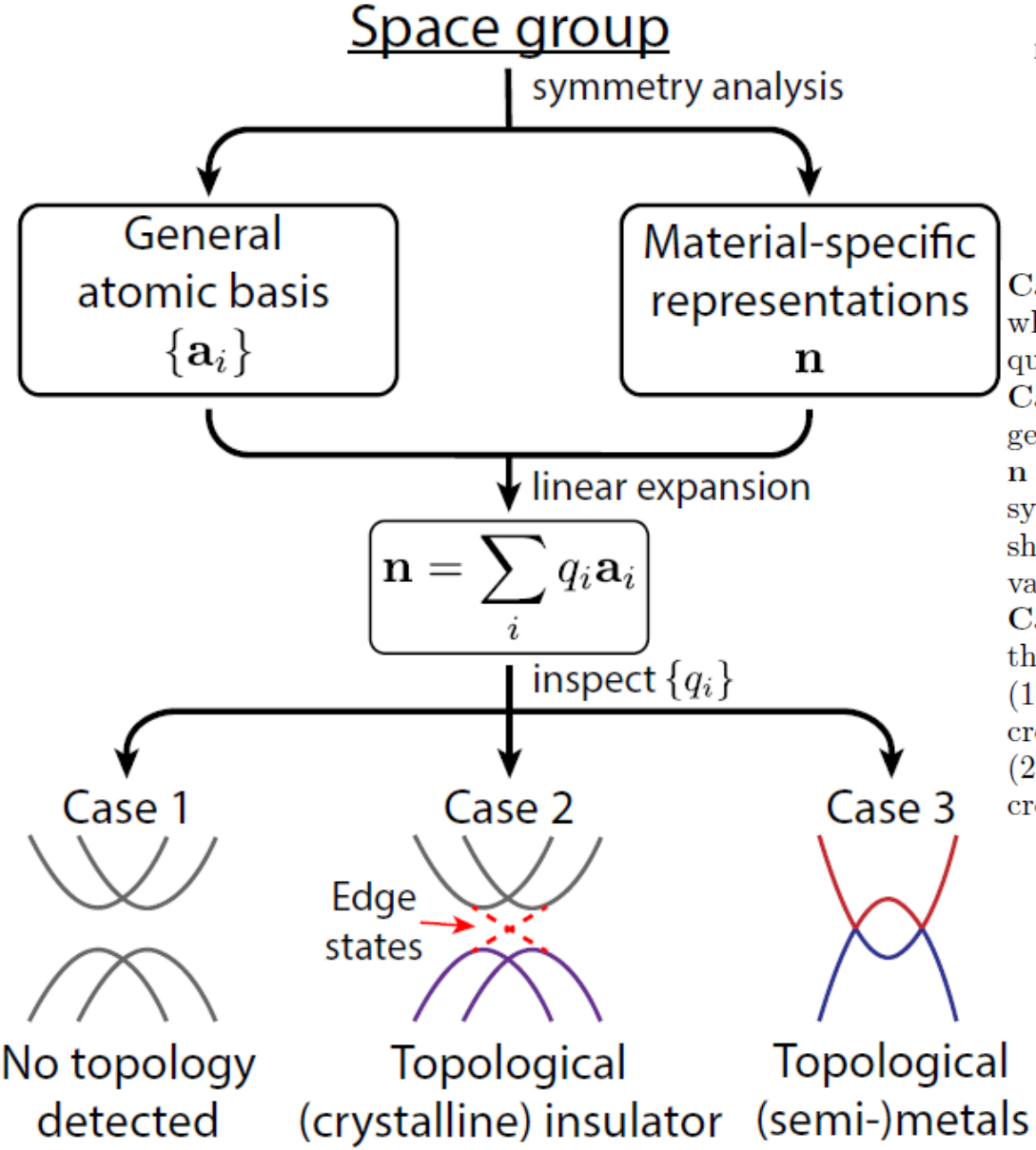
$$X_{\mathrm{BS}} \equiv \frac{\{\mathrm{BS}\}}{\{\mathrm{AI}\}}$$

Atomic limit

Provide no insight into how to find or engineer materials in any non-trivial class

X_{BS}	Space groups
$\mathbb{Z}_2$	81, 82, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 215, 216, 217, 218, 219, 220
$\mathbb{Z}_3$	188, 190
$\mathbb{Z}_4$	52, 56, 58, 60, 61, 62, 70, 88, 126, 130, 133, 135, 136, 137, 138, 141, 142, 163, 165, 167, 202, 203, 205, 222, 223, 227, 228, 230
$\mathbb{Z}_8$	128, 225, 226
$\mathbb{Z}_{12}$	176, 192, 193, 194
$\mathbb{Z}_2 \times \mathbb{Z}_4$	14, 15, 48, 50, 53, 54, 55, 57, 59, 63, 64, 66, 68, 71, 72, 73, 74, 84, 85, 86, 125, 129, 131, 132, 134, 147, 148, 162, 164, 166, 200, 201, 204, 206, 224
$\mathbb{Z}_2 \times \mathbb{Z}_8$	87, 124, 139, 140, 229
$\mathbb{Z}_3 \times \mathbb{Z}_3$	174, 187, 189
$\mathbb{Z}_4 \times \mathbb{Z}_8$	127, 221
$\mathbb{Z}_6 \times \mathbb{Z}_{12}$	175, 191
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$	11, 12, 13, 49, 51, 65, 67, 69
$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	83, 123
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$	2, 10, 47

Our Algorithm



$$\mathbf{n} = (\nu, n^1_{\mathbf{k}_1}, \ldots, n^{\alpha_1}_{\mathbf{k}_1}, n^1_{\mathbf{k}_2}, \ldots, n^{\alpha_2}_{\mathbf{k}_2}, \ldots, n^1_{\mathbf{k}_N}, \ldots, n^{\alpha_N}_{\mathbf{k}_N})$$

230 space group

Go beyond one-by-one

Case 1: the expansion coefficients $q_i's$ are all integers, which indicates that $\mathbf{n}$ is an AI, thus the material is equivalent to an atomic insulator;

Case 2: the expansion coefficients $q_i's$ are not all integers, but all $q_iC_i's$ are integers. This indicates that the $\mathbf{n}$ is a BS and the material is equivalent to a BI, but this system must been topological since some remainder(s) should be nonzero as shown in Eq. 3, i.e. the SI is non-vanishing;

Case 3: Not only the expansion coefficients $q_i's$ but also the $q_iC_i's$ are not all integers:

(1) some $n^{\alpha}_{\mathbf{k}}$ is non-integer which indicates that band crossing happens at this k point;

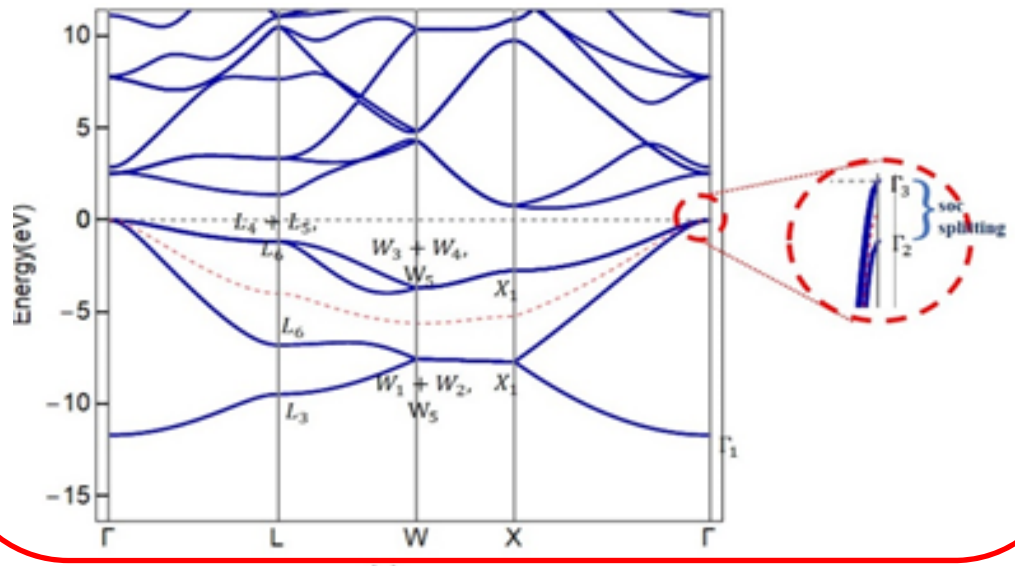
(2) all the $n^{\alpha}_{\mathbf{k}}{}'s$ are integers, then there must be band crossing in high symmetry line or plane.

Tang, Po, Vishwanath, ***Wan****

15*, 470 Nature Physics (2019)*

Band Structure

Band structure of Si (SG227)



高对称点	坐标	Irreps
Γ	(0，0，0)	G_{96}^{8}: 4(2)，5(2)，8(4)，12(2)，13(2)，16(4)
X	(0，1，0)	G_{64}^{2}: 19 (4)
L	(1/2，1/2，1/2)	G_{24}^{3}: 3(1)，4(1)，6(2)，9(1)，10(1)，12(2)
W	(1/2，1，0)	G_{64}^{3}: 13(1)，14(1)，15(1)，16(1)，20(2)

Topological is Global

What is detail:
If nothing pass the Fermi level, then all is detail!

BZ

《物理》48， 341 (2019)

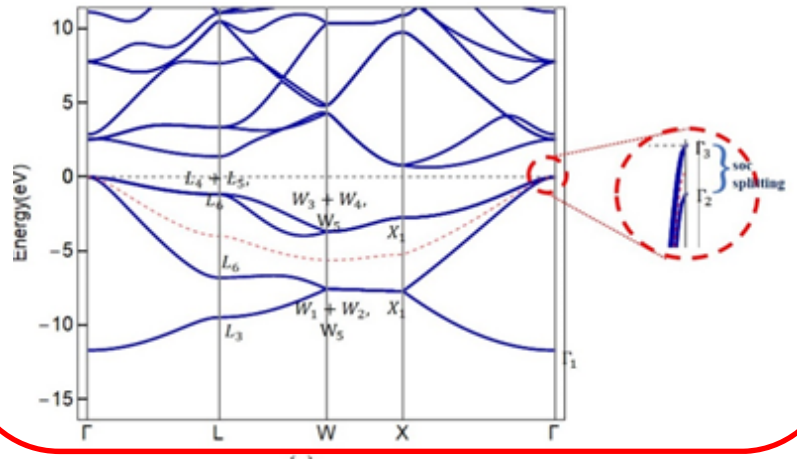
Bands can cross when they carry different symmetry labels

Dimensions of the irreps determine how the bands are “stuck”

High symmetry point, High symmetry line, irreps, ……..

Band Structure

Band structure of Si



高对称点	坐标	Irreps
Γ	(0, 0, 0)	G_{96}^{8}: 4(2), 5(2), 8(4), 12(2), 13(2), 16(4)
X	(0, 1, 0)	G_{64}^{2}: 19 (4)
L	(1/2, 1/2, 1/2)	G_{24}^{3}: 3(1), 4(1), 6(2), 9(1), 10(1), 12(2)
W	(1/2, 1, 0)	G_{64}^{3}: 13(1), 14(1), 15(1), 16(1), 20(2)

What is detail:
If nothing pass the Fermi level, then all is detail!

$$\boldsymbol{n}_{\mathrm{BS}} = \left(v,\ n_{k_1}^{1},\ n_{k_1}^{2},\ \cdots,\ n_{k_1}^{r_1},\ n_{k_2}^{1},\ n_{k_2}^{2},\ \cdots,\ n_{k_2}^{r_2},\ \cdots,\ n_{k_N}^{1},\ n_{k_N}^{2},\ \cdots,\ n_{k_N}^{r_N}\right).$$

$$\boldsymbol{n}_{\mathrm{BS}} = (8,\ 1,\ 1,\ 1,\ 0,\ 0,\ 0,\ 2,\ 0,\ 0,\ 1,\ 1,\ 1,\ 2,\ 1,\ 1,\ 1,\ 1,\ 2).$$

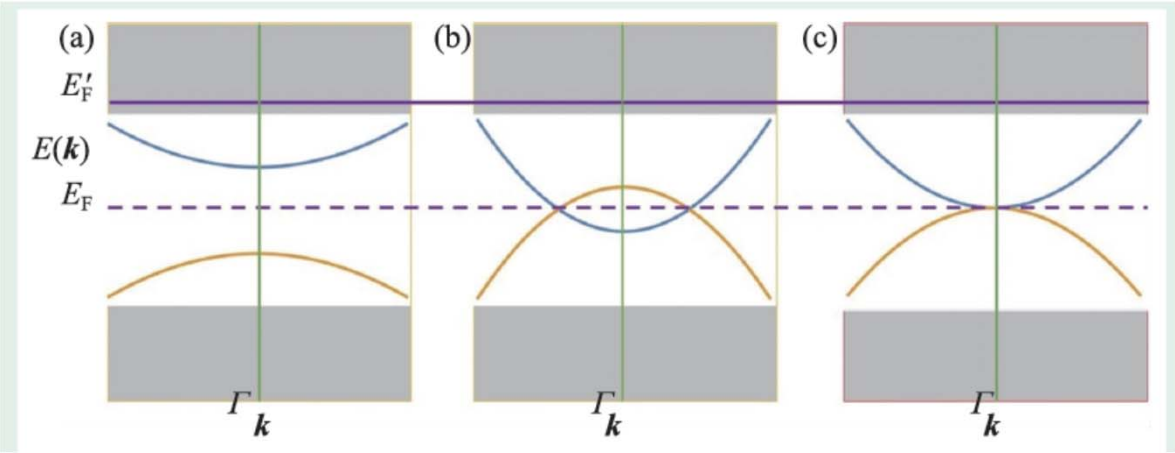
$$\boldsymbol{n}_{\mathrm{BS},\,1} = (4,\ 0,\ 0,\ 1,\ 0,\ 0,\ 0,\ 1,\ 0,\ 0,\ 0,\ 1,\ 1,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1),$$

$$\boldsymbol{n}_{\mathrm{BS},\,2} = (4,\ 1,\ 1,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 0,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 0,\ 0,\ 1).$$

$$\boldsymbol{n}_{\mathrm{BS}} = \boldsymbol{n}_{\mathrm{BS},\,1} + \boldsymbol{n}_{\mathrm{BS},\,2}$$

- **Labels become simple counting!**
- **Gap conditions above and below ensure counting is well defined**

Atomic limit



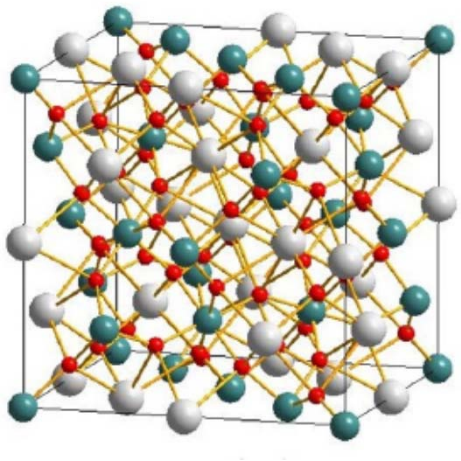
- Unit cell has one atom
- One *s* orbit at this atom

230 Space group

- Wyckoff Positions
- Site symmetry

Wyckoff Positions of Group 2 (P -1)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
2	i	1	(x, y, z) (- x, - y, - z)
1	h	-1	(1/2 , 1/2 , 1/2)
1	g	-1	(0, 1/2 , 1/2)
1	f	-1	(1/2 , 0, 1/2)
1	e	-1	(1/2 , 1/2 , 0)
1	d	-1	(1/2 , 0, 0)
1	c	-1	(0, 1/2 , 0)
1	b	-1	(0, 0, 1/2)
1	a	-1	(0, 0, 0)



$Y_2Ir_2O_7$

Wyckoff Positions of Group 227 (F d -3 m) [origin choice

Multiplicity	Wyckoff letter	Site symmetry	Coordinates		
			(0,0,0)+	(0,1/2,1/2)+	(1/2,0,1/2)+ (1/2,1/2,0)+
192	i	1	(x, y, z)	(- x, - y + 1/2 , z + 1/2)	(- x + 1/2 , y + 1/2 , - z)
			(z, x, y)	(z + 1/2 , - x, - y + 1/2)	(- z, - x + 1/2 , y + 1/2)
			(y, z, x)	(- y + 1/2 , z + 1/2 , - x)	(y + 1/2 , - z, - x + 1/2)
			(y + 3/4 , x + 1/4 , - z + 3/4)	(- y + 1/4 , - x + 1/4 , - z + 1/4)	(y + 1/4 , - x + 3/4 , z + 3/4
			(x + 3/4 , z + 1/4 , - y + 3/4)	(- x + 3/4 , z + 3/4 , y + 1/4)	(- x + 1/4 , - z + 1/4 , - y +
			(z + 3/4 , y + 1/4 , - x + 3/4)	(z + 1/4 , - y + 3/4 , x + 3/4)	(- z + 3/4 , y + 3/4 , x + 1/4
			(- x + 1/4 , - y + 1/4 , - z + 1/4)	(x + 1/4 , y + 3/4 , - z + 3/4)	(x + 3/4 , - y + 3/4 , z + 1/4
			(- z + 1/4 , - x + 1/4 , - y + 1/4)	(- z + 3/4 , x + 1/4 , y + 3/4)	(z + 1/4 , x + 3/4 , - y + 3/4
			(- y + 1/4 , - z + 1/4 , - x + 1/4)	(y + 3/4 , - z + 3/4 , x + 1/4)	(- y + 3/4 , z + 1/4 , x + 3/4
			(- y + 1/2 , - x, z + 1/2)	(y, x, z)	(- y, x + 1/2 , - z + 1/2)
			(- x + 1/2 , - z, y + 1/2)	(x + 1/2 , - z + 1/2 , - y)	(x, z, y)
			(- z + 1/2 , - y, x + 1/2)	(- z, y + 1/2 , - x + 1/2)	(z + 1/2 , - y + 1/2 , - x)
96	h	..2	(1/8 , y, - y + 1/4)	(7/8 , - y + 1/2 , - y + 3/4)	(3/8 , y + 1/2 , y + 3/4) (5/8 , - y, y + 1/4)
			(- y + 1/4 , 1/8 , y)	(- y + 3/4 , 7/8 , - y + 1/2)	(y + 3/4 , 3/8 , y + 1/2) (y + 1/4 , 5/8 , - y)
			(y, - y + 1/4 , 1/8)	(- y + 1/2 , - y + 3/4 , 7/8)	(y + 1/2 , y + 3/4 , 3/8) (- y, y + 1/4 , 5/8
			(1/8 , - y + 1/4 , y)	(3/8 , y + 3/4 , y + 1/2)	(7/8 , - y + 3/4 , - y + 1/2) (5/8 , y + 1/4 , - y)
			(y, 1/8 , - y + 1/4)	(y + 1/2 , 3/8 , y + 3/4)	(- y + 1/2 , 7/8 , - y + 3/4) (- y, 5/8 , y + 1/4
			(- y + 1/4 , y, 1/8)	(y + 3/4 , y + 1/2 , 3/8)	(- y + 3/4 , - y + 1/2 , 7/8) (y + 1/4 , - y, 5/8)
96	g	..m	(x, x, z)	(- x, - x + 1/2 , z + 1/2)	(- x + 1/2 , x + 1/2 , - z)
			(z, x, x)	(z + 1/2 , - x, - x + 1/2)	(- z, - x + 1/2 , x + 1/2)
			(x, z, x)	(- x + 1/2 , z + 1/2 , - x)	(x + 1/2 , - z, - x + 1/2)
			(x + 3/4 , x + 1/4 , - z + 3/4)	(- x + 1/4 , - x + 1/4 , - z + 1/4)	(x + 1/4 , - x + 3/4 , z + 3/4)

Pyrochlore structure: Space Group 227

Y→16d

Ir→16c

O1→8b

O2→48f

Calculation of Atomic Insulator Basis

Taking SG2 as an example

Step 1:

Obtaining HSPs.

$\mathcal{SG}2's$ HSP	Γ	X	Y	Z	U	T	S	R
coordinate	(0,0,0)	$(\frac{1}{2},0,0)$	$(0,\frac{1}{2},0)$	$(0,0,\frac{1}{2})$	$(\frac{1}{2},\frac{1}{2},0)$	$(0,\frac{1}{2},\frac{1}{2})$	$(\frac{1}{2},0,\frac{1}{2})$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

Step 2: *Give all the Wyckoff positions.*

2 ◀ 8 1 17

$\mathcal{SG}2's$ Wyckoff position	site-group	Wyckoff orbits
2i	C_1	$(x,y,z),(-x,-y,-z)$
1h	C_i	$(1/2,1/2,1/2)$
1g	C_i	$(0,1/2,1/2)$
1f	C_i	$(1/2,0,1/2)$
1e	C_i	$(1/2,1/2,0)$
1d	C_i	$(1/2,0,0)$
1c	C_i	$(0,1/2,0)$
1b	C_i	$(0,0,1/2)$
1a	C_i	$(0,0,0)$

TABLE VII. The nine Wyckoff positions for $\mathcal{SG}2$.

Calculation of Atomic Insulator Basis

$\mathcal{SG}2$	n^1_{2i}	n^1_{1h}	n^2_{1h}	n^1_{1g}	n^2_{1g}	n^1_{1f}	n^2_{1f}	n^1_{1e}	n^2_{1e}	n^1_{1d}	n^2_{1d}	n^1_{1c}	n^2_{1c}	n^1_{1b}	n^2_{1b}	n^1_{1a}	n^2_{1a}
ν	4	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
Γ^1_1	1	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0
Γ^1_2	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1
X^1_1	1	1	0	0	1	1	0	0	1	0	1	0	1	1	0	1	0
X^1_2	1	0	1	1	0	0	1	1	0	1	0	1	0	0	1	0	1
Y^1_1	1	1	0	0	1	0	1	1	0	0	1	1	0	0	1	1	0
Y^1_2	1	0	1	1	0	1	0	0	1	1	0	0	1	1	0	0	1
Z^1_1	1	1	0	0	1	0	1	0	1	1	0	1	0	1	0	0	1
Z^1_2	1	0	1	1	0	1	0	1	0	0	1	0	1	0	1	1	0
U^1_1	1	1	0	1	0	0	1	0	1	1	0	0	1	0	1	1	0
U^1_2	1	0	1	0	1	1	0	1	0	0	1	1	0	1	0	0	1
T^1_1	1	1	0	1	0	1	0	0	1	0	1	1	0	0	1	0	1
T^1_2	1	0	1	0	1	0	1	1	0	1	0	0	1	1	0	1	0
S^1_1	1	1	0	1	0	0	1	1	0	0	1	0	1	1	0	0	1
S^1_2	1	0	1	0	1	1	0	0	1	1	0	1	0	0	1	1	0
R^1_1	1	1	0	0	1	1	0	1	0	1	0	0	1	0	1	0	1
R^1_2	1	0	1	1	0	0	1	0	1	0	1	1	0	1	0	1	0

TABLE X. The 17 AI vectors for $\mathcal{SG}2$.

n $n^1_{\cdot}, n^2_{\cdot}, n^1_X, n^2_X, n^1_Y, n^2_Y, n^1_Z, n^2_Z, n^1_U, n^2_U, n^1_T, n^2_T, n^1_S, n^2_S, n^1_R, n^2_R$

The BS can be represented by an integer-valued vector, $\mathbf{n} =$: 2 8 1 17

$$(\nu, n^1_{\mathbf{k}_1}, n^2_{\mathbf{k}_1}, \ldots, n^{\alpha_1}_{\mathbf{k}_1}, \ldots, n^{r_1}_{\mathbf{k}_1}, n^1_{\mathbf{k}_2}, n^2_{\mathbf{k}_2}, \ldots, n^{\alpha_2}_{\mathbf{k}_2} \ldots, n^{r_2}_{\mathbf{k}_2},$$
$$n^1_{\mathbf{k}_i}, \ldots, n^{\alpha_i}_{\mathbf{k}_i}, \ldots, n^{r_i}_{\mathbf{k}_i}, \cdots, n^1_{\mathbf{k}_N}, \ldots, n^{\alpha_N}_{\mathbf{k}_N}, \ldots, n^{r_N}_{\mathbf{k}_N}).$$

Calculation of Atomic Insulator Basis

We choose our basis such that the values of C_i are maximized: **Smith decomposition**.

(a)The 9 AI basis vectors for $\mathcal{SG}2$. Here ν is the number of the bands. It is also called the filling number. Staring from the 3rd row, we give the number $n_{\mathbf{k}}^{\alpha}$ in order. We omit the notation n for clarity: The first column of these rows gives the information of the HSP and its irrep completely.

$\mathcal{SG}2$	$\mathbf{a}_1$	$\mathbf{a}_2$	$\mathbf{a}_3$	$\mathbf{a}_4$	$\mathbf{a}_5$	$\mathbf{a}_6$	$\mathbf{a}_7$	$\mathbf{a}_8$	$\mathbf{a}_9$
ν	4	2	2	2	2	4	4	4	8
Γ_1^1	1	1	1	1	1	2	2	2	4
Γ_2^1	1	0	0	0	0	0	0	0	0
X_1^1	1	1	0	1	0	2	2	0	4
X_2^1	1	0	1	0	1	0	0	2	0
Y_1^1	1	1	0	0	1	2	0	2	4
Y_2^1	1	0	1	1	0	0	2	0	0
Z_1^1	1	1	0	0	0	0	0	0	0
Z_2^1	1	0	1	1	1	2	2	2	4
U_1^1	1	1	1	0	0	0	2	2	4
U_2^1	1	0	0	1	1	2	0	0	0
T_1^1	1	1	1	1	0	2	2	2	4
T_2^1	1	0	0	0	1	0	0	0	0
S_1^1	1	1	1	0	1	2	2	2	4
S_2^1	1	0	0	1	0	0	0	0	0
R_1^1	1	1	0	1	1	2	2	2	4
R_2^1	1	0	1	0	0	0	0	0	0

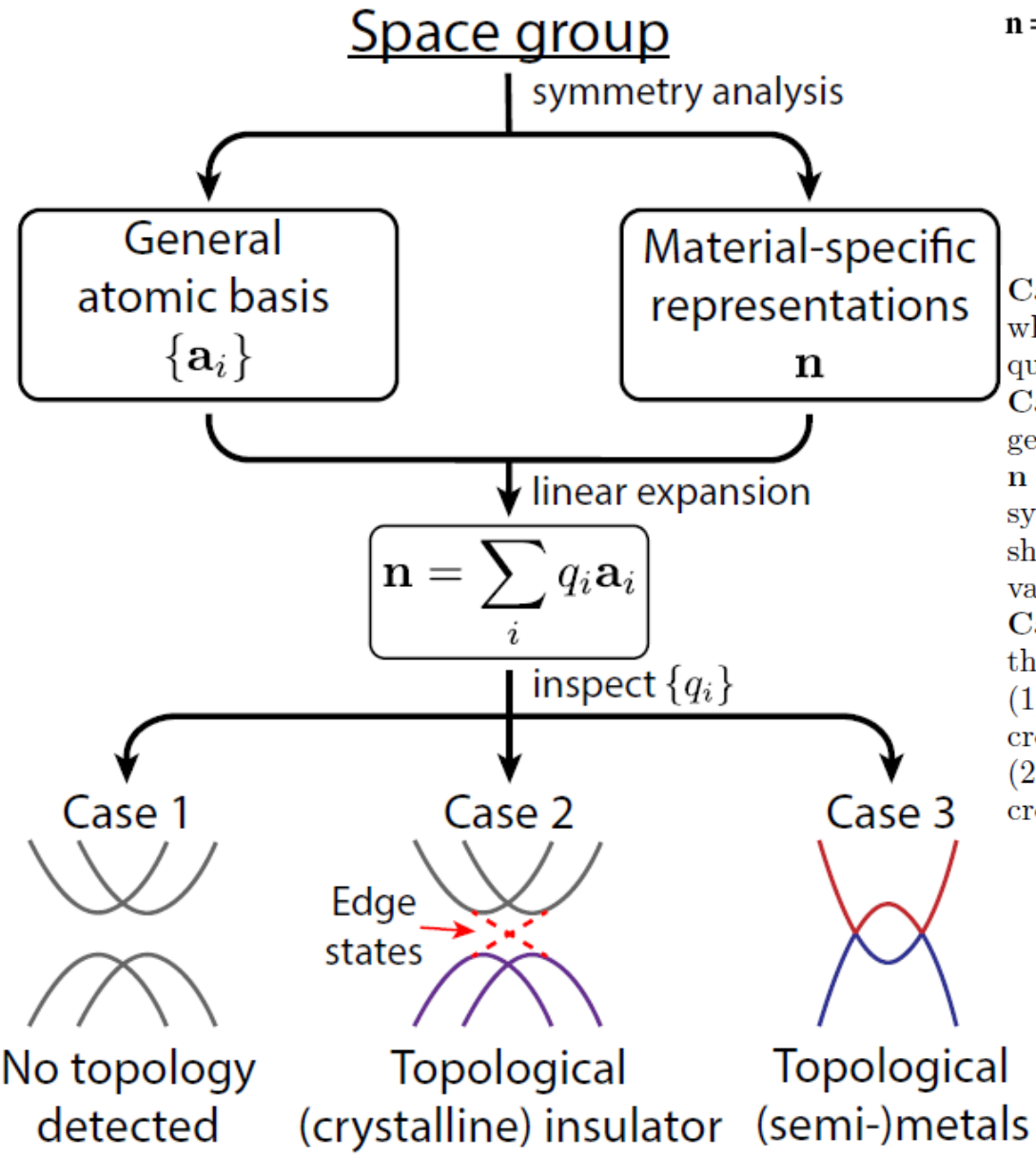
$$Z_2 \blacktriangleleft Z_2 \blacktriangleleft Z_2 \blacktriangleleft Z_4$$

$$\mathrm{BS} = \sum_{i=1}^{d_{\mathrm{BS}}} m_i \mathbf{b}_i,$$

Common factors

$d_{\mathrm{AI}} = d_{\mathrm{BS}}$ Po *et al.*, NC (2017)

Our Algorithm



$$\mathbf{n} = (\nu, n^1_{\mathbf{k}_1}, \ldots, n^{\alpha_1}_{\mathbf{k}_1}, n^1_{\mathbf{k}_2}, \ldots, n^{\alpha_2}_{\mathbf{k}_2}, \ldots, n^1_{\mathbf{k}_N}, \ldots, n^{\alpha_N}_{\mathbf{k}_N})$$

230 space group

Go beyond one-by-one

Case 1: the expansion coefficients $q_i's$ are all integers, which indicates that $\mathbf{n}$ is an AI, thus the material is equivalent to an atomic insulator;

Case 2: the expansion coefficients $q_i's$ are not all integers, but all $q_i C_i's$ are integers. This indicates that the $\mathbf{n}$ is a BS and the material is equivalent to a BI, but this system must been topological since some remainder(s) should be nonzero as shown in Eq. 3, i.e. the SI is non-vanishing;

Case 3: Not only the expansion coefficients $q_i's$ but also the $q_i C_i's$ are not all integers:

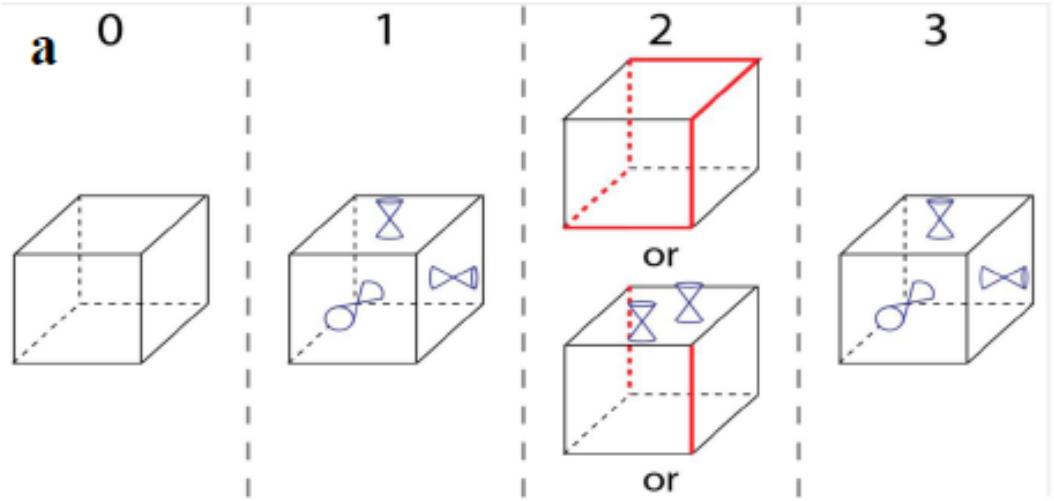
(1) some $n^{\alpha}_{\mathbf{k}}$ is non-integer which indicates that band crossing happens at this k point;

(2) all the $n^{\alpha}_{\mathbf{k}}{}'s$ are integers, then there must be band crossing in high symmetry line or plane.

Tang, Po, Vishwanath, ***Wan****

15*, 470 Nature Physics (2019)*

Z_4 TCI



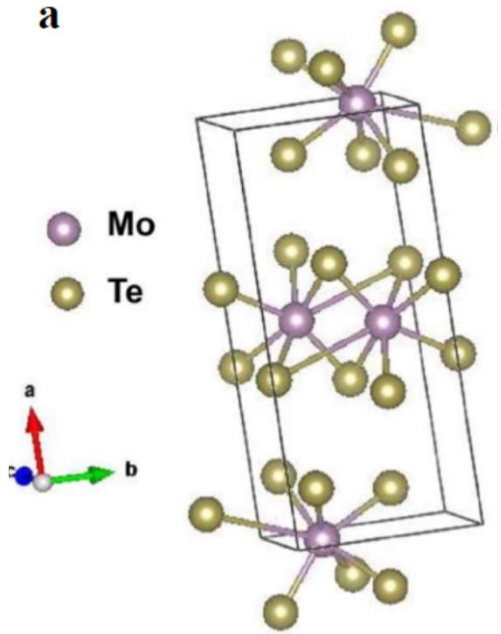
2 of Z_4

TABLE I. We focus on the following space groups ($\mathcal{SG}$s), in which a strong topological insulators generate a $\mathbb{Z}_4$ subgroup in the group of symmetry indicators, X_{BS}. The entry $2 \in \mathbb{Z}_4$ corresponds to various kinds of topological crystalline insulators, and the predicted materials candidates for such phases are tabulated.

X_{BS}	$\mathbb{Z}_2^3 \times \mathbb{Z}_4$	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$\mathbb{Z}_4$
$\mathcal{SG}$	**2**	**11,12**	**166**	**61, 136, 227**
Materials	Ag_2F_5	β-$MoTe_2$,BiBr	A7-P	c-TiS_2

Topological Hinge states in β-$MoTe_2$

(SG) **11** ($P2_1/m$).



α-phase：

β-phase：room temperature

Monolayer—QSH *(Qian, Liu, Fu & Li, Science 2014)*

γ-phase：

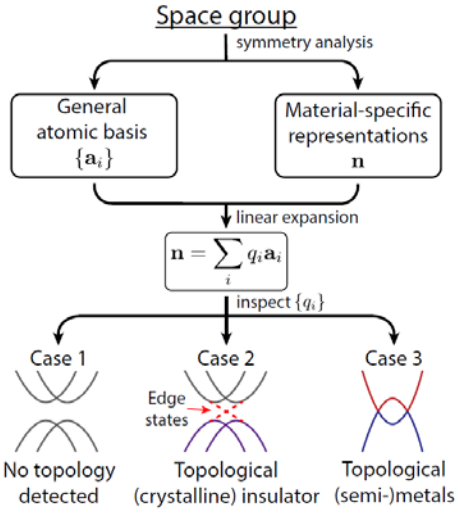
Type-II Weyl Semimetal:

Deng et al., Nature Phys. (2016)

Tamai et al., PRX (2016)

Huang et al., Nature Mater. (2016)

Jiang et al., Nature Commun. (2016)



DFT results of β-$MoTe_2$

- 2 inequivalent Mo's and 4 in-equivalent Te's
- all occupy 2e Wyckoff positions.
- total 12 atoms (56 valence electrons) primitive unit cell

→ν=56 SG11

TABLE I. For $\mathcal{SG}\mathbf{11}$, the HSPs are given by the labels $\Gamma, B, \ldots$ in order. For the labeling of the irreps of $\mathcal{G}(\mathbf{k}_i)$, we use (j, m) where j means the jth irrep and m denotes the dimension of the corresponding irrep. They are all listed in Ref. [2]. We use the same order of the irrep as Ref. [2]. The red color means that due to $\mathcal{T}$, the irrep must occur with its $\mathcal{T}$ pair (belonging to the same irrep) simultaneously. Thus $\mathcal{T}$ requires that the red colored irreps must happen even times. So it is necessary to divide them by 2 [1] to obtain the physical common factors.

HSP	Γ				B				Y				Z	C	D	A				E
irrep	(1,1)	(2,1)	(3,1)	(4,1)	(1,1)	(2,1)	(3,1)	(4,1)	(1,1)	(2,1)	(3,1)	(4,1)	(1,2)	(1,2)	(1,2)	(1,1)	(2,1)	(3,1)	(4,1)	(1,2)
$n^{\alpha_i}_{\mathbf{k}_i}$	16	16	12	12	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14	14

DFT

$$\mathbf{n} = (\nu, n^1_{\mathbf{k_1}}, n^2_{\mathbf{k}_1}, \ldots n^{\alpha_1}_{\mathbf{k}_1}, \ldots, n^1_{\mathbf{k_2}}, n^2_{\mathbf{k_2}}, \ldots, n^{\alpha_2}_{\mathbf{k_2}}, \ldots, n^1_{\mathbf{k_N}}, n^2_{\mathbf{k_N}}, \ldots, n^{\alpha_N}_{\mathbf{k}_N}, \ldots),$$

n 🖬 🐭 $n^1_{\searrow}, n^2_{\searrow}, n^3_{\searrow}, n^4_{\searrow}, n^1_B, n^2_B, n^3_B, n^4_B, n^1_Y, n^2_Y, n^3_Y, n^4_Y, n^1_Z, n^1_C, n^1_D, n^1_A, n^2_A, n^3_A, n^4_A, n^1_E$

$$\mathbf{n} = (56, 16, 16, 12, 12, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14)$$

Expansion of β-$MoTe_2$

(b)The 5 AI basis vectors for $\mathcal{SG}11$.

$\mathcal{SG}11$	$\mathbf{a}_1$	$\mathbf{a}_2$	$\mathbf{a}_3$	$\mathbf{a}_4$	$\mathbf{a}_5$
ν	4	4	0	0	0
Γ_1^1	1	2	0	0	0
Γ_2^1	1	2	0	0	0
Γ_3^1	1	0	0	0	0
Γ_4^1	1	0	0	0	0
B_1^1	1	0	0	2	0
B_2^1	1	0	0	2	0
B_3^1	1	2	0	-2	0
B_4^1	1	2	0	-2	0
Y_1^1	1	0	2	0	0
Y_2^1	1	0	2	0	0
Y_3^1	1	2	-2	0	0
Y_4^2	1	2	-2	0	0
Z_1^2	1	1	0	0	0
C_1^2	1	1	0	0	0
D_1^2	1	1	0	0	0
A_1^1	1	2	-2	-2	4
A_2^1	1	2	-2	-2	4
A_3^1	1	0	2	2	-4
A_4^1	1	0	2	2	-4
E_1^2	1	1	0	0	0

$$C_1 = C_2 = 1,\ C_3 = C_4 = 2,\ \text{and}\ C_5 = 4$$

$$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$$

$$\mathbf{n} = (56, 16, 16, 12, 12, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14)$$

$$= 12\mathbf{a}_1 + 2\mathbf{a}_2 + \mathbf{a}_3 + \mathbf{a}_4 + \frac{1}{2}\mathbf{a}_5,$$

$$(q_1, q_2, q_3, q_4, q_5) = (12, 2, 1, 1, \tfrac{1}{2})$$

$$\text{SI}\ \ (0, 0, 2)$$

$$2 \in \mathbb{Z}_4$$

2 of Z_4

Topological feature of β-$MoTe_2$

$$\kappa_1 = \sum_{\mathbf{k}\in \mathrm{TRIM}} (n_{\mathbf{k}}^{+} - n_{\mathbf{k}}^{-})/2 \mod 4$$

Z. Song, T. Zhang, Z. Fang, and C. Fang, ArXiv e-prints (2017), arXiv:1711.11049.
E. Khalaf, H. C. Po, A. Vishwanath, and H. Watanabe, ArXiv e-prints (2017), arXiv:1711.11589.

$\mathbf{k} \in$ TRIM	Γ	X	Y	Z	U	T	S	R
$n_{\mathbf{k}}^{+}$	16	14	14	14	14	14	14	14
$n_{\mathbf{k}}^{-}$	12	14	14	14	14	14	14	14

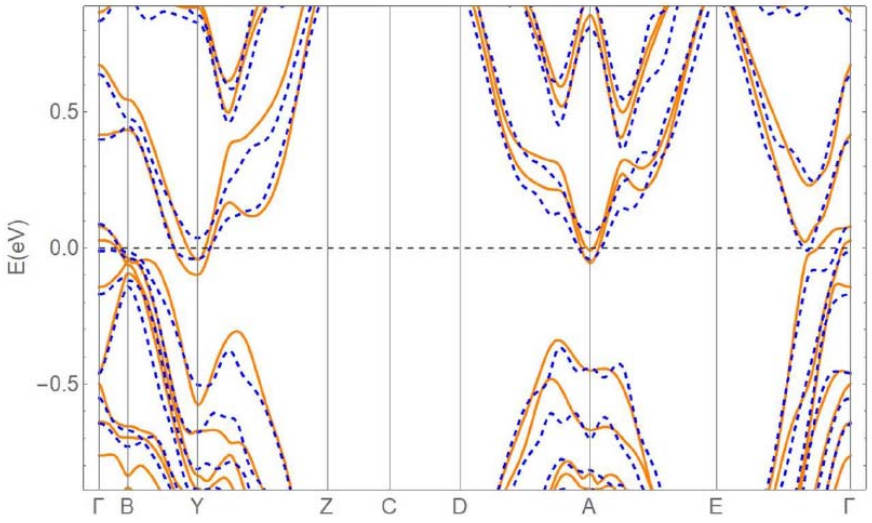
$n_k^{\pm}$ is the number of the occupied even/odd Kramers pairs

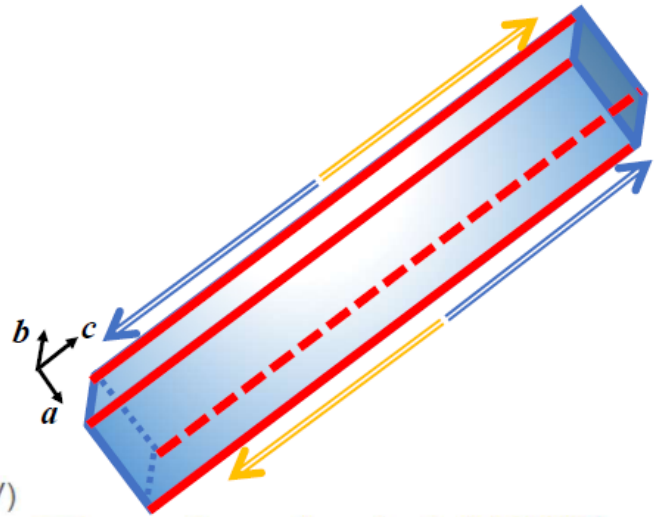
For this compound, 2 of Z_4→ mirror Chern/hinge states

WIEN2K→ mirror Chern number for $k_z = 0$ and $k_z = \pi/c$
They all vanish

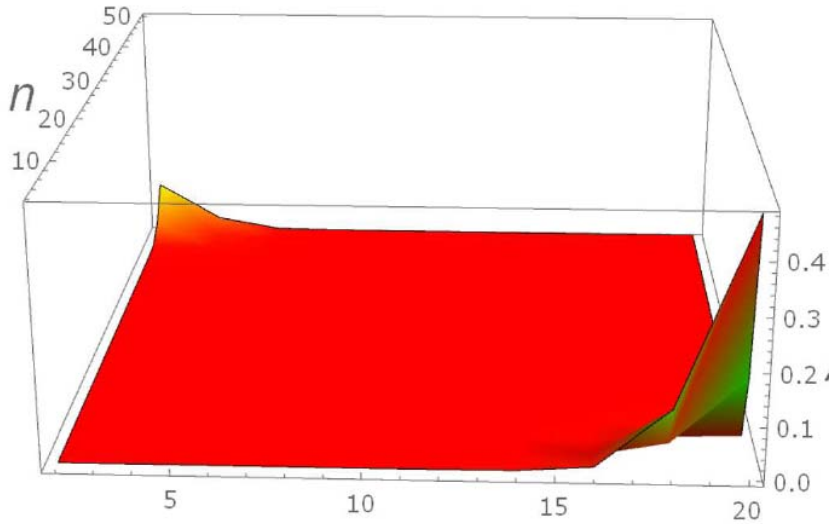
So hinge state!

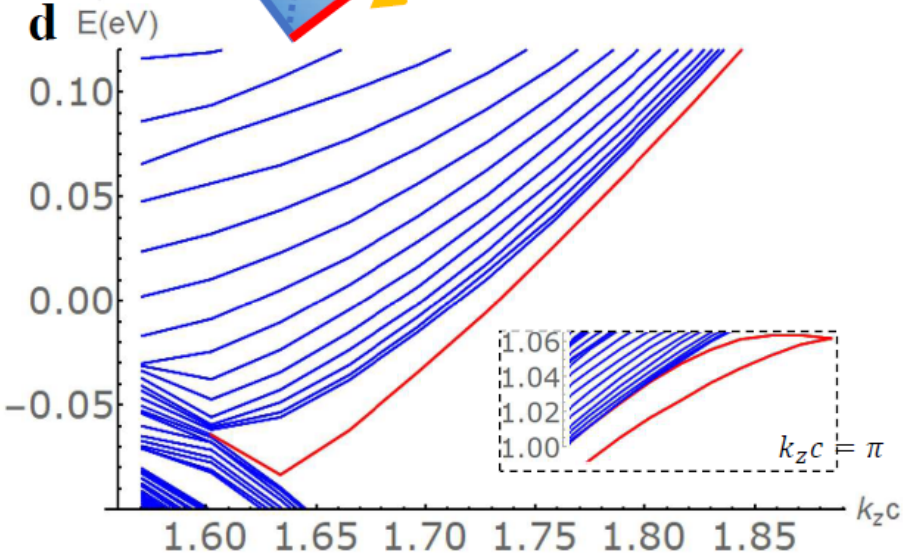
Hinge state from TB calculation





TB reproducts topo-feature and band dispersion





Had been confirmed by
Wang, Wieder, Li, Yan &Bernevig,
arXiv:1806.11116 (2018)

BiBr： Dirac Surface Sates Coexisting with Hinge State

$\mathcal{SG}\mathbf{12}\ (C2/m)$

TABLE III. For $\mathcal{SG}\mathbf{12}$, the HSPs are given by the labels $\Gamma, A, \ldots$ in order, and their coordinates can be referred to Ref. [2]. For the labeling of the irreps of $\mathcal{G}(\mathbf{k}_i)$, we use (j, m) where j means the jth irrep as listed in order by Ref. [2] and m denotes the dimension. The red color means that due to $\mathcal{T}$, the irrep must occur simultaneously with its $\mathcal{T}$ pair which belongs to the same irrep.

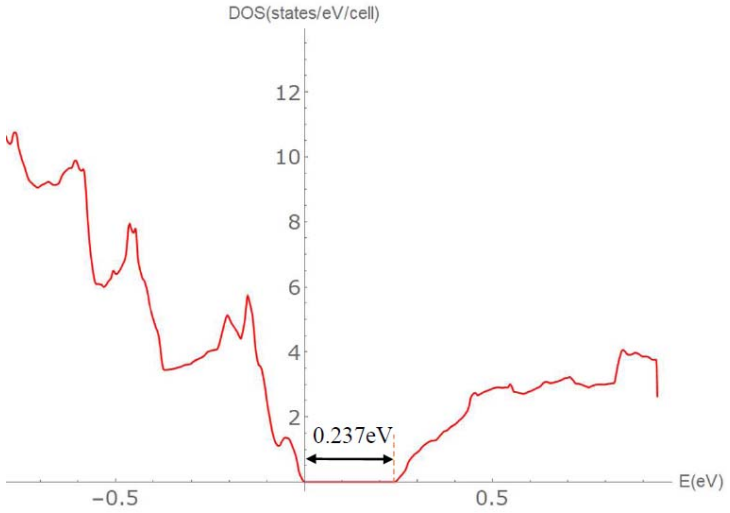
HSP	Γ				A				Z				M				L		V	
irrep	(1,1)	(2,1)	(3,1)	(4,1)	(1,1)	(2,1)	(3,1)	(4,1)	(1,1)	(2,1)	(3,1)	(4,1)	(1,1)	(2,1)	(3,1)	(4,1)	(1,1)	(2,1)	(1,1)	(2,1)
$n_{\mathbf{k}_i}^{\alpha_i}$	18	18	14	14	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16

$$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$$

$$\mathbf{n} = (64, 18, 18, 14, 14, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16)$$

$$= 14\mathbf{a}_1 + 2\mathbf{a}_2 + 2\mathbf{a}_3 + 2\mathbf{a}_4 + \mathbf{a}_6 - \frac{1}{2}\mathbf{a}_7,$$

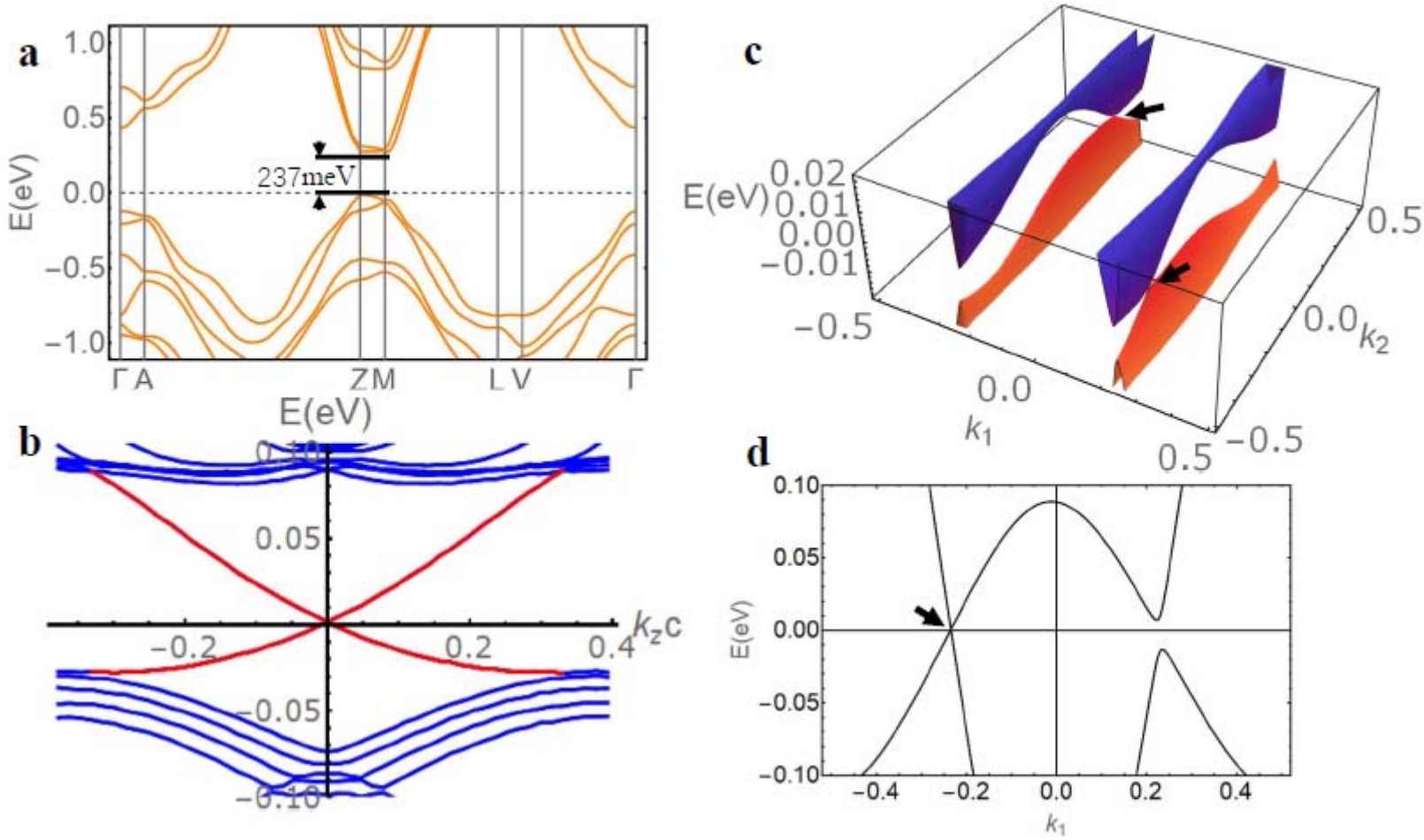
SI of $(0, 0, 2)$



(c)The 7 AI basis vectors for $\mathcal{SG}\mathbf{12}$.

$\mathcal{SG}\mathbf{12}$	$\mathbf{a}_1$	$\mathbf{a}_2$	$\mathbf{a}_3$	$\mathbf{a}_4$	$\mathbf{a}_5$	$\mathbf{a}_6$	$\mathbf{a}_7$
ν	4	4	-8	2	-4	8	-8
Γ_1^1	1	2	-4	1	-2	4	-4
Γ_2^1	1	2	-4	1	-2	4	-4
Γ_3^1	1	0	0	0	0	0	0
Γ_4^1	1	0	0	0	0	0	0
A_1^1	1	0	-1	0	0	2	-4
A_2^1	1	0	-1	0	0	2	-4
A_3^1	1	2	-3	1	-2	2	0
A_4^1	1	2	-3	1	-2	2	0
Z_1^1	1	0	-2	1	0	2	-4
Z_2^1	1	0	-2	1	0	2	-4
Z_3^1	1	2	-2	0	-2	2	0
Z_4^1	1	2	-2	0	-2	2	0
M_1^1	1	2	-3	0	-2	4	0
M_2^1	1	2	-3	0	-2	4	0
M_3^1	1	0	-1	1	0	0	-4
M_4^1	1	0	-1	1	0	0	-4
L_1^1	1	1	-1	1	-2	0	0
L_2^1	1	1	-3	0	0	4	-4
V_1^1	1	1	0	0	0	0	0
V_2^1	1	1	-4	1	-2	4	-4

Topological states in BiBr



- **Mirror Chern number = 0**
- **Hinge-State + Surface Dirac State**
- **TB→topo-feature**

Confirmed by:

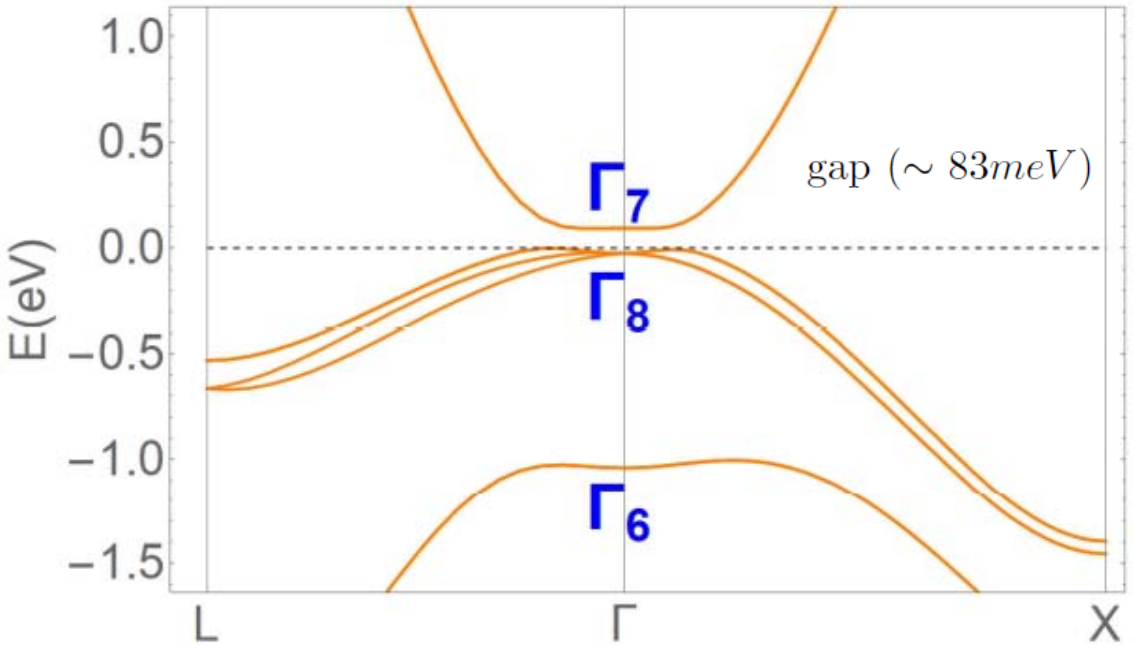
Hsu C H *et al.* 2D Mater., 2019, 6:031004

Non-Centrosymmetric Strong TI in AgNaO

- Inversion → Fu-Kane parity criterion
- Non-inversion → calculate Z_2 invariant

SG **216** ($F\bar{4}3m$), which are non-centrosymmetric and contains S_4

Expansion→ be insulators with the SI 1 □ Z_2



$s(d)$ band is mainly above (below) the Fermi level.

band inversion near the Gamma point,

results in an S_4 invariant

Other $2 \in Z_4$ Materials

- Cubic crystal TiS_2 (SG227) is a glide-protected TCI with **hourglass** surface states

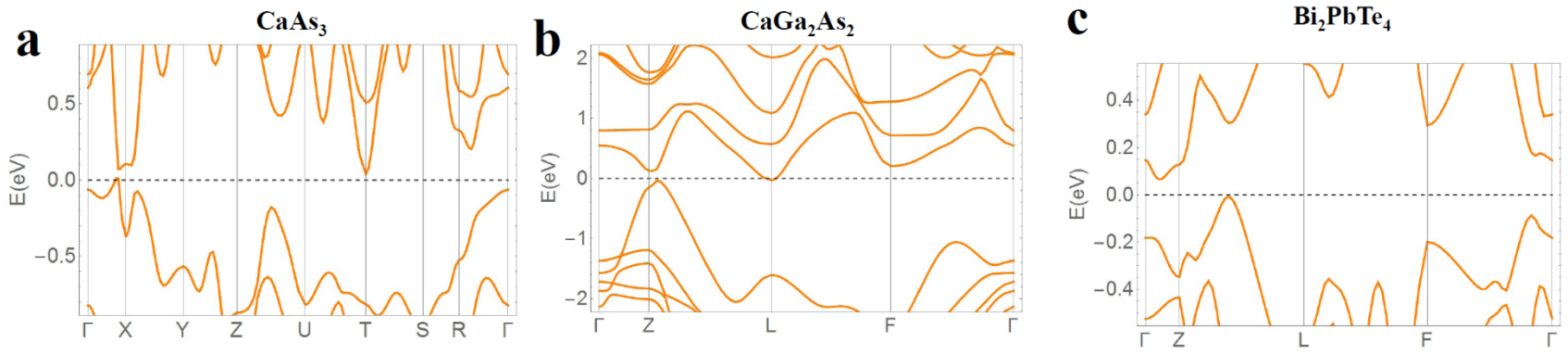
- Elemental phosphorus in the A7 structure (SG166), which occurs at about 9GPa, is predicted to be an inversion-protected TCI with 1D **hinge** states

- Ag_2F_5 (SG2) is a **weak TI** with additional inversion-protected band topology characterized by the invariant $\kappa_1=2$

Strong TI Found by 1,3 of Z_4

TABLE V. Table of centrosymmetric STI candidates discovered by 1, 3 in $\mathbb{Z}_4$

$\mathcal{SG}$	Material	X_{BS}	SI	$(\nu_0;\nu_1,\nu_2,\nu_3)$	κ_1
2	$CaAs_3$ [17]	$\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_4$	(0,0,1,1)	(1;1,0,0)	1
166	Bi_2PbTe_4 [18]	$\mathbb{Z}_2\times\mathbb{Z}_4$	(1,1)	(1;1,1,1)	3
166	$CaGa_2As_2$ [19]	$\mathbb{Z}_2\times\mathbb{Z}_4$	(1,1)	(1;1,1,1)	1

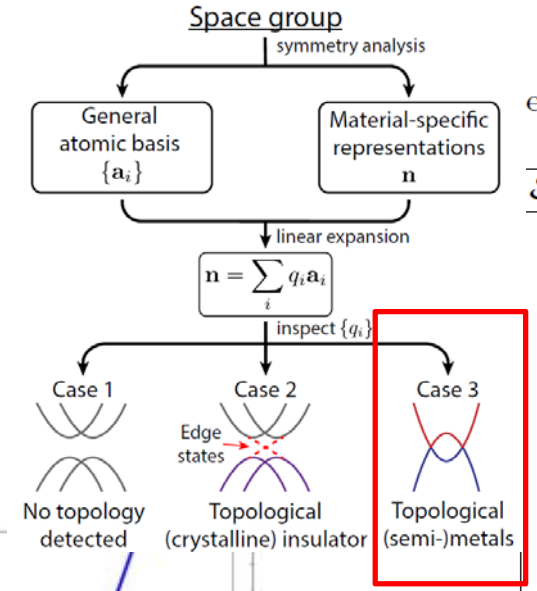


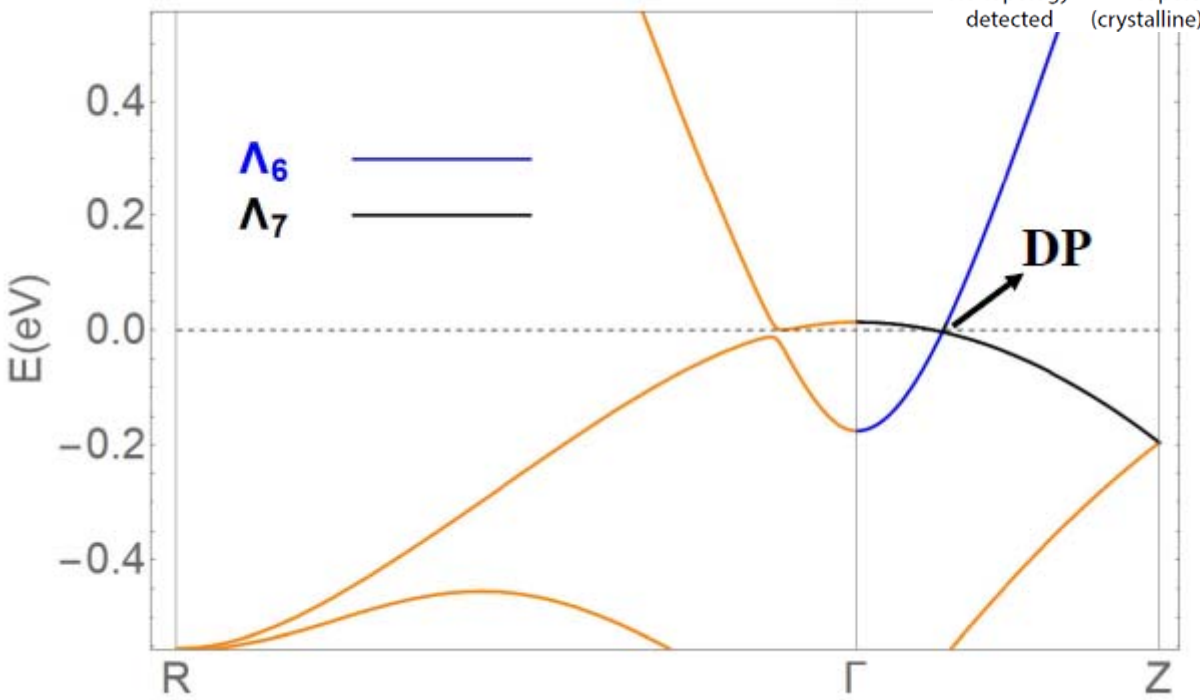
Dirac Semimetal $MgBi_2O_6$

$\mathcal{SG}136$

Expansion → case 3

So topological Semimetal



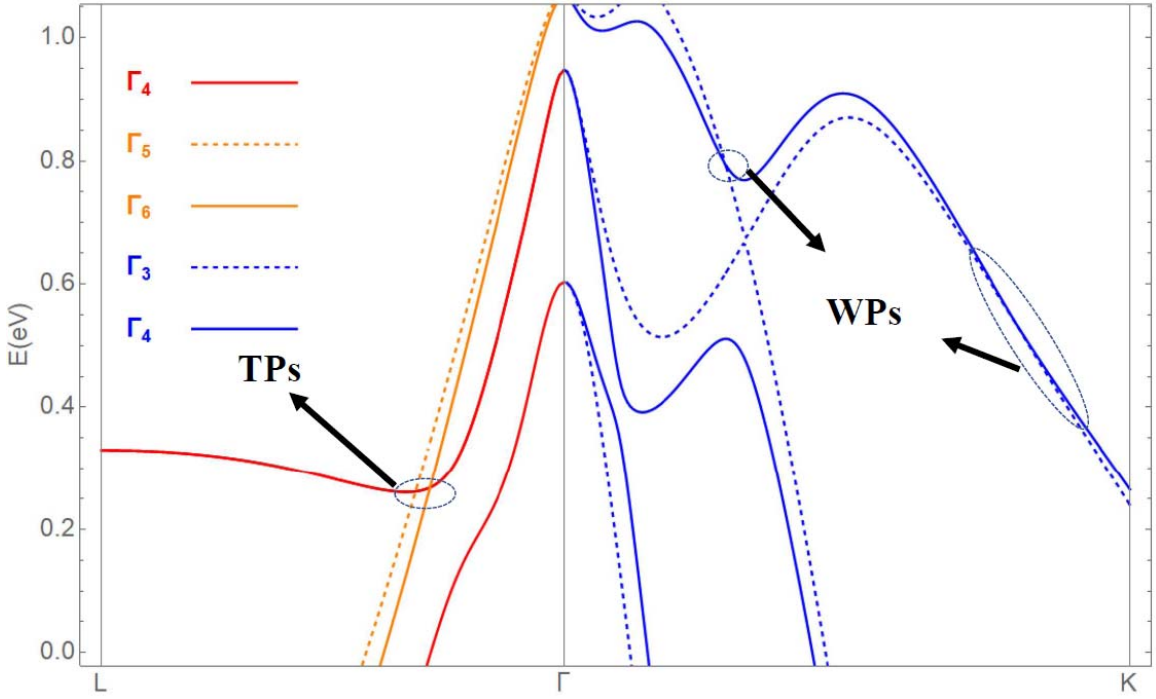


e)The 8 AI basis vectors for $\mathcal{SG}136$.

$\mathcal{SG}136$	$\mathbf{a}_1$	$\mathbf{a}_2$	$\mathbf{a}_3$	$\mathbf{a}_4$	$\mathbf{a}_5$
ν	8	8	8	4	-48
Γ_1^2	1	2	2	1	-12
Γ_2^2	1	0	2	1	-8
Γ_3^2	1	0	0	0	0
Γ_4^2	1	2	0	0	-4
K_1^2	1	1	0	1	-4
K_2^2	1	1	0	1	-4
K_3^2	1	1	2	0	-8
K_4^2	1	1	2	0	-8
K_1^4	2	2	2	1	-12
K_1^4	2	2	2	1	-12
K_1^1	1	1	1	0	-4
K_2^1	1	1	1	0	-4
K_3^1	1	1	1	0	-4
K_4^1	1	1	1	0	-4
K_5^1	1	1	1	1	-8
K_6^1	1	1	1	1	-8
K_7^1	1	1	1	1	-8
K_8^1	1	1	1	1	-8
K_1^2	2	2	2	1	-12
K_2^2	2	2	2	1	-12

Three-Fold Degenerate Fermions

- AuLiMgSn (SG216)
- DFT→ n_k^{α} are all integers thus there are finite direct gaps in all the HSPs.
- However expansion on the SG216′s AI basis vectors shows that they cannot constitute a BS at all, namely case 3 in the main text



The Nodal-line Semimetal AgF_2

AgF_2 (SG61)

$\left(\frac{11}{2}, \frac{19}{2}, \frac{13}{4}\right)$

(d)The 3 AI basis vectors for $\mathcal{SG}61$.

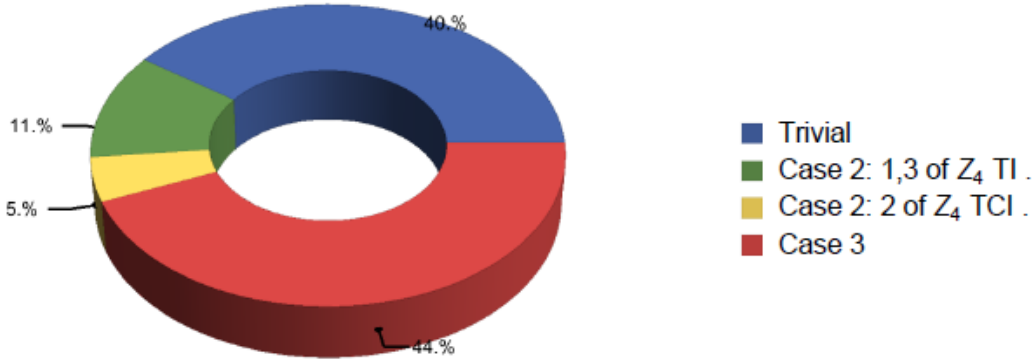
$\mathcal{SG}61$	$\mathbf{a_1}$	$\mathbf{a_2}$	$\mathbf{a_3}$
ν	16	8	-32
Γ_1^2	4	4	-12
Γ_2^2	4	0	-4
Y_1^2	4	2	-8
Y_2^2	4	2	-8
X_1^2	4	2	-8
X_2^2	4	2	-8
Z_1^2	4	2	-8
Z_2^2	4	2	-8
U_1^2	2	1	-4
U_2^2	2	1	-4
T_1^2	2	1	-4
T_2^2	2	1	-4
S_1^2	2	1	-4
S_2^2	2	1	-4
R_1^1	1	0	0
R_2^1	1	0	0
R_3^1	1	0	0
R_4^1	1	0	0
R_5^1	1	1	-4
R_6^1	1	1	-4
R_7^1	1	1	-4
R_8^1	1	1	-4

Comprehensive database searches

- Around 180000 compounds at ICSD database
- Consider stoichiometric compound
- Do not consider 3*d*/4*f*/5*f* and several 4*d*/5*d* element
- → **19143** compounds with SOC+time-reverse symmetry

- Highly efficient (main jobs is around 1 month within a cluster 28-node/one-node-32 CPU core)

GGA calculation
Check by MBJ calculation



$\mathcal{SG}$	X_{BS}	Topological insulators
2	$\mathbb{Z}_2^3 \times \mathbb{Z}_4$	AgO_4S[3],Ag_2F_5[4],As_3Ca[5, 6],As_3Sr[7, 8],Bi[9],Br_5W[10],$CaMo_6S_8$[11],CaP_3[8, 12]
11	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$BBeLi$[13],$GeHfPd$[14],HfS_3[15],Mo_2S_3[16],$NbPt_3$[17],Nb_2Se_3[18],Se_3Ta_2[18, 19]
12	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$Ag_4K_2Se_3$[20],$Al_2Ge_4Sr_3$[21],Al_8Mo_3[22],As_3Ba[8, 23],As_3Sr[8, 24],Au_2P_3[25],$BaSb_3$[26] $Ba_2Cd_2Sb_3$[27], $Ba_2Hg_3O_{14}Pd_7$[28],$Ba_3Li_4Sn_8$[29],$BaTl_4$[30], $Ba_{11}Bi_{14}Cd_8$[31],$Bi_2Pb_3S_6$[32],Bi_2Pd[33] $Bi_4Pb_7Se_{13}$[34],$Br_4Cs_2I_2Pd$[35],Hg_2Sn_2Sr[36],Nb_2PdS_5[37],Nb_2PdS_6[38],Nb_2PdSe_6[38],P_3Sr[39] ,$PdSe_6Ta_2$[38],$PtSe_7Ta_2$[40]
14	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$Ag2Te$[41, 42]
51	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$AlPt_2$[43], $AuITe_2$[44], Au_3Rb_2Tl[45]
55	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$Al_2Bi_6Ca_5$[46],$Bi_6In_2Sr_5$[47]
57	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	STa_2[48]
58	$\mathbb{Z}_4$	Bi_2Hf[49],S_2Ti[50]
59	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Ag_3Sb[51], $AuCs_3Pb_4$[52], $AuPb_4Rb_3$[52], $AuRb_3Sn_4$[52]
60	$\mathbb{Z}_4$	Au_2Pb[53, 54], O_2Pb[55]
61	$\mathbb{Z}_4$	$AuSn_2$[56],Bi_2Pt[57]
62	$\mathbb{Z}_4$	$AsCdNa$[58],As_2Hf[59],As_2Zr[60, 61],Ba_2Pb[62],Ba_2Si[63, 64],Ca_3GeO[65],$CdGeSr$[66],$CdNaSb$[67, 68],$FSeY$[69] $GaPtSc$[70], $GaPtY$[70],$GeHfPt$[71, 72],$GeMoZr$[73],$GePdZr$[74, 75],$GePtZr$[75, 76],$GeZr$[77],$Ge_2InLiSr_2$[78],Ge_2Mo[79] Ge_2W[80],$HfNbP$[81],HfP_2[82],$HfSi$[83],NNa_3[84],N_5Ta_3[85],$NbPZr$[86],$PPtSc$[75, 87],P_2Ti[88] P_2Zr[89],$PbSr_2$[90, 91],$PdSiTi$[75, 92],$PdSiZr$[93],$PtSiTi$[75, 94],$PtSiZr$[75, 94],Sb_2SrZn[95, 96],$SiSr$[97],$SiTi$[98],$SiZr$[98]
63	$\mathbb{Z}_2 \times \mathbb{Z}_4$	AgS_3Ta[99],$AlBMo$[100],$AlBW$[100], Al_2BaSi_2[101], $AuClTe_2$[102], B_7WY_3[103],$BaIn$[104],$CaSi$ [105] Ga[106],$GeNa_2Zn$[107], $HfPd$[108],$HfTe_5$[109, 110],$PdZr$[111]
64	$\mathbb{Z}_2 \times \mathbb{Z}_4$	As[112], C_2B_2Mg[113], $LiTl$[114]
65	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Ag_3Te_2Tl[115],Ba_3Ge_4[116]
69	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Be_2Zn[117]
71	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$AsTeTi$[118],Br_2Ca_3Si[119]
72	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$Br_2Hg_5O_4$[120]
87	$\mathbb{Z}_2 \times \mathbb{Z}_8$	As_4Mo_5[121],Hf_5Te_4[122],Se_4Ti_5[123],Te_4Zr_5[124]
114	$\mathbb{Z}_2$	Pd_4S[125]
121	$\mathbb{Z}_2$	Ag_2S_4SnZn[126]
122	$\mathbb{Z}_2$	As_2CdGe[127],As_2CdSn[128],As_2SnZn[129],$CdSb_2Sn$[130]
123	$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	$BaGe_3Mg_4$[131],$BiLi$[132],$BiNa$[133],$ClNa_2$[134],$ClNa_3$[134]
127	$\mathbb{Z}_4 \times \mathbb{Z}_8$	B_4Y[135],CsI_3Sn[136, 137], Pt_3Si[138]
129	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$HfSb_2$[139]
136	$\mathbb{Z}_4$	Ag_5CsSe_3[140],Ag_5CsTe_3[141]
139	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Ag_2Zr[142],Au_2Hf[143],Au_2Zr[144],$BaCd_2Ge_2$[145], $BaGe_2Mg_2$[146],$Be_{12}W$ [147] $Bi_{10}Ca_{11}$[148],$CaGe_2Zn_2$[146],Cd_2Ge_2Sr[149],Ge_2SrZn_2[150],Hf_2Pd[151],$InPd_3$[152],$PdZr_2$[153],Pd_2Ti[154]
140	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Bi_3In_5[155],Hf_2Si[156],In_5Sb_3[157],Pb_2Pt[158],Sc[159],$SiZr_2$[160],Sb_2Ti[161],Si_3Sr_5[162],Sn_3Sr_5[163]
164	$\mathbb{Z}_2 \times \mathbb{Z}_4$	Ag_2O[164],$As_2Ge_5Te_8$[165],As_4GeTe_7[166],$BaSn_2$[167, 168],Be[169],Bi_2Li_3Y[170],Bi_2Mg_3 [171, 172] $Bi_2Pb_2Se_5$[173, 174],Bi_4SnTe_7[175],CNb_2[176],CTa_2[177],$C_6K_2N_6PtS_6$[178],$C_6N_6PtRb_2S_6$ [178] $CaGe_2$[179, 180],$CaSi_2$[180, 181],$GeSb_4Te_7$[182],Ge_2Sr[180, 183],$PdTe_2$[184, 185],$PtTe_2$[186, 187],Sb_2Te_2[188],$SiTe_2$ [189]
166	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$CsGa_7$[190],$Cl_8Na_2Ti_3$[191],Ga_7Rb[192],$PtTe$[193], Pt_2Te_3[193],STi[194],$SeTi$[195],$AgGeLi_2$[196] $Al_{10}Ba_7$[197],As[198],As_2CaGa_2[199] $As_2Ge_4Te_7$[200],As_2Sn_2Sr[201, 202],Bi_2GeTe_4[203, 204], Bi_2PbTe_4[205],Bi_2SeTe_2[206, 207],Bi_2Se_3[208, 209],Bi_2Te_3[209, 210] Bi_6PbTe_{10}[210],Bi_8Te_9 [211], CS_2Ta_2[212],CY_2[213],C_5Ti_8[214] $CaGe_2$[215],$CaSi_2$[216, 217],$GaGeTe$[218] GaP[219],Ga_2Te_3[220],In_2Te_3[220],Li_8Pb_3 [221] N_2W[222],Sb[223],$SbTe_2Tl$[224, 225],Sb_2SeTe_2[226, 227] Sb_2SnTe_4[228, 229],Sb_2Te_3[209, 230],Sb_8Te_3[231],$Sb_{48}Te_9$[231]
191	$\mathbb{Z}_6 \times \mathbb{Z}_{12}$	B_2Sr[232],$BaSi_2$[233],$CaSi_2$[234],Li_2Pd[235],Li_2Pt[236],Ti[237]
193	$\mathbb{Z}_{12}$	Pb_3TeZr_5[238],Sn_3Zr_5[239]
194	$\mathbb{Z}_{12}$	$AgSbSr$[240],AlN_3Ti_4[241],Al_2Hf[242],$AuBaBi$[243],C_2AlTa_3[244],Ca_2IN[245] $MgPo$[246],$PbPt$[247],$SiSr_2$[248],$BeHfSi$[249]
216	$\mathbb{Z}_2$	$AgKO$[250],$AgNaO$[250],$AgORb$[250],HgS[251],InN[252],NTl [253]
221	$\mathbb{Z}_4 \times \mathbb{Z}_8$	$AlSc$[254],AlY[255],B_6Ca[256],B_6Sr[256],$BeTi$[257] Br_3CsGe[258],Br_3CsPb[259],CsI_3Sn[260] $MgPd$[261],$PbSe$[262],$SnTe$[263]
223	$\mathbb{Z}_4$	$BiNb_3$[264],Nb_3Sb[265],$SbTa_3$[266, 267]
225	$\mathbb{Z}_8$	BiY[268],CPd[269],CZr[270],Li_2MgSi[271],N_2Pd[272]
227	$\mathbb{Z}_4$	CTi_2[273],Se[274]

TABLE I. The list of all the TIs with relatively clean Fermi surfaces discovered by GGA calculations: when the MBJ calculation doesn't change the band topology predicted by GGA calculations, we print the material in blue, while the red color means that the MBJ calculation results in a topological crystalline phase.

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$\mathcal{SG}$	X_{BS}	Topological crystalline insulators
2	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$CsHg$[275],HgK[276]
11	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$BaSb_2$[277],$MoTe_2$[278],Sb_2Sr[279],Se_3Ta[280, 281]
12	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$Al_4Cl_{51}Zr_{12}$[282],$Al_4Na_4P_{12}Sr_8$[283],As_2Nb[284, 285],As_2Ta[285, 286],As_3Mo_2[287],As_3W_2 [288] $As_4Ba_3Zn_2$[289],$Ba_3Cd_2Sb_4$[290],$BiBr$[291],$BiHf_2$[292],Bi_2ITe[293, 294],CdK_6Pb_8[295],$ClZr$ [296] Cl_8NSc_5[297],NbP_2[298],$NbSb_2$[299],Sb_2Ta[300, 301],Se_4Ti_3[302],Ta_2Te_3[303]
51	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$GaPt_2$[304],$CdMg$[305]
55	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$Ca_5Ga_2Sb_6$[306]
58	$\mathbb{Z}_4$	Bi_3RbS_5[307]
59	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$BrNTi$[308]
62	$\mathbb{Z}_4$	$HgSr_3$[309],$PdSi$[310],$PdSn$[311]
63	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$BaGe$[312],$BaSi$[313], $BaSn$[314],Ba_3Pb_5[315],$Ba_5Cd_2FSb_5$[316], $CaGe$[317],$CaSn$ [318] $Cd_2FSb_5Sr_5$[319],$PbSr$[320],$SnSr$[321]
64	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$Ca_5Ga_2N_4$[322],Li[323]
65	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	Au_7Rb_3[324]
69	$\mathbb{Z}_2^2 \times \mathbb{Z}_4$	$Ge_6Li_2Sr_4$[325]
71	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$Ba_3Bi_4Li_4$[326],$Ba_3Li_4Sb_4$[326]
87	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Au_4Ti[327]
88	$\mathbb{Z}_4$	O_4PbPd_2[328]
123	$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	As_3CsZn_4[329],As_3RbZn_4[329],CPd_3Sn[330], Pd_3Sn[331]
127	$\mathbb{Z}_4 \times \mathbb{Z}_8$	B_4Ca[332]
129	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$AsGeNb$[333],$GeHfS$[334, 335],$GeHfSe$[334, 335],$GeHfTe$[334, 335],$GeNbSb$[336],$GeSZr$ [337] $GeSeZr$[334],$HfSSi$[334, 335],$HfSeSi$[334, 335],$OSiZr$[334],$SSiZr$[338],$SeSiZr$[338],$SiTeZr$[338],$SnTeZr$[338]
137	$\mathbb{Z}_4$	Ba_2LiN[339]
139	$\mathbb{Z}_2 \times \mathbb{Z}_8$	$AsBa_2$[340],$AsCa_2$[341] Ba_2Bi[342],Ba_2Sb[343],$Ba_{11}Bi_{10}$[344],$BiSr_2$[343],$Bi_2F_2OSr_2Ti_2$[345],Br_2Ca_3Si [346] $CaIn$[347],$F_2OSb_2Sr_2Ti_2$[348],Hf_2Hg[349],Pd_2Si_2Sr[350],$SbSr_2$ [351]
140	$\mathbb{Z}_2 \times \mathbb{Z}_8$	Bi[352],$GePt_3$[353],Mg_2Pt[354]
164	$\mathbb{Z}_2 \times \mathbb{Z}_4$	$BaSi_2$[355],$BiTe$[356],$Bi_2Pb_2Te_5$[357, 358], Bi_2Se_2[359],Bi_3STe_2[360],$HgPt_2Se_3$[361],Te_2Zr[362]
166	$\mathbb{Z}_2 \times \mathbb{Z}_4$	B_2Mo[363],$Ba_3O_9Sc_4$[364],Pt_3Te_4[365],$TeZr_3$[366],$AsNaTe_2Zr_2$[367],As_3Cd_4K[368] As_3Cd_4Na[368],As_3Cd_4Rb[368],Bi[369],Bi_4Se_3[370, 371],Bi_8Se_9[372],$BrZr$[373],CNb_2S_2[374],$C_3Al_6N_2$ [375] $ClZr$[376],Hg[377],P[378],$Pd_3S_2Tl_2$ [379]
187	$\mathbb{Z}_3 \times \mathbb{Z}_3$	Br_2Ca_3Si[380],CHf[381],$InNbS_2$[382, 383],$InNbSe_2$[383, 384],NY[385]
189	$\mathbb{Z}_3 \times \mathbb{Z}_3$	$AgAsCa$[386, 387],$AgCaP$[387, 388] $GeLiY$[389]
191	$\mathbb{Z}_6 \times \mathbb{Z}_{12}$	B_2Ca[390],B_2Mg[391],B_2Ti[392],B_2Zr[393], $Be_{12}Ti$[394],Ga_2Sr[395],Pd_5Sr[396]
193	$\mathbb{Z}_{12}$	Pb_3SZr_5[397]
194	$\mathbb{Z}_{12}$	$AlLi$[398],$AsHgK$[399, 400] ,B_2W[401], Be[402],C[403],$CdNa_2Sn$[404], $HgKSb$[400, 405],$SnTi_2$[406]
221	$\mathbb{Z}_4 \times \mathbb{Z}_8$	$CPbPd_3$[407],CPt_3Sn[407],$CaPd$[408],Ca_3GeO[409, 410],Ca_3OPb[410, 411],$HfPd_3$[412],$HgPt_3$[413],NTi_3Tl[414] NY[415],$PbPt_3$[416],Pt_3Sn[417],Pt_3Zn[418]
225	$\mathbb{Z}_8$	$AsSc$[419],Au_2InSc[420],Au_2InY[421],Ba[422],BiI_3[423],$BiSc$[424] CPt[425],Ca[426],$PbPo$[427, 428],SSn[429],$SbSc$[430],$SeSn$[431], $SnTe$[432, 433]
227	$\mathbb{Z}_4$	$Mo_2O_7Y_2$[434],S_2Ti[435]

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$\mathcal{SG}$	Topological (semi-)metals
11	Br_9TeW[436],$CBrHgNS$[437],Li_7Sn_3[438],Mo_2S_2Sb[439]
51	$AuCd$[440],$AuTi$[441]
52	Ag_2BiO_3[442],Bi_3Sr_2[443]
55	Al_3Pd_5[444],Al_3Pt_5[445],BCl_6Sc_4[446], $Bi_9Ca_9Cd_4$[447], $Bi_9Ca_9Zn_4$[448],$Bi_9Cd_4Sr_9$[447],$In_5S_{13}Y_4$[449]
57	$AlCaPd$[450], BiK_2Sn[451]
58	$C_{60}K$[452]
59	Ag_3Sn[453]
60	F_4NaTi[454]
61	AgF_2[455]
62	$AgAuF_7$[456],AgF_3K[457],$AlPt_2$[458] Bi_3Ca_5[459],Bi_3Sr_5[460],Ca_5Sb_3[461] $GeNb_3Te_6$[462],$GePd_2Y$[463],N_3Nb_2[464],Nb_3Si[465] $PdSbZr$[466],$SiTa_3Te_6$[466]
63	$AgCa$[467], $AuCa$[468], $BiZr$[469], Ga_3PdSr[470], Ga_5Zr_3[471], $GeSc$[472], GeY[473], $HfSb$[474],$K_3O_4Pd_2$[475],$K_3O_4Pt_2$[476],K_4P_3[477, 478], N_5NaTa_3[479],PdY[480],SiY[481], Sr_3Tl_5[482]
64	$AgCs_2F_4$[483],$Au_{10}Ca_4In_3$[484],Bi[485, 486]
87	Ba_9In_4[487],$In_4Pd_{17}Se_4$[488],$Pt_{11}Zr_9$[489], $Pt_{12}Si_5$[490]
88	$Al_{21}Pt_8$[491],$CsFO_3S$[492],Ge_8Pd_{21}[493]
123	$AgPPt_5$[494],$AlPPt_5$[494],$AsInPd_5$[495],$AsPd_5Tl$[496] $AsPt_5Tl$[496],As_2BaPd_2[497],BaP_2Pd_2[498],$CaPb$[499] $CdPd$[500],$CdPd_5Se$[501],$CdPt$[502],Cd_3Zr[503] $FKNb_4O_5$[504],$HgPd$[505],$HgPd_5Se$[506],$HgPt$[507],Hg_2Pt[507] $InPPd_5$[508],$InPPt_5$[508],PPd_5Tl[508],PPt_5Tl[508] $PdTi$[509],Pd_5SeZn[510],$SiSr$[511],Sr[512]
127	$AlSc_2Si_2$[513],Au_2Ca_2Pb[514],Au_2InY_2[515],B_2Ta_3[516] B_4W[517],C_2B_2Y[518],Ga_2MgSc_2[519],Ca_3Hg_2[520] Ga_2Nb_3[521],Ga_2Ta_3[522],Ge_2Hf_3[523],Hg_2Sr_3[524, 525] $InPd_2Y_2$[526],In_5Ti_2[527],$LiSi_2Y_2$[528],$PbPd_2Y_2$[529]
129	$AgMgSb$[530],$AsNbSi$[531],$AsSiTa$[532], $BaMgSi$[533],$BiKMg$[534],$GeTeZr$[535],$MoNTa$[536]
130	$AlMg_4Si_3$[537],Se_3Tl_5[538]
131	OPd[539]
136	$AlNb_2$[540],$AlTa_2$[541],Bi_2MgO_6[542], O_2Pb[543, 544],O_2Pd[545],O_2Pt[546]
137	As_2Cd_3[547, 548],Bi_2Se_3[549]
139	Ag_2CaGe_2[550],Ag_2Ge_2Sr[550],Ag_2Si_2Sr[551],Ag_2Sn_2Sr[552],Al_2BaSi_2[553],Al_2Pb_2Sr[554],Al_3Nb[555] Al_3Ta[556],Al_3Zr[557],Al_4Ba[558],Au_4CaCd_2[559],$BaBi_4Cl_2O_6$[560],$BaIn_4$[561],$Be_{12}Pd$[562],$Be_{12}Pt$[562] $CaGa_4$[563],$Ca_{11}Sb_{10}$[564],Ga_3Nb[565, 566],Ga_3Ta[567],In_4Sr[568],Pt_3Sb[569],S_2Ti[570],$Sb_{10}Sr_{11}$[571] Si_2W[572],$ZnZr_2$[573]
140	$AgCsF_3$[574],AgF_3Rb[574],$AgIn_2$[575],$AlZr_2$[576],$AuSe_3Tl_4$[577],$AuTl_2$[578],Au_3Cd_5[579] Au_4In_2K[580],Au_4In_2Rb[580] BGe_2Nb_5[581],BMo_2[582],BTa_2[583],BTi_2[584],BW_2[585],Ba[586],$BeTa_2$[587],Bi_3In_4Pb[588] Ca_5Pt_3[589],Ca_5Si_3[590] Cs_9InO_4[591],$GaHf_2$[592],$GaPt_3$[593],$GaZr_2$[594],Ga_5Pd[595],$GeHf_2$[596],Ge_3Mo_5[597] Ge_3Nb_5[598],Ge_3W_5[599],Nb_5SiSn_2[600] Nb_5Si_3[601],Pb_3Sr_5[602],$PdTl_2$[603],SZr_2[604] Si_3W_5[605],Sr[606],Te_3Tl_5[607]
163	AlF_6LiPd[608],$F_6GaLiPd$[609],In_2Pt_3[610]
164	$AlCl_3$[611],CSc_2[612],$CaHg_2$[613],$CaSb_2Zn_2$[614],Cl_2Ti[615],$HfTe_2$[616, 617],Hg_7K_2 [618] Hg_7Rb_2[618],OTi_2[619],Sb_2SrZn_2[620],Se_2Ti [621]
166	$BaPb_3$[622],$Be_{17}Hf_2$[623],$Be_{17}Nb_2$[624],$Be_{17}Ta_2$[623],$GeTe$[625, 626],$Pb_2Pd_3S_2$[627] $Pb_2Pd_3Se_2$[628],Po[629],$SbSn$ [630] $AgInSe_2$[631],As_3NaZn_4[632],Bi_4Te_3[633],$C_3Al_8N_4$[634],Cd_4KP_3[635],GeP_3[636],In_2Se_3[637],$Pd_3Se_2Tl_2$ [638],Ag_4Sb_2Sr[639]
167	Al_5Mo[640],Cs_8Ga_{11}[641],F_3Mo[642],F_3Pd[643],F_3Ti[644],$In_{11}K_8$ [645] K_8Tl_{11}[646],$Mo_9S_{11}Tl_2$[647],NPd_3 [648]

List 489 good topological Semimetal

176	$AgCd_3F_{20}Hf_3$[649],$AgCd_3F_{20}Zr_3$[649],$AgMo_3Se_3$[650],$AsNb_3Te_3$[651] $CsMo_3S_3$[652],$CsMo_3Se_3$[653],$CsMo_3Te_3$[654],$InMo_3Se_3$[655, 656] $InMo_3Te_3$[655, 656],KMo_3S_3[655],KMo_3Se_3[655, 656],KMo_3Te_3[656, 657],$LiMo_3Se_3$[658] Mo_3NaSe_3[655, 656],Mo_3NaTe_3[656, 658],Mo_3RbS_3[655],Mo_3RbSe_3[658, 659] Mo_3RbTe_3[660],Mo_3Se_3Tl[656, 658],$Mo_6Se_6Tl_2$[661],$NbSe_2$[662]
187	AgN[663],$CLiNaO_3$[664],CMo[665],CPt[666],CTa[666],CW[667] InS_2Ta[668],$InSe_2Ta$[669],MoP[670],NNb[671],NPd[672],NW[673] NZr[674],N_2Pt[675],N_2Ta[675],NbS[676],STa[677] STi[678],TeZr[679]
188	I_3LiSc[680]
189	AlHfPt[681],AlPdY[682],AlPtZr[681],Al_2Hf_6Pt[683],$AsPd_2$[684] AuInY[685],GaPtZr[681],GePdSc[686],$GePd_2$[687],$GePt_2$[688],InPdY[689] InPtSc[690],InPtY[691],MgPdY[692],NTa[693],PdTlY[694],PdYZn[695] Pd_2Si[696],$PtSb_2Zr_6$[697],Pt_2Si[698]
190	AlHfPt[699],AlPtZr[700],$B_4Ga_3Pt_9$[701], GaHfPd[702],GaPtZr[703],Li_2Sb[704],PdScSn[705]
191	Au_2Ba[706],Au_5K[707],Au_5Rb[707],B_2Mo[708],$BaGa_2$[709],$BaPd_5$[710],Be_2Hf[711] Be_5Hf[712],Be_5Zr[713],$CaGa_2$[714],$CaHg_2$[715],Hf[716],Hf_2N_3Ta[717],Hg[718] $LiNNa_2$[719],NNa_3[720],NOTa[721],NTa[722],N_3TaTi_2[723],N_3TaZr_2[723],N_4Ta_2[724],S_2Ti[725]
193	$AgIn_3Zr_5$[726],$AgPb_3Zr_5$[727],$AgSb_3Zr_5$[728],$AlSn_3Zr_5$[729],Al_3Hf_5[730] Al_3Hf_5N[731],Al_3Ta_5[732],Al_3Zr_5[733],Al_4Zr_5[734] $AsPb_3Zr_5$[735],$AsSb_3Zr_5$[736],$AsSn_3Zr_5$[737],As_3Ca_5[738],As_3Sr_5[739] BNb_5Si_3[740],BSn_3Zr_5[741],Ba_3N[742],Ba_5Bi_3[743] Ba_5Sb_3[743],Bi_3Sr_5[744],CSb_3Zr_5[745],CSn_3Zr_5[746],Ca_5Sb_3[747],$CdPb_3Zr_5$[748] Cl_3Ti[749, 750],Cl_3Zr[750, 751],$GaSn_3Zr_5$[752],$Ga_3Hf_3Nb_2$[753] Ga_3Nb_5[754],Ga_3Sc_5[755],Ga_3Ta_5[756],Ga_4Nb_5[757],Ga_4Ti_5[758] Ga_4Zr_5[758],$GePb_3Zr_5$[759],Ge_3Mo_5[760],Ge_3Nb_5[761] Ge_3Sc_5[762],Ge_3Ta_5[763],Ge_3Y_5[764],HfI_3[765, 766],Hf_5Sb_3Zn[767],Hf_5Si_3[768] Hf_5Sn_3[769],Hf_5Sn_4[770],Hg_3Mg_5[771],I_3Nb[772] I_3Ti[773, 774],I_3Zr[775],$InPb_3Zr_5$[776],$K_3Nb_8O_{21}$[777] Mo_5Si_3[778],NSn_3Zr_5[779],N_6Nb_5[780],N_6Ta_5[781] Nb_5OPt_3[782],Nb_5PSi_3[783],Nb_5Si_3[784],PPb_3Zr_5[785] PSn_3Zr_5[786],P_3Ti_5[787],Pb_3SbZr_5[788],Pb_3Sc_5[789] Pb_3SeZr_5[788],Pb_3SiZr_5[788],Pb_3SnZr_5[788],Pb_3Y_5[790] SSb_3Zr_5[791],SSn_3Zr_5[792],Sb_3SiZr_5[793] Sb_3Sr_5[794],Sb_4Zr_5[795],$SeSn_3Zr_5$[796],$SiSn_3Zr_5$[796] Si_3Ta_5[797],Si_3Y_5[798],Sn_4Zr_5[799]

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Symmetry indicator

- TaAs family

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- Magnetic

Conclusion

- We propose a highly efficient method to explore topological materials

What one need to do is to look the expansion coefficient!

- We propose numbers of new topological materials.

Thank you very much for your attention

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当前的问题和可能的方案

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