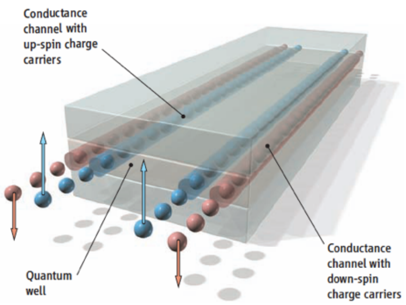
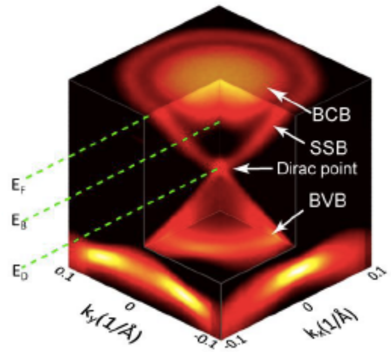
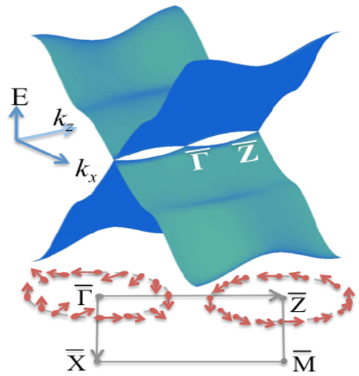






Topological insulators

Binghai Yan

Max Planck Institute for Chemical Physics of Solids, Dresden

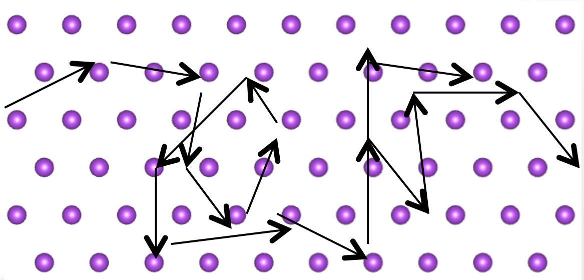
Outlines

Topological insulator (TI)

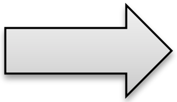
- Where did TI come from?
- What is topology?
- What is a TI?
- Who are TIs?
  Graphene, HgTe, Bi2Se3, Heuslers
- What is the recent progress?
- Topological mirror insulator

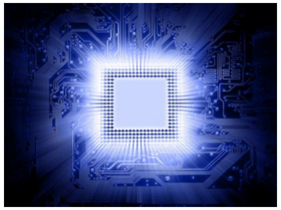
Travel of electrons in the device

Joule's heat: $Q=I^2\mathbf{R}\,t$
R: resistance



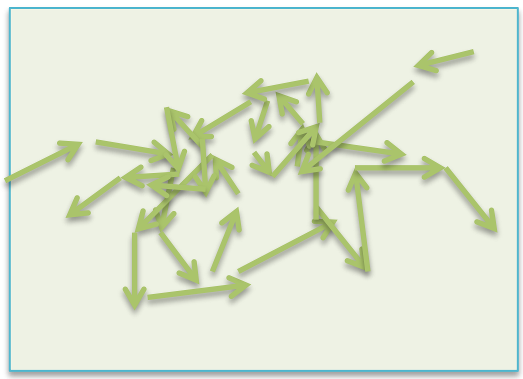
Human society

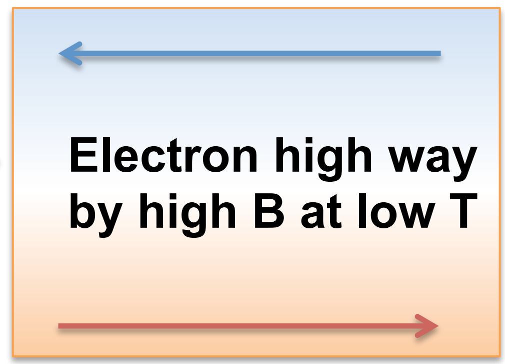




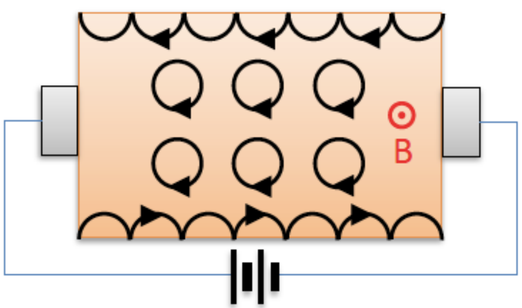
Information highway ?

Separate the electron motion

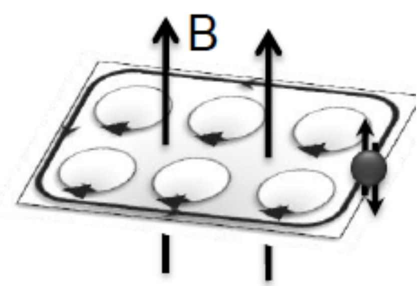




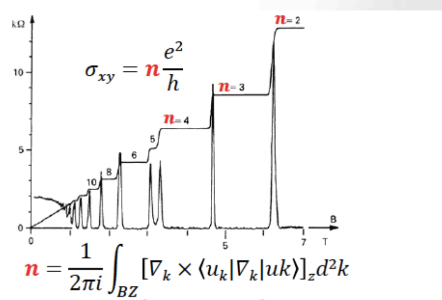
K. von Klitzing
1985 Nobel Prize in Physics



Avoid backscattering



Edge conduction

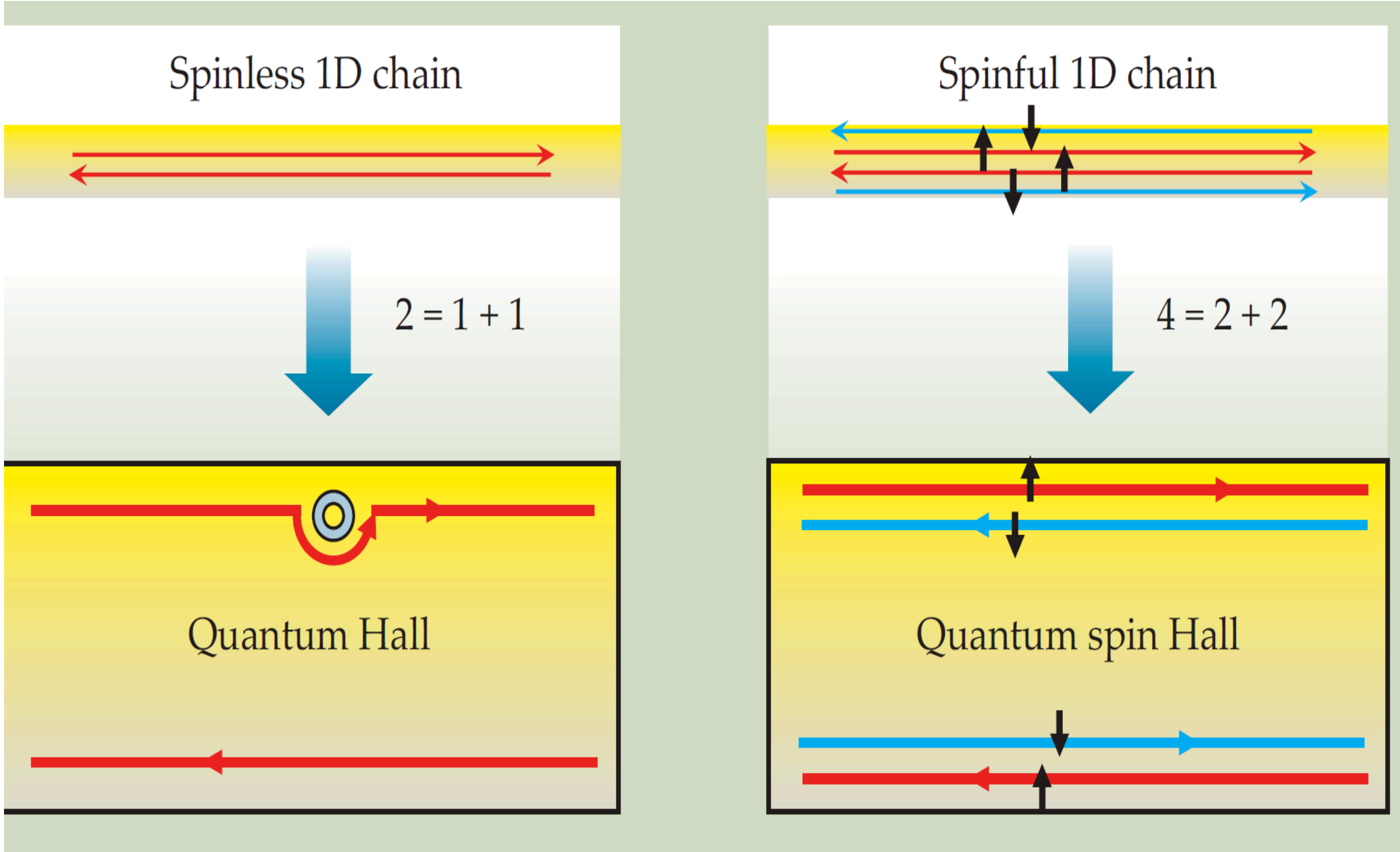


$$n = \frac{1}{2\pi i}\int_{BZ} [\nabla_k \times \langle u_k|\nabla_k|uk\rangle]_z d^2k$$

n **: Chern number**

"Topological invariant"
(TKNN, 1982)

Quantum Spin Hall effect (2D TI)



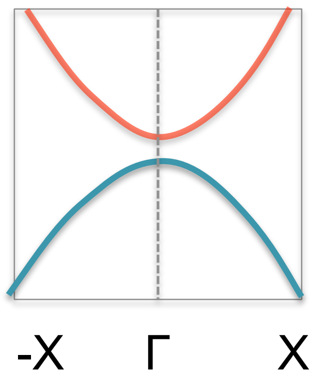
GaAs

Predicted for HgTe in 2006
by Bernevig, Huges and Zhang.

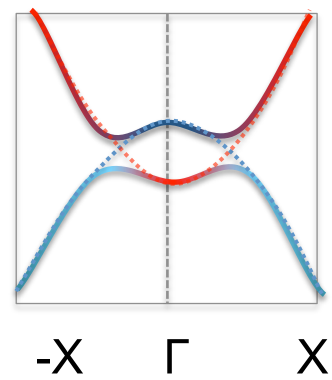
X.-L. Qi and S.-C. Zhang, Physics Today **63**, 33 (2010).

Band inversion

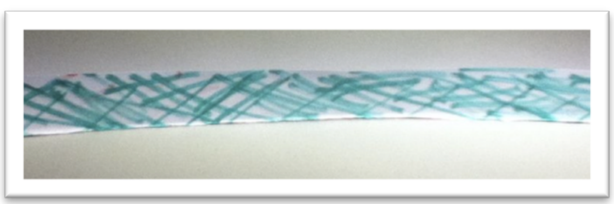
Normal insulator

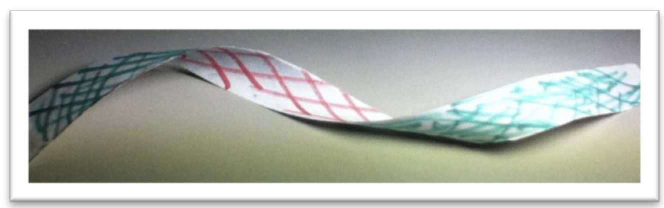


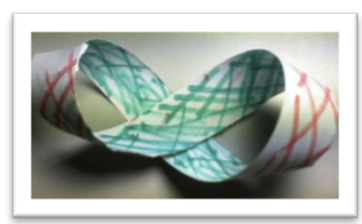
Topological insulator



k-space





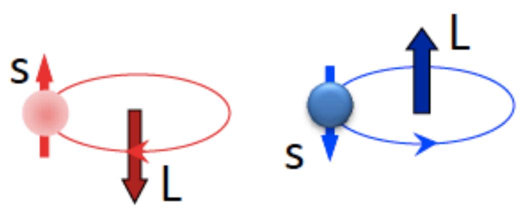


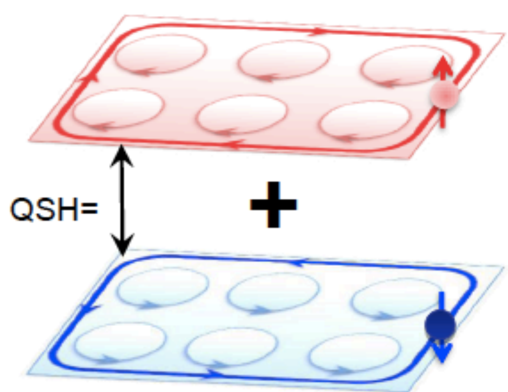
From QHE to QSHE

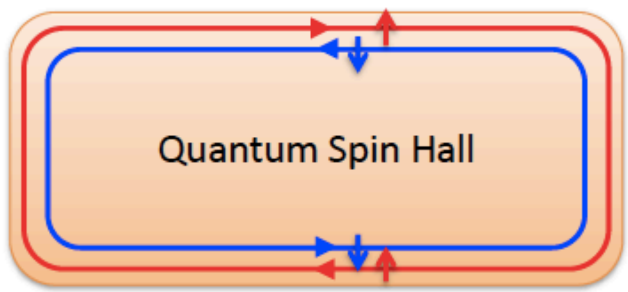
Quantum Spin Hall State Time reversal symmetry (TRS)

Spin-orbital coupling:

$$H_{SO} = \alpha \mathbf{L} \cdot \mathbf{S}$$

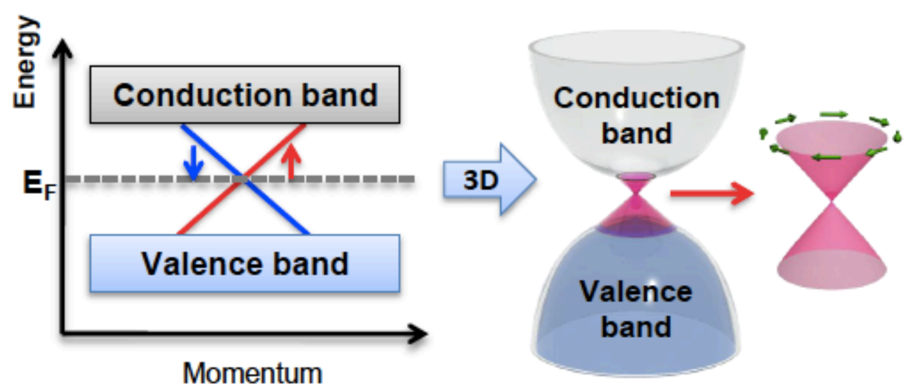






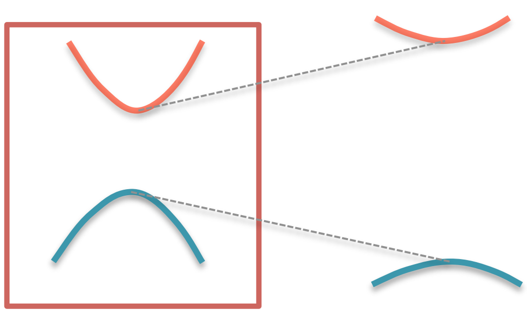
$$\sigma_{xy} = 0$$

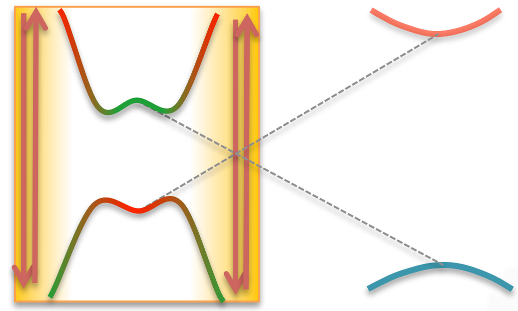
Kane & Mele, 2005, Z_2 invariant

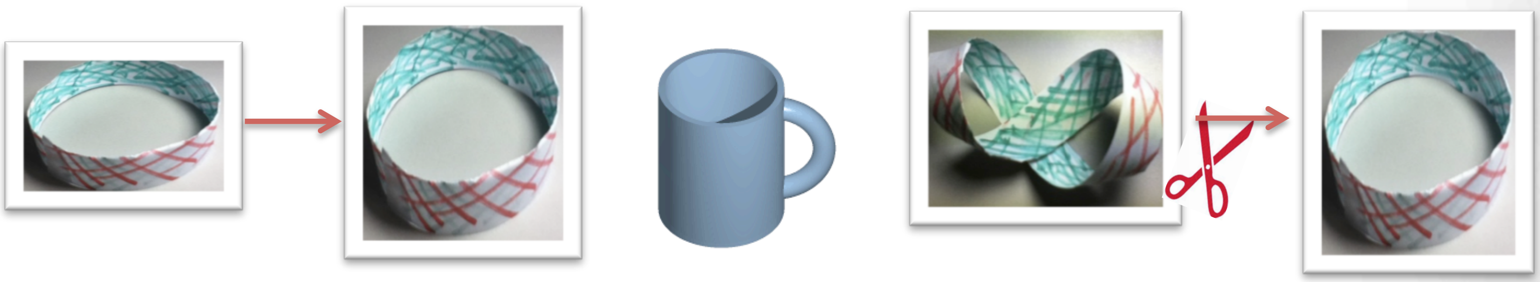


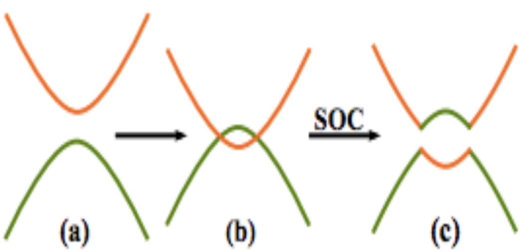
Surface states due to band inversion

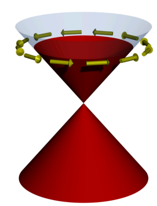
Understand the **topology**









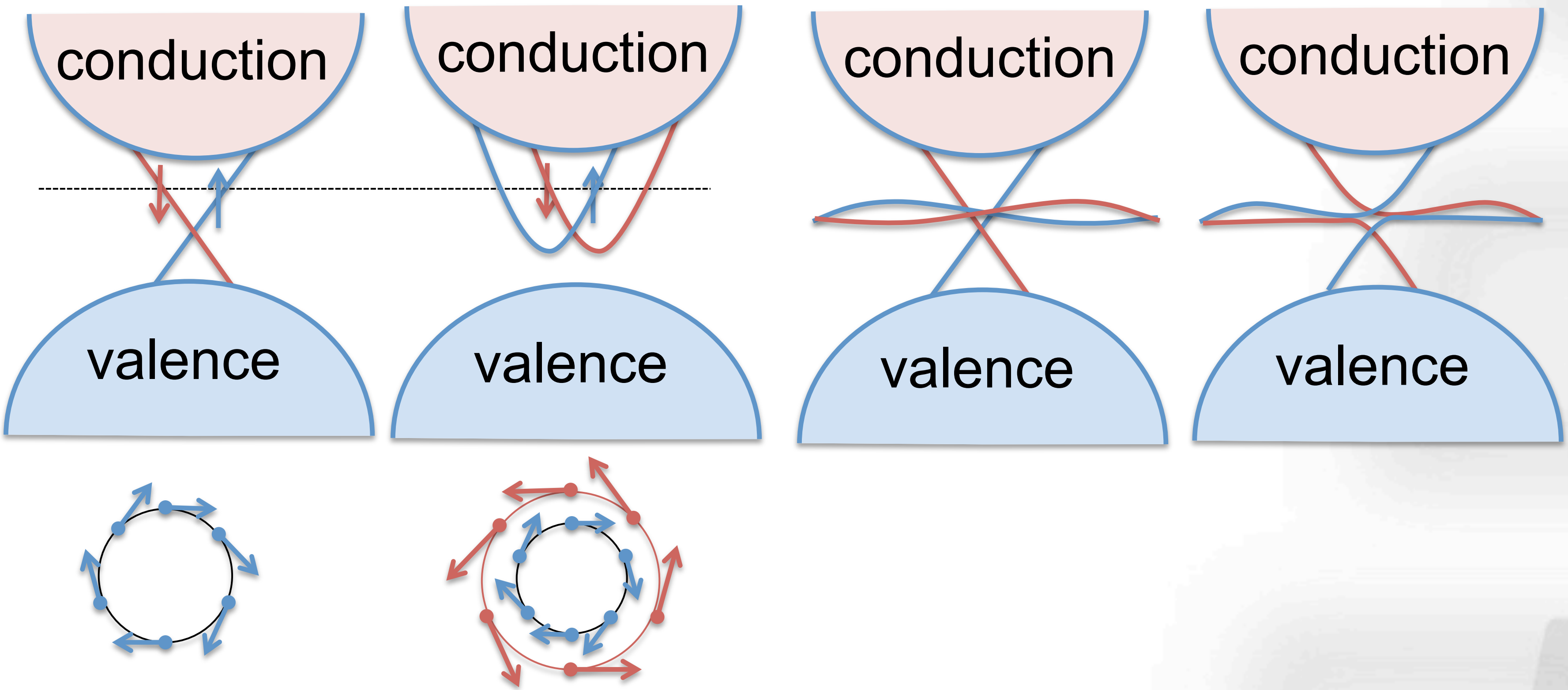


Think the bulk!

Band inversion inside the bulk

Topological states on the boundary

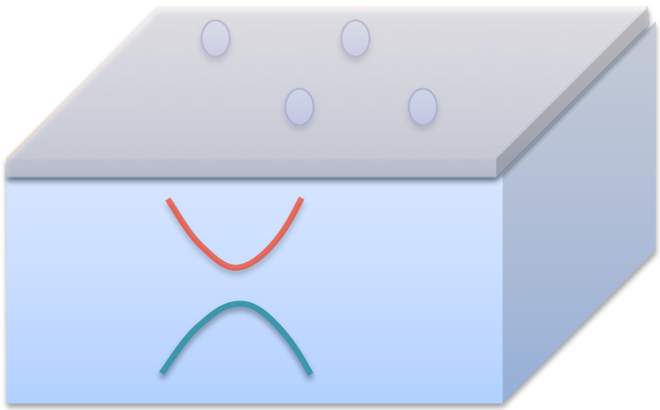
Different from trivial surface states



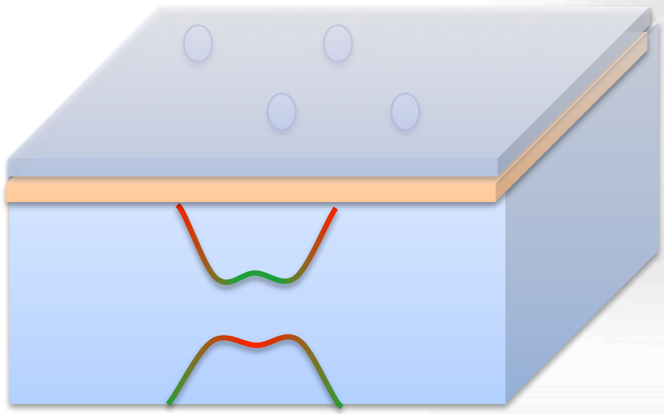
Only in a small energy region, they do look quite similar.

Robustness of topological states

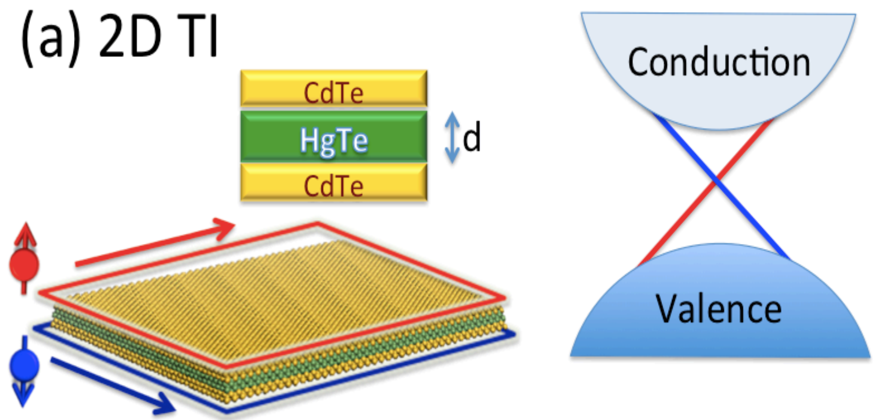
Normal surface states



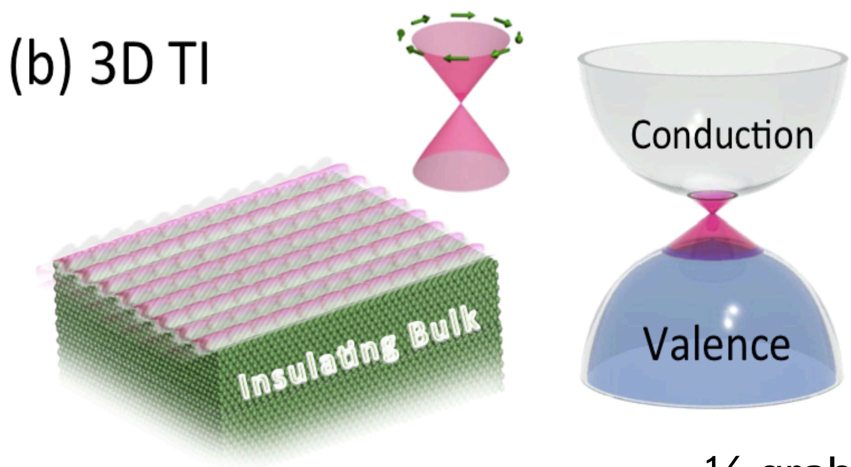
Topological surface states

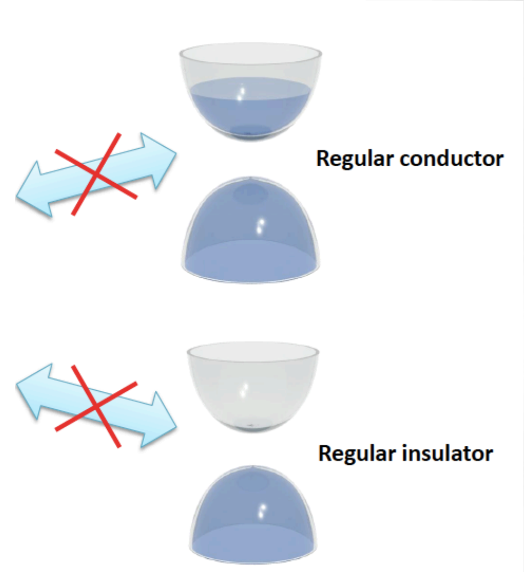


Topological Insulators



- Metallic edge or surface states
- Spin-momentum locking

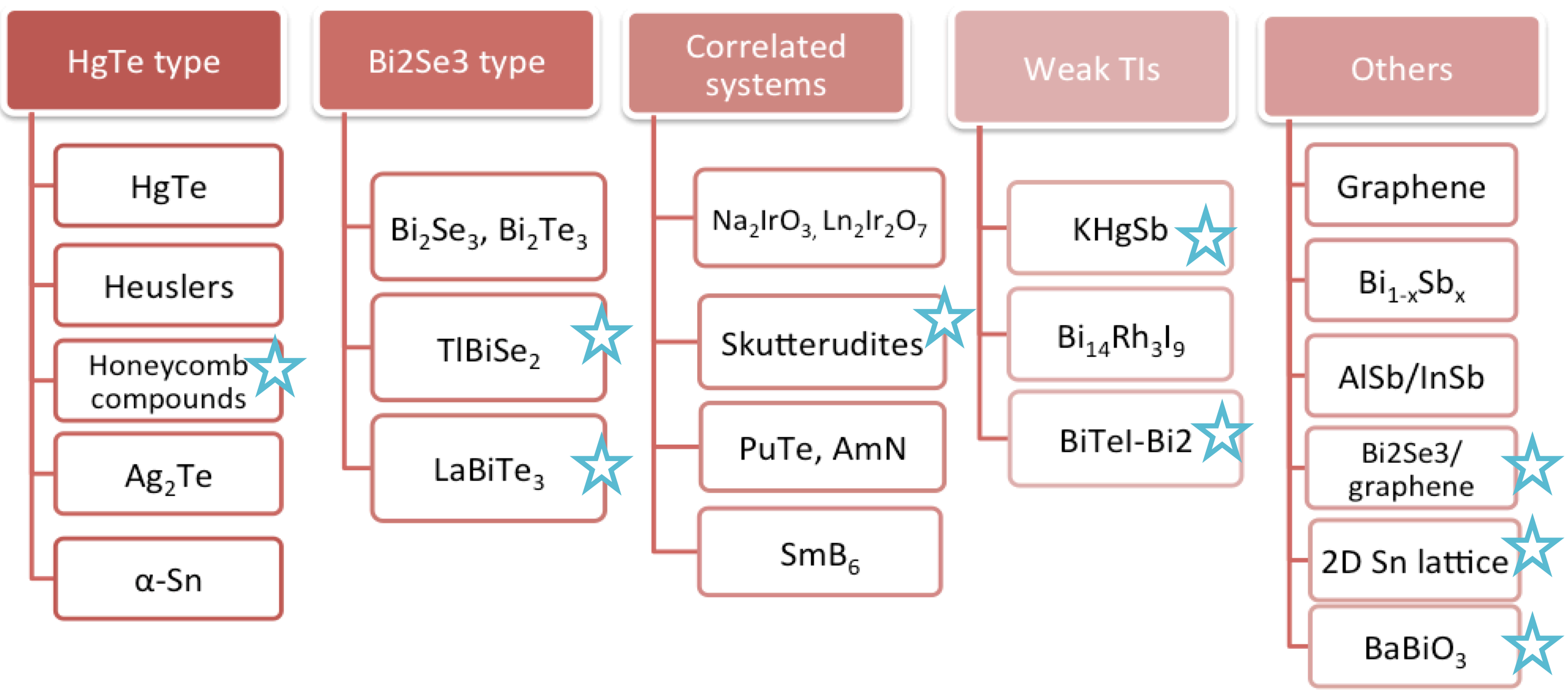




¼ grahene

TI is an insulator but conducts.

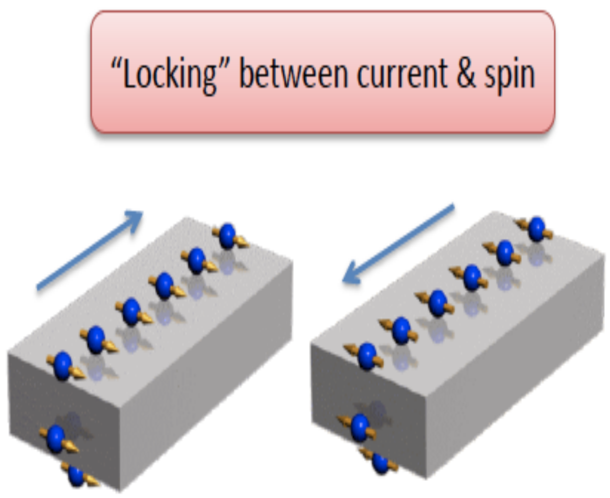
Materials for TIs

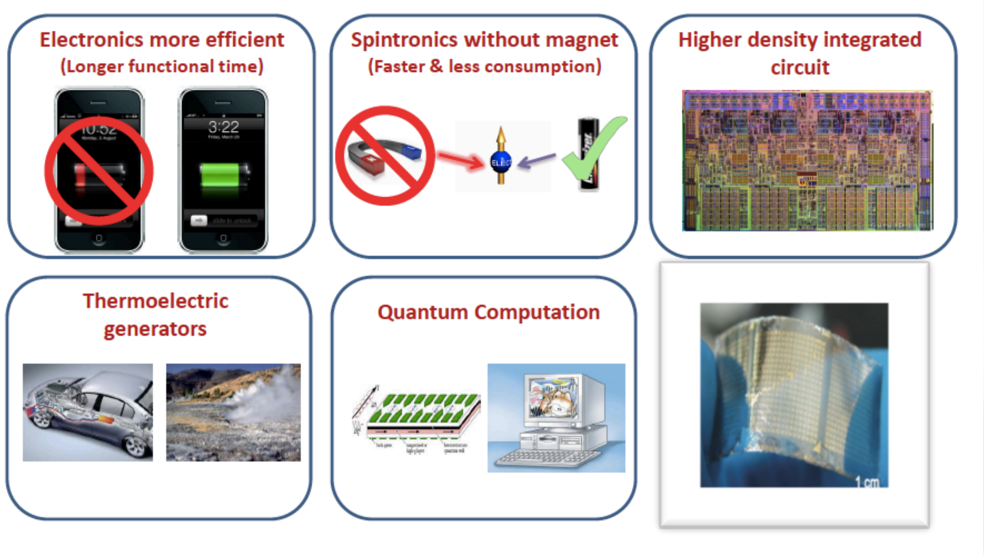


For a review on materials,
BY and S.-C. Zhang, Rep. Prog. Phys. 75, 096501 (2012).

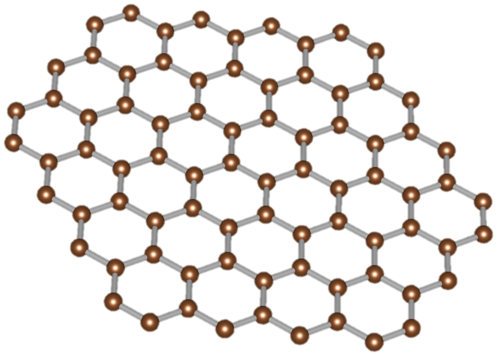
Interesting Physics and applications

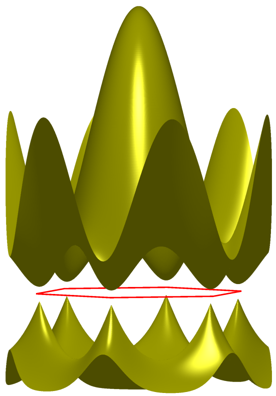
- ✧ Spin-momentum locked, pure spin current. Spintronics application.
- ✧ Majorana particles. Quantum computation.
- ✧ Topological magnetoelectric effects $$S_\theta = \frac{\theta\alpha}{4\pi^2}\int d^3x dt E \cdot B$$
- ✧ Thermoelectric devices
- ✧ Transparent conducting layer

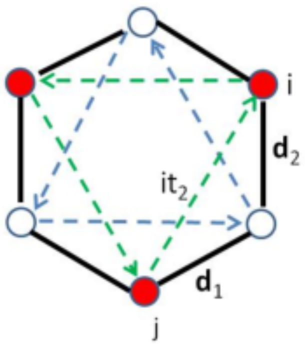




Graphene

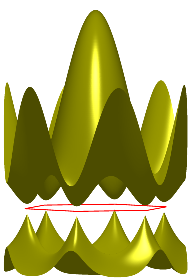


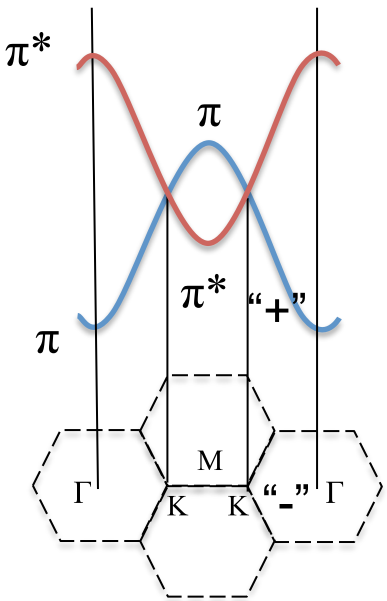


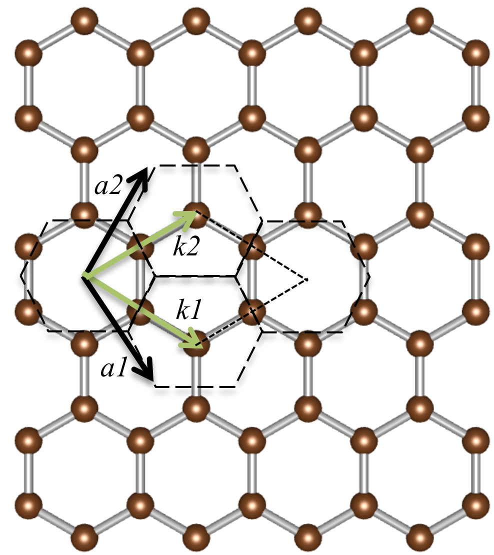


$$\mathcal{H} = \sum_{\langle ij\rangle\alpha} t c^{\dagger}_{i\alpha} c_{j\alpha} + \sum_{\langle\langle ij\rangle\rangle\alpha\beta} i t_2 \nu_{ij} s^{z}_{\alpha\beta} c^{\dagger}_{i\alpha} c_{j\beta}.$$

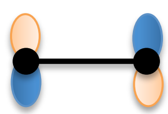
Graphene



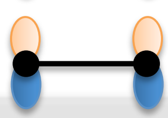




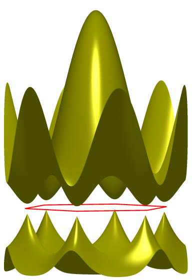
Anti-bonding state “+” parity

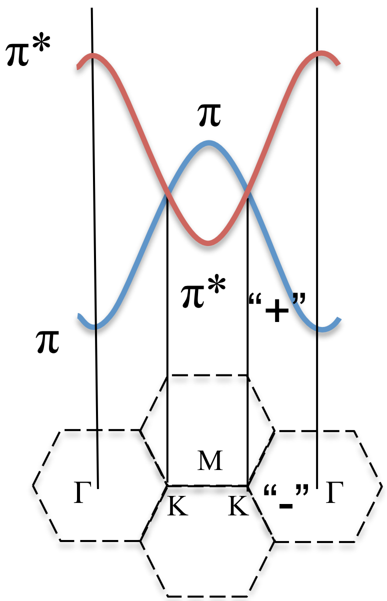


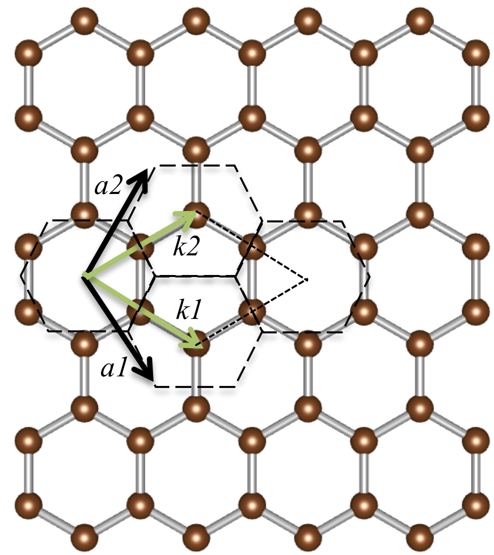
Bonding state “-” parity

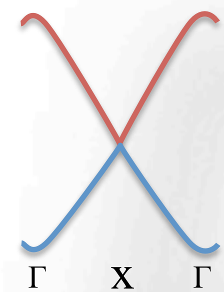


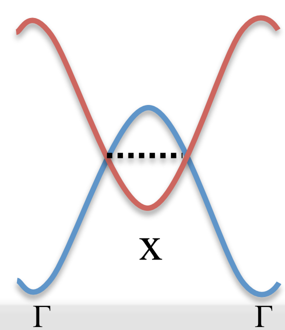
Graphene











Graphene

Shockley edge states (spinless)

AUGUST 15, 1939 PHYSICAL REVIEW VOLUME 56

On the Surface States Associated with a Periodic Potential

WILLIAM SHOCKLEY
Bell Telephone Laboratories, New York, New York
(Received June 19, 1939)

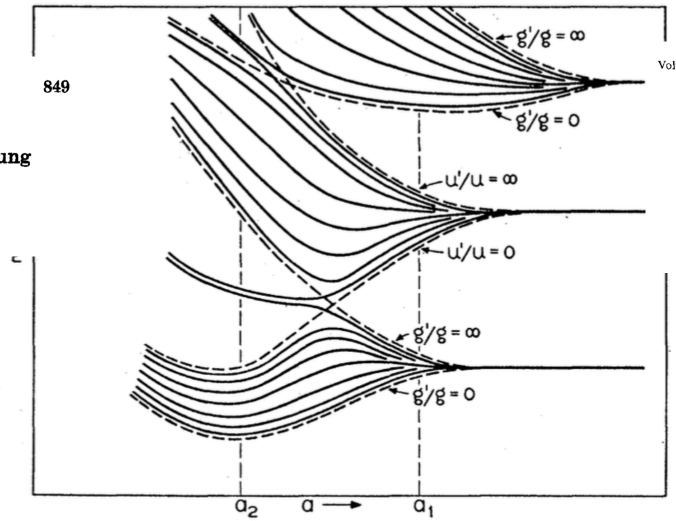


FIG. 2. Energy spectrum for a one-dimensional lattice with eight atoms.

849

Über eine mögliche Art der Elektronenbindung an Kristalloberflächen.

Von **Ig. Tamm** in Moskau.
(Eingegangen am 13. Mai 1932.)

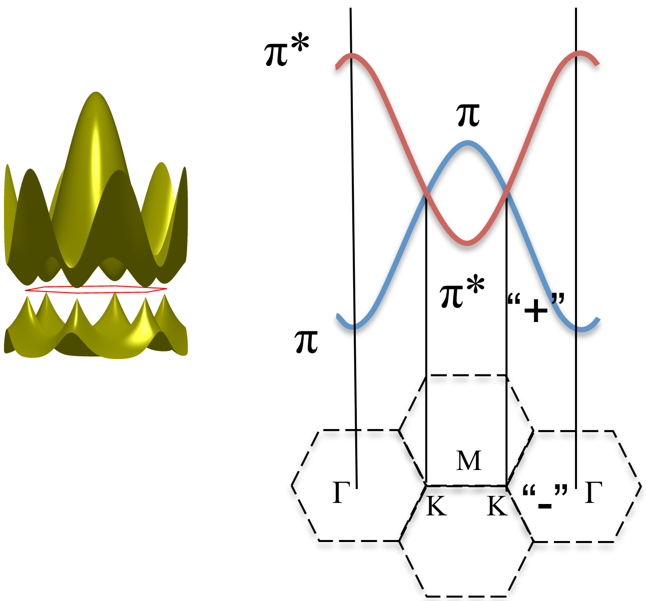
Volume 106A, number 8 PHYSICS LETTERS 24 December 1984

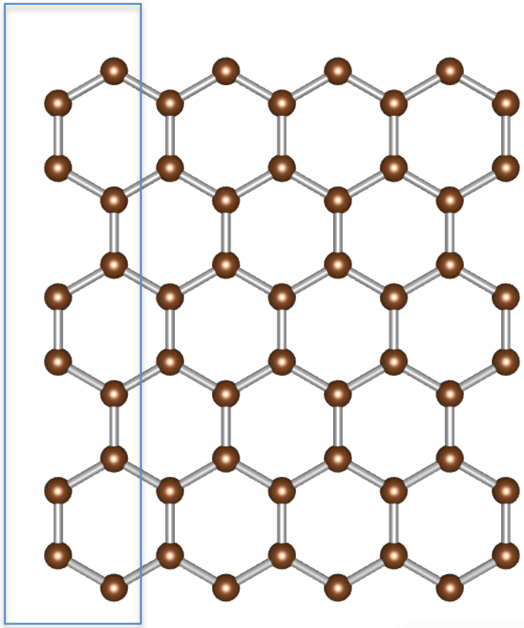
BAND CROSSING AND SURFACE STATES IN SOLIDS

J. ZAK
Department of Physics, Technion – Israel Institute of Technology, Haifa, Israel

Received 13 September 1984

Graphene





Polyacetylene
(Su, Schrieffer, and Heeger, 1979, 1980) model,

Quantum Spin Hall Effect in Graphene

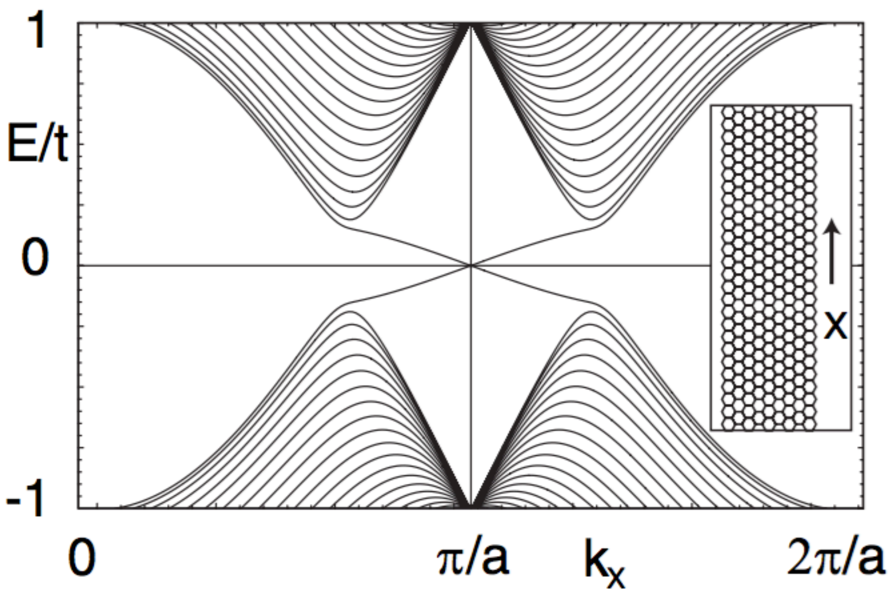
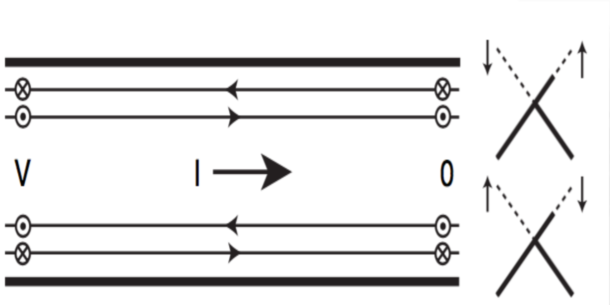


FIG. 1. (a) One-dimensional energy bands for a strip of graphene (shown in inset) modeled by (7) with $t_2/t = 0.03$. The bands crossing the gap are spin filtered edge states.

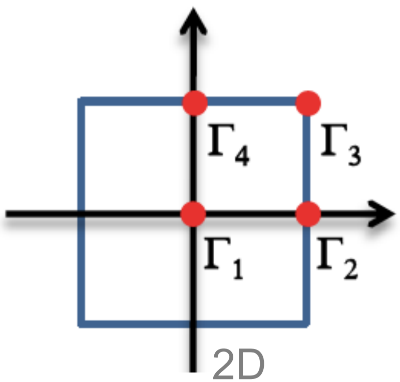


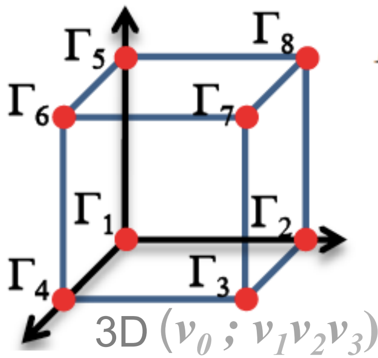
Kane, Mele PRL **95,** 226801 (2005)

The bulk band structure of TIs

Z_2 topological invariant

Band theory [Fu, Kane & Mele (2007), Moore & Balents (2007), Roy (2007)]





$$B_{\alpha\beta}(\mathbf{k}) = \langle -\mathbf{k}, \alpha | T | \mathbf{k}, \beta \rangle \quad \delta_i = \frac{\sqrt{\det[B(\Gamma_i)]}}{\mathrm{Pf}[B(\Gamma_i)]} = \pm 1$$

$$(-1)^{\nu_0} = \prod_i \delta_i = \pm 1$$

$$\nu_0 = \begin{cases} 1: \text{topological insulator} \\ 0: \text{regular insulator} \end{cases}$$

Inversion symmetry: δ_i is the parity product of all valence Bloch states.

Time reversal invariant k-point

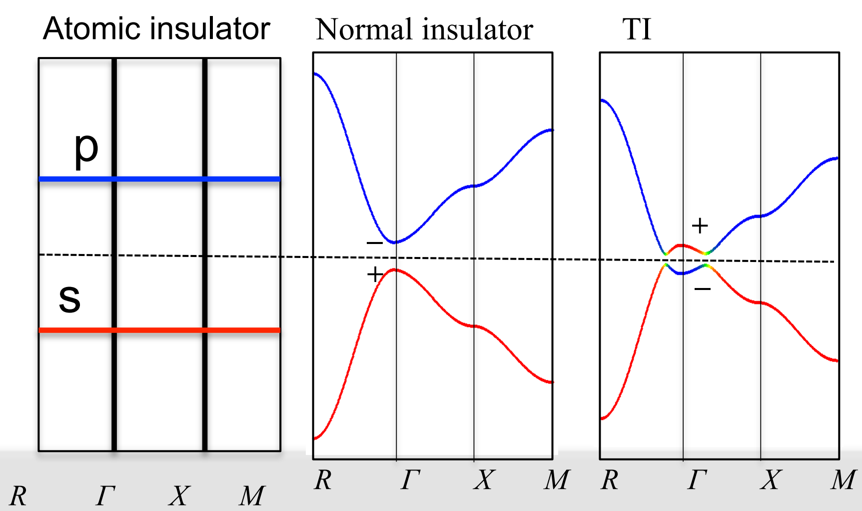
$K^i = - K^i + n\, \boldsymbol{K_0}$

Γ (0 0 0)

X (½ 0 0)

M (½ ½ 0)

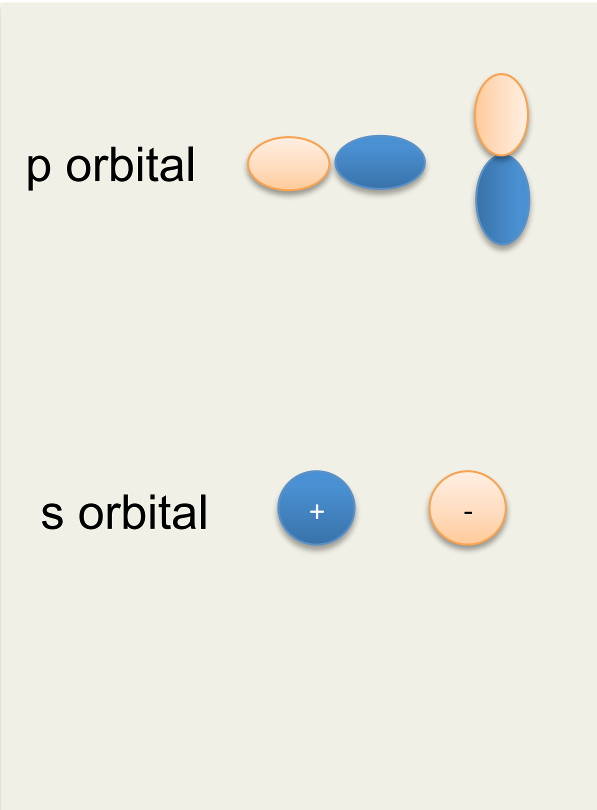
R (½ ½ ½)

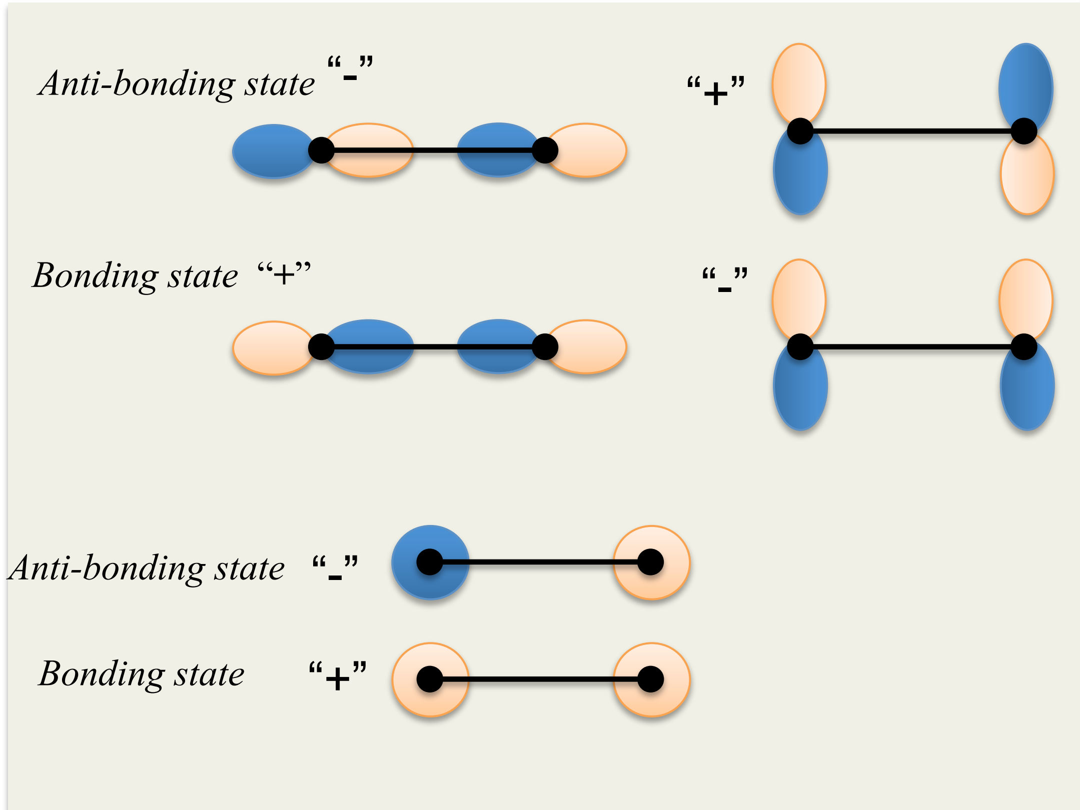


Parity of valence bands

K^i	*Normal*	*TI*
1 Γ	+	−
3 X	+	+
3 M	+	+
1 R	+	+
ν_0	0	1

A note about the Parity



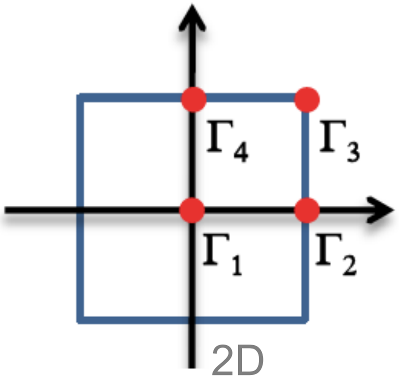


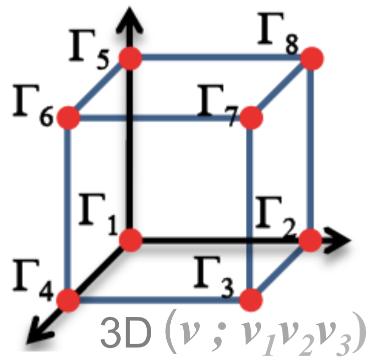
The parity of the Bloch wave function in a lattice is **NOT** equivalent to the parity of the local orbital, when the inversion center does not locate at the atom center.

Characterize TIs

Z_2 topological invariant

Band theory [Fu, Kane & Mele (2007), Moore & Balents (2007), Roy (2007)]

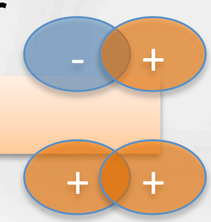




$$B_{\alpha\beta}(\mathbf{k}) = \langle -\mathbf{k}, \alpha | T | \mathbf{k}, \beta \rangle \quad \delta_i = \frac{\sqrt{\det[B(\Gamma_i)]}}{\mathrm{Pf}[B(\Gamma_i)]} = \pm 1$$

$$(-1)^{\nu} = \prod_i \delta_i = \pm 1$$

$\nu =$
- 1: topological insulator
- 0: regular insulator



Inversion symmetry: δ_i is the parity product of all valence Bloch states.

Field theory [Qi, Zhang, et. al. (2008, 2009), Wilczek, (1987,2009)]

$$S_0 = (8/\pi) \int d^3x dt \,(\epsilon \mathbf{E}^2 - (1/\mu)\mathbf{B}^2)$$

+

$$\boxed{S_\theta = \frac{\theta \alpha}{4\pi^2} \int d^3x dt E \cdot B}$$

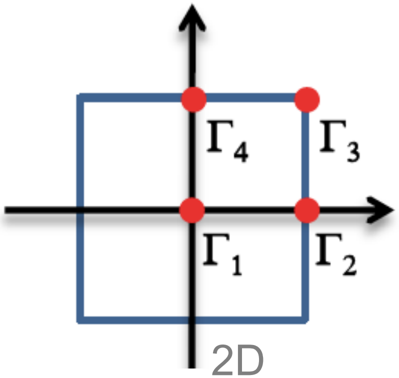
$\theta =$
- π: topological insulator
- 0: regular insulator

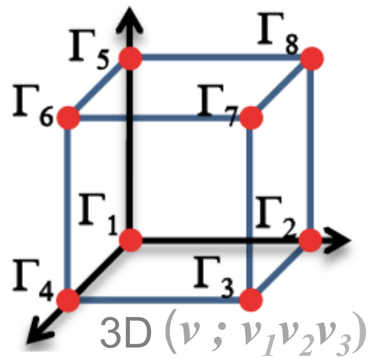
Wang & Zhang (2012) Simplified Topological Invariants, G(w=0,k)

Characterize TIs

Z_2 topological invariant

Band theory [Fu, Kane & Mele (2007), Moore & Balents (2007), Roy (2007)]

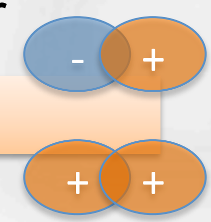




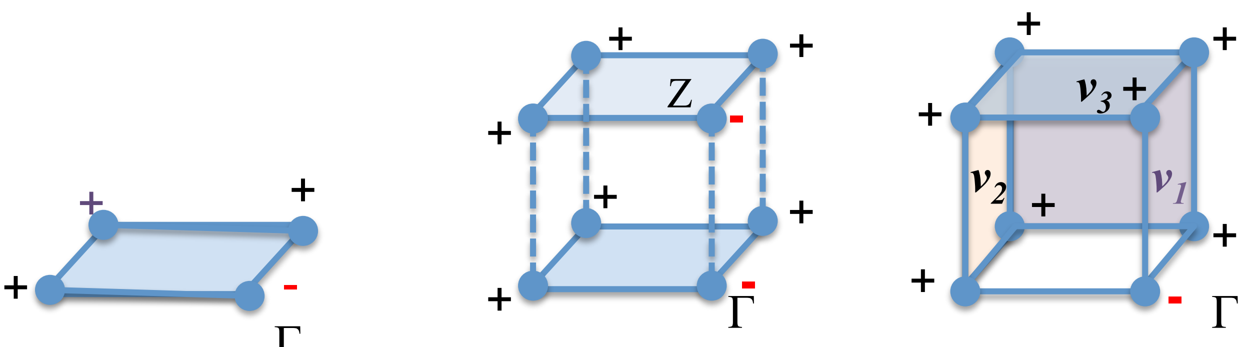
$$B_{\alpha\beta}(\mathbf{k}) = \langle -\mathbf{k}, \alpha | T | \mathbf{k}, \beta \rangle \quad \delta_i = \frac{\sqrt{\det[B(\Gamma_i)]}}{\mathrm{Pf}[B(\Gamma_i)]} = \pm 1$$

$$(-1)^{\nu} = \prod_i \delta_i = \pm 1$$

$\nu =$ 1: topological insulator; 0: regular insulator



Inversion symmetry: δ_i is the parity product of all valence Bloch states.



$\nu=1$ 2D TI

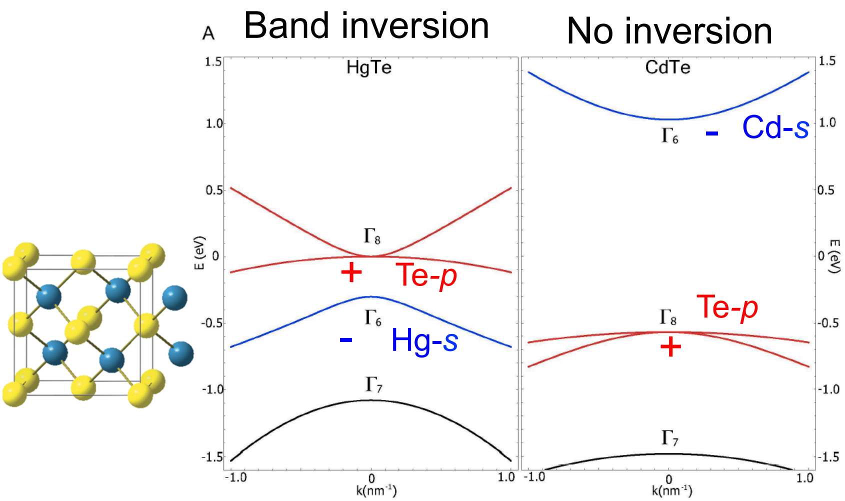
(0;001) Weak 3D TI

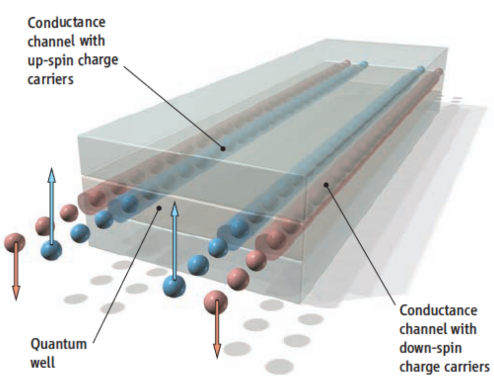
(1;000) Strong 3D TI

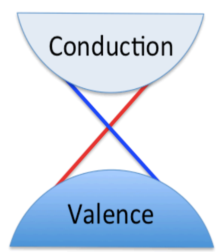
Topological Crystalline/Valley Insulators.
Fu, PRL 106, 106802 (2011).
Slager *et al.* arXiv:1209.2610 (2012)

TI materials

HgTe QWs (2D TIs)

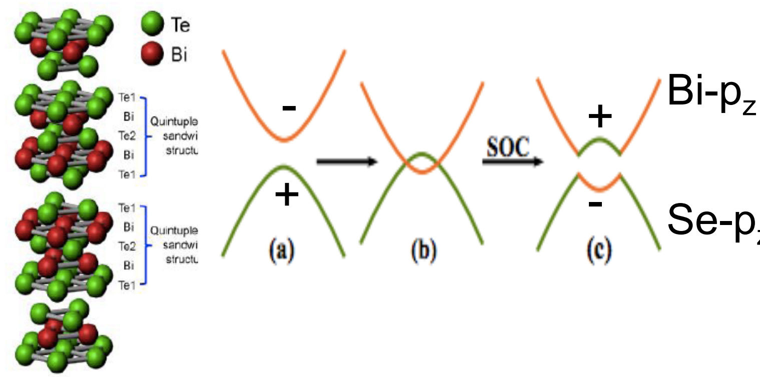


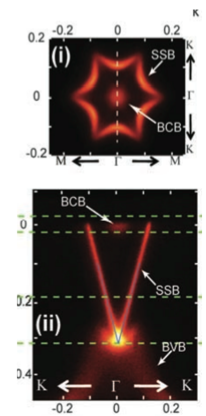


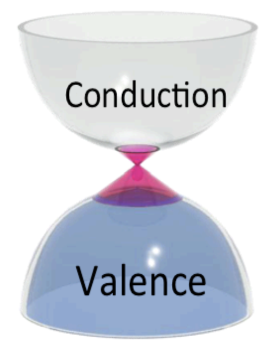


Zhang group, Science 314, 1757 (2006);
Molenkamp group, Science 318, 766 (2007).

Bi_2Te_3, Bi_2Se_3 and Sb_2Te_3 (3D TIs)

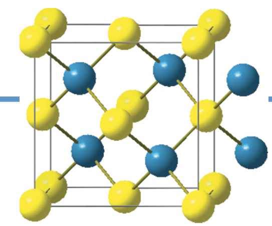




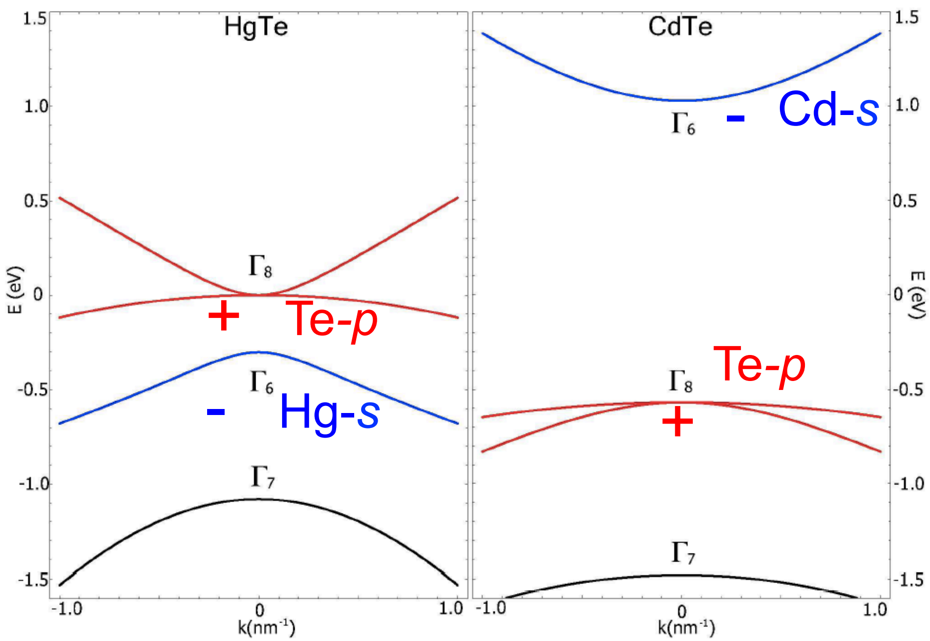


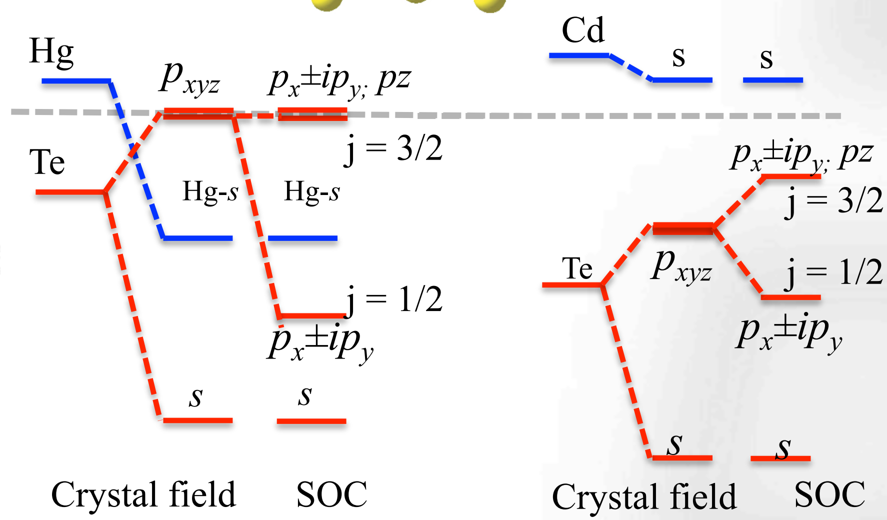
Zhang *et al. Nature Phys.* 5, 438 (2009).
Xia et al. *Nature Phys.* 5, 398 (2009).
Chen et al. *Science* 325, 178 (2009).

HgTe QWs

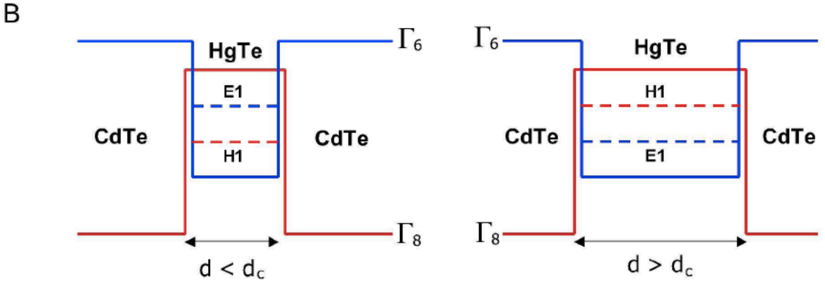


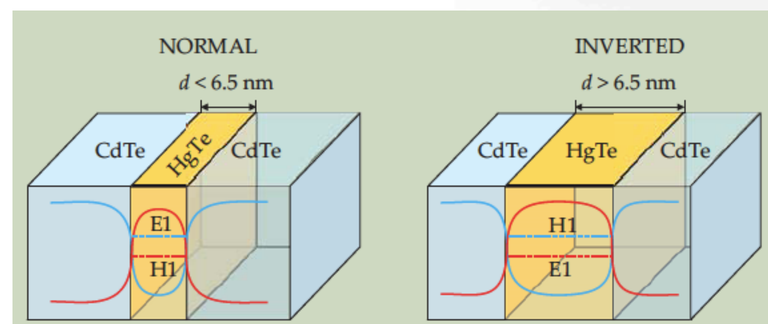
A Band inversion





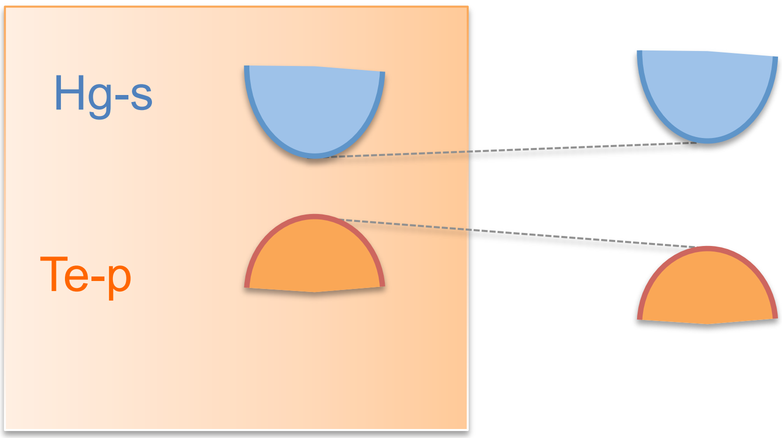
B



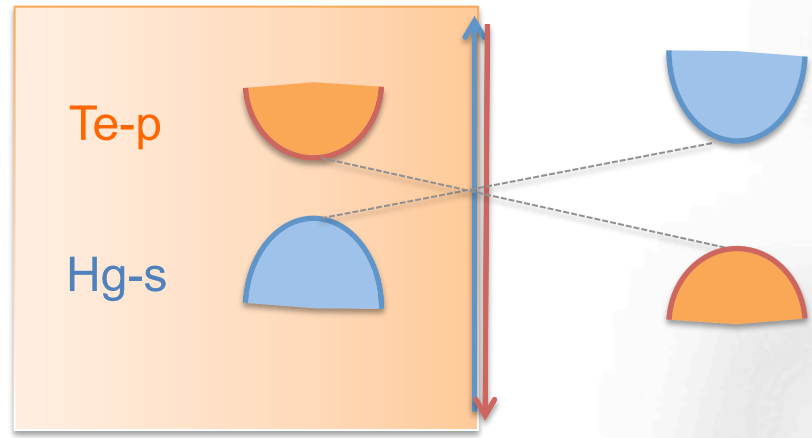


B. A. Bernevig, T. L. Hughes, S.-C. Zhang, Science 314, 1757 (2006).

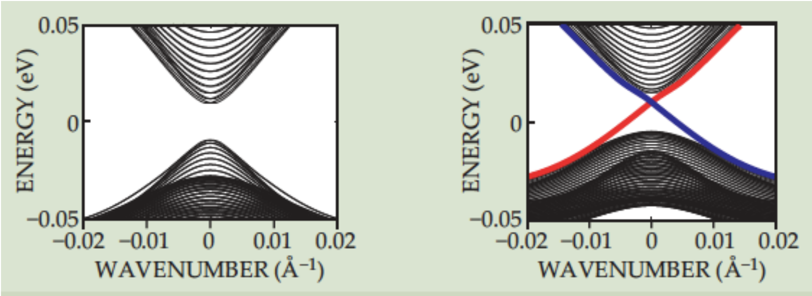
HgTe QWs

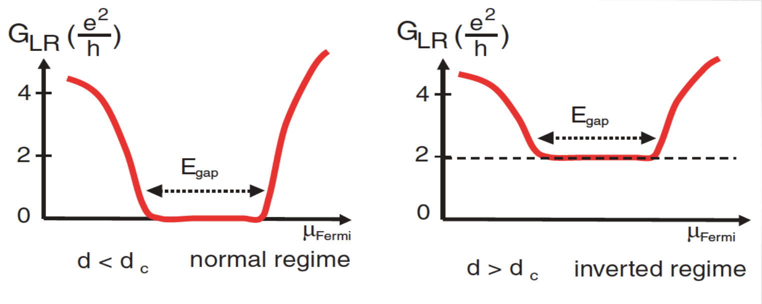


$d < d_c$=6.3 nm



$d > d_c$=6.3 nm

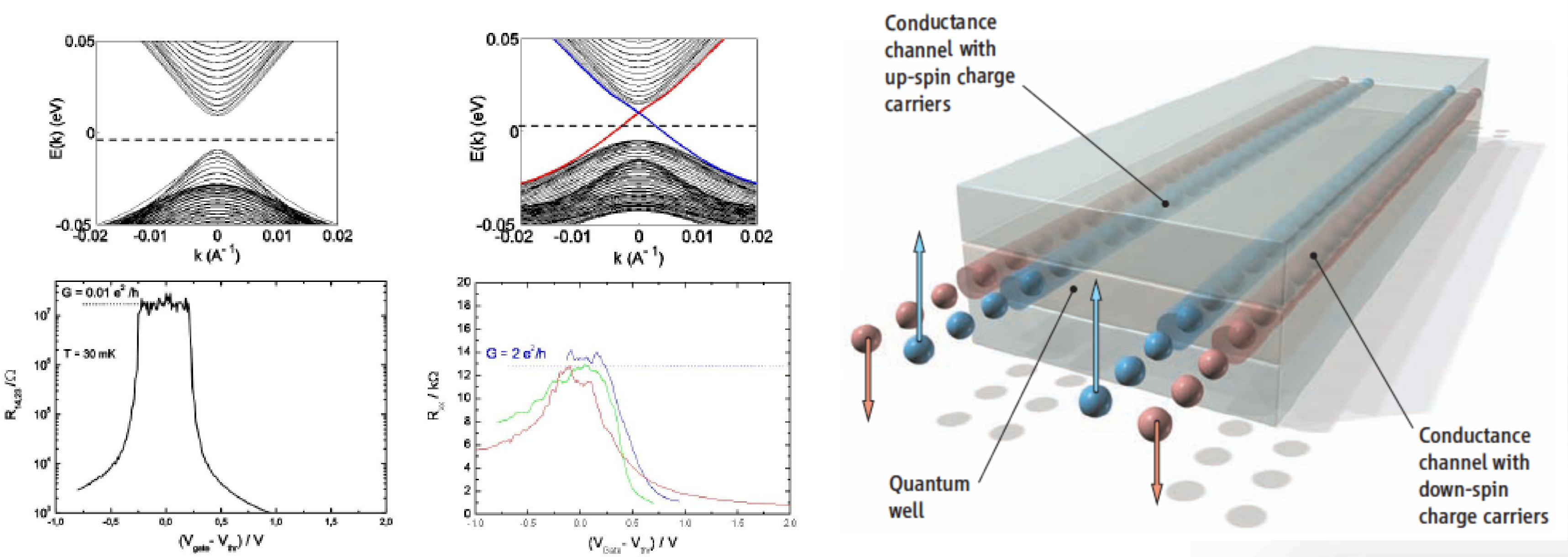




B. A. Bernevig, T. L. Hughes, S.-C. Zhang, Science 314, 1757 (2006).

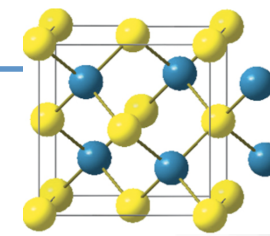
HgTe QWs

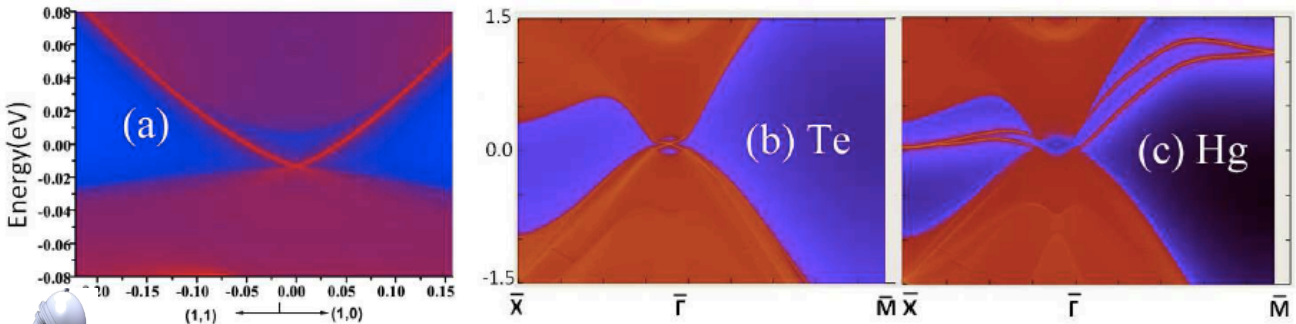
Transport measurements of the edge state conductance.

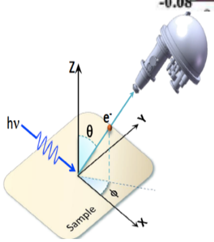


M. König *et al.* Science 318, 766 (2007)

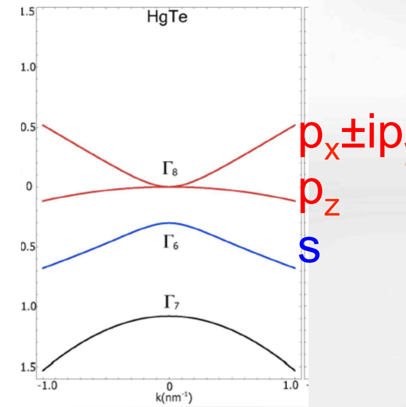
Strained HgTe, 3D TI

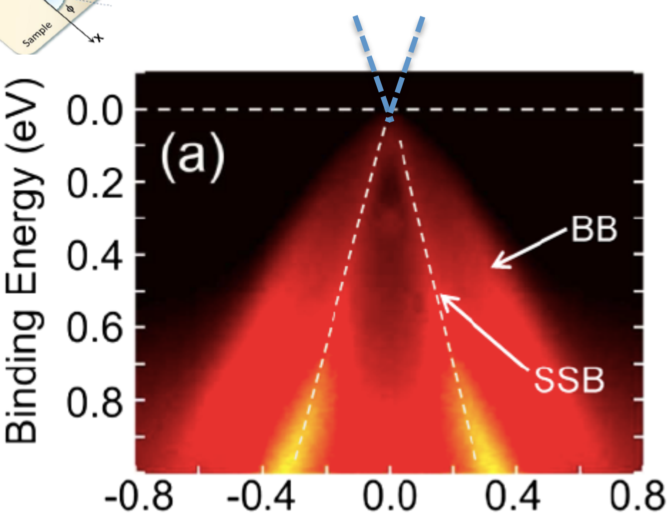


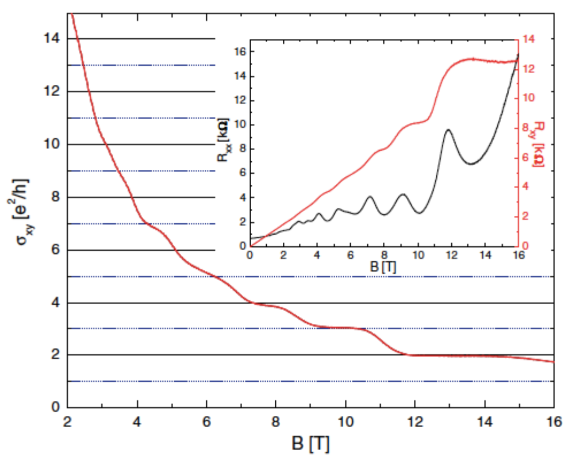


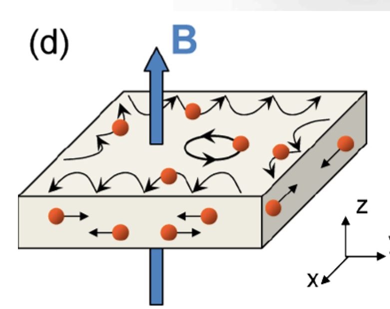


X. Dai et al. Phys. Rev. B **77**, 125319 (2008).
S.C. Wu et al. EPL, 107 (2014) 57006.



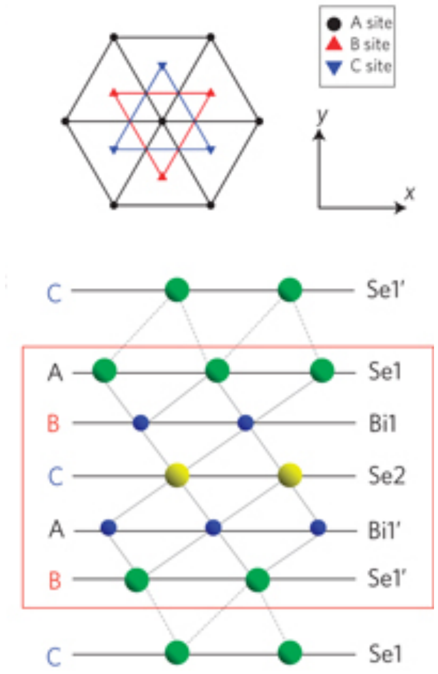


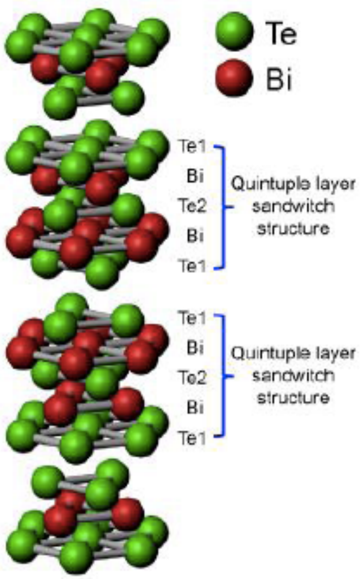




Brüne *et al.* PRL106, 126803 (2011).

Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3

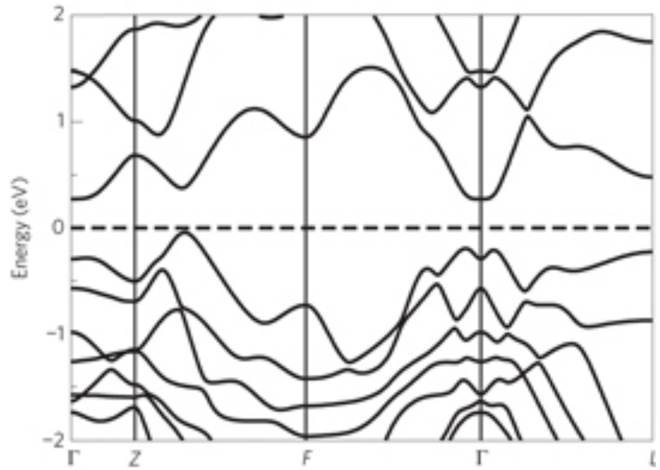


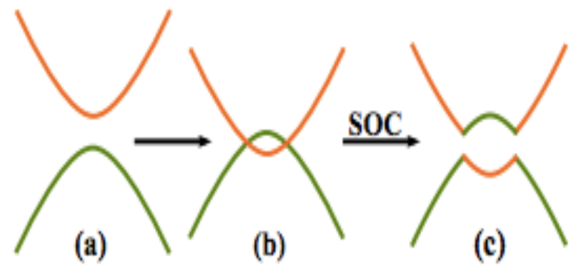


Layered semiconductor with strong SOC.

Zhang *et al. Nature Physics* 5(6) 438 (2009).

Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3

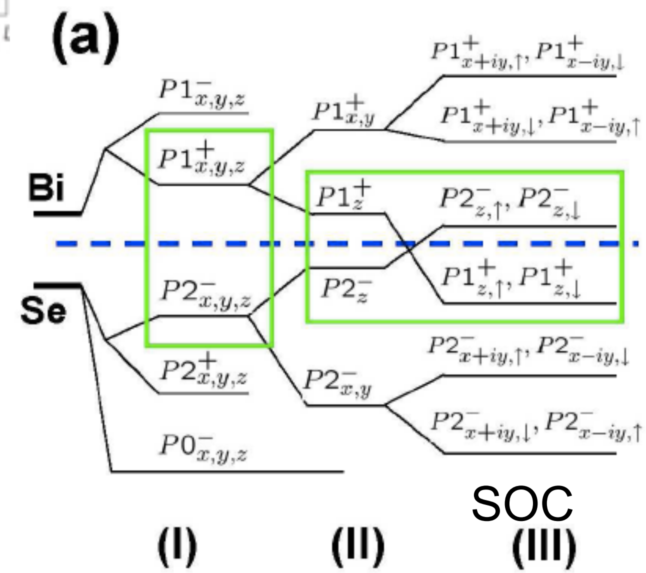




With SOC

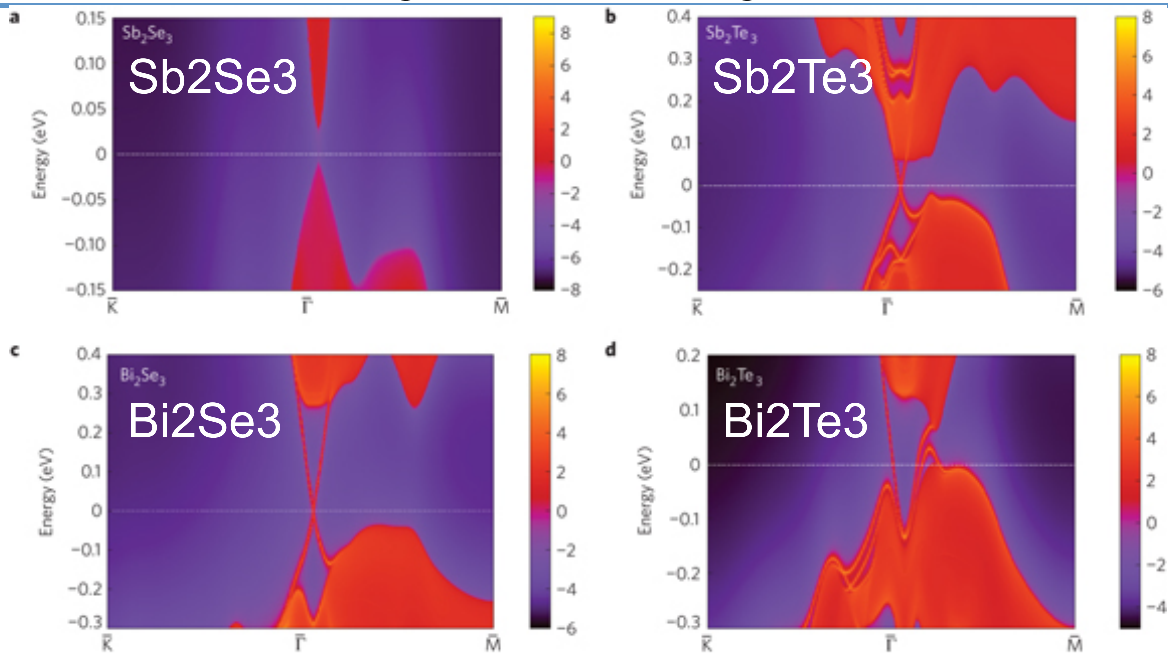
Z_2= (1;000)

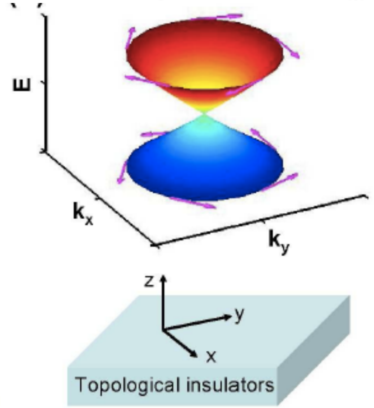
Sb_2Se_3	+ − + − + − + − + − + − − −; +	(+)
Sb_2Te_3	+ − + − + + − + − + − − − +; −	(−)
Bi_2Se_3	+ − + − + − + − + − + − − +; −	(−)
Bi_2Te_3	+ − + − + − + + − + − − − +; −	(−)

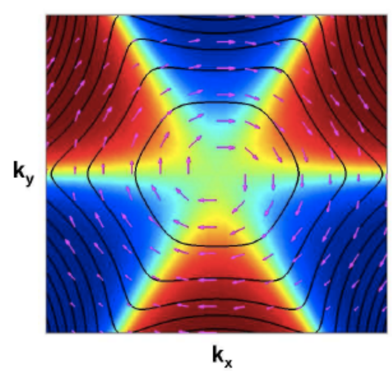


Zhang *et al. Nature Physics* 5(6) 438 (2009).

Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3



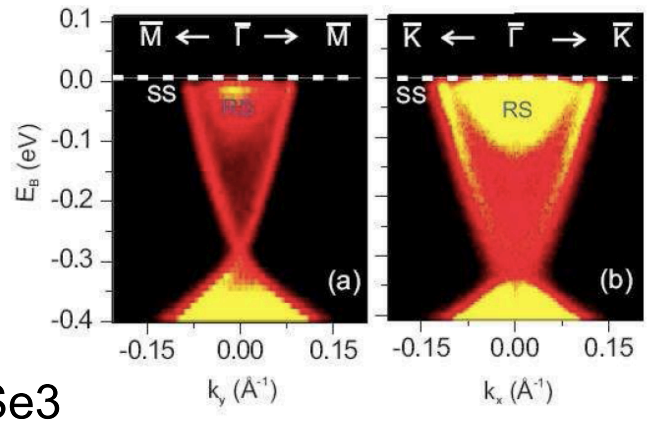




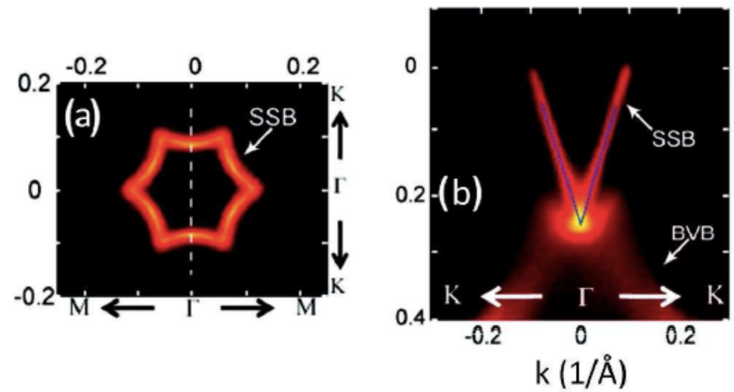
Zhang *et al. Nature Physics* 5(6) 438 (2009).

Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3

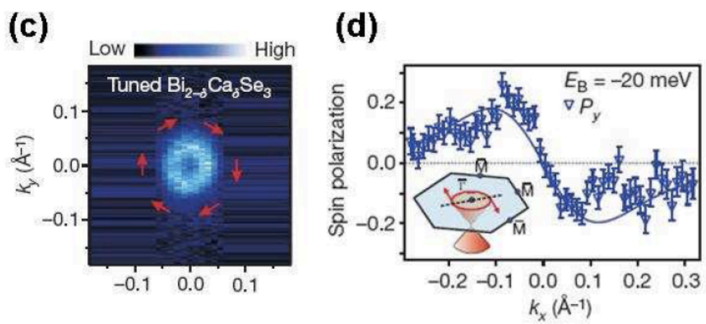
ARPES experiments



Bi2Se3



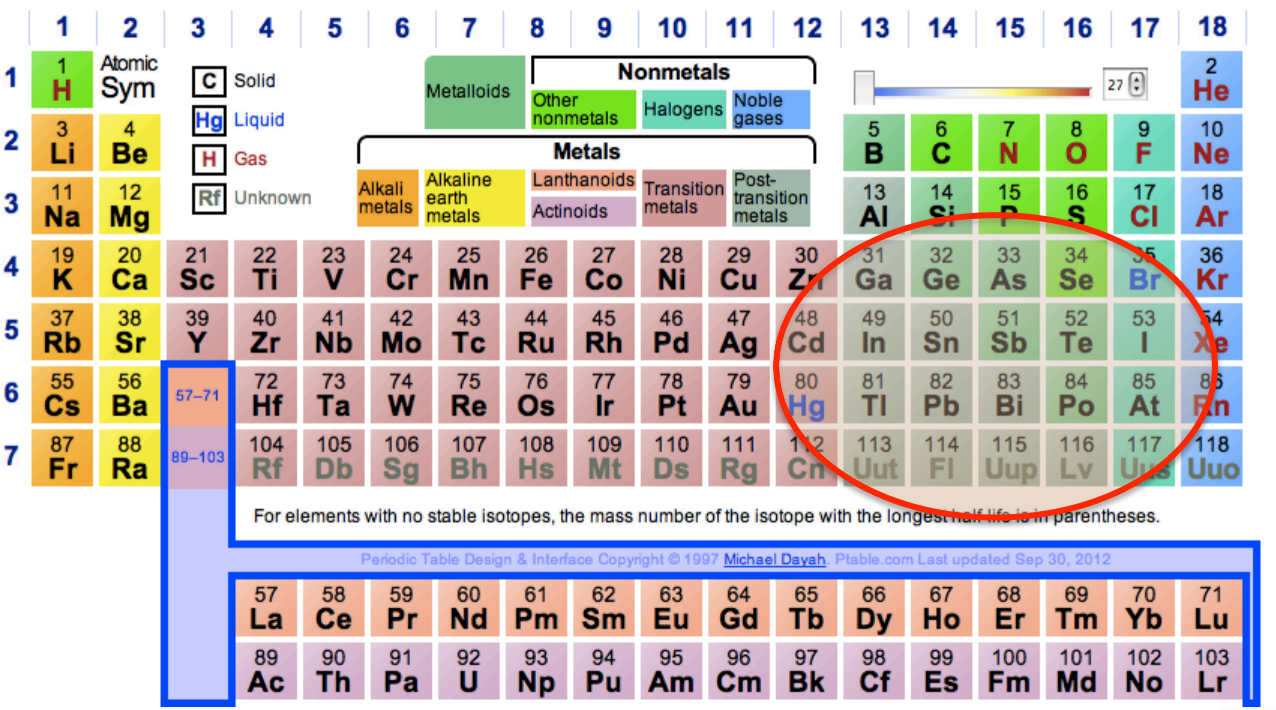
Bi2Te3



Problem:
Bi2Se3, n-type, Se vacacny
Bi2Te3, n-type, Bi-Te antisite defect
Sb2Te3, p-type, Sb vacancy

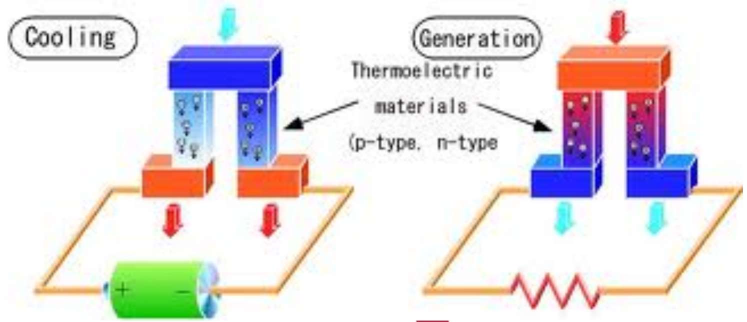
Xia et al. 2009 *Nature Physics* 5(6) 398. Chen et al. 2009 *Science* 325(5937) 178.
Hsieh et al. 2009 *PRL* 103(14) 146401. Hsieh et al. 2009 *Nature* 460(7259) 1101.

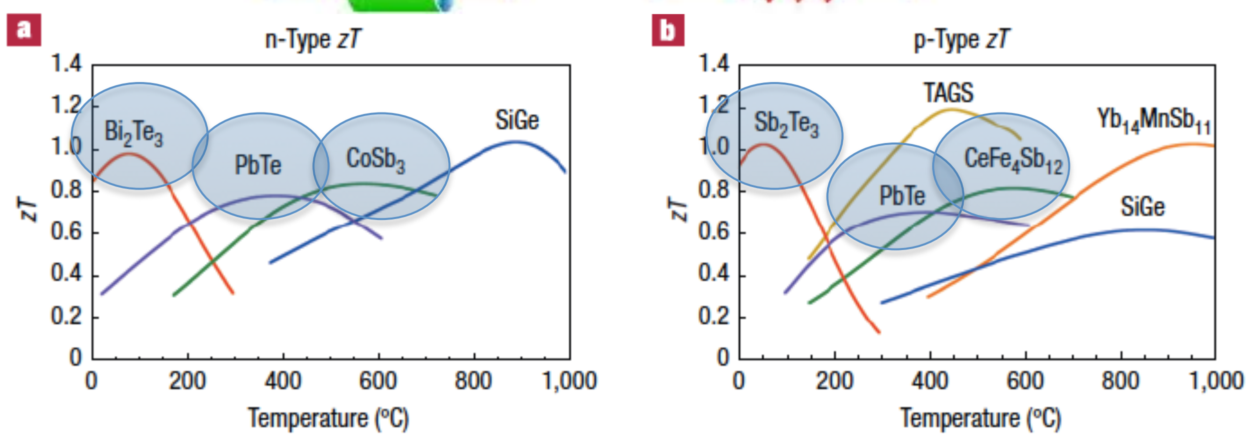
Find new TI materials



Strong SOC , λ_{so} is proportional to Z^4.

Thermoelectric materials





Snyder & Toberer
Nature Mater.
7,105 (2008).

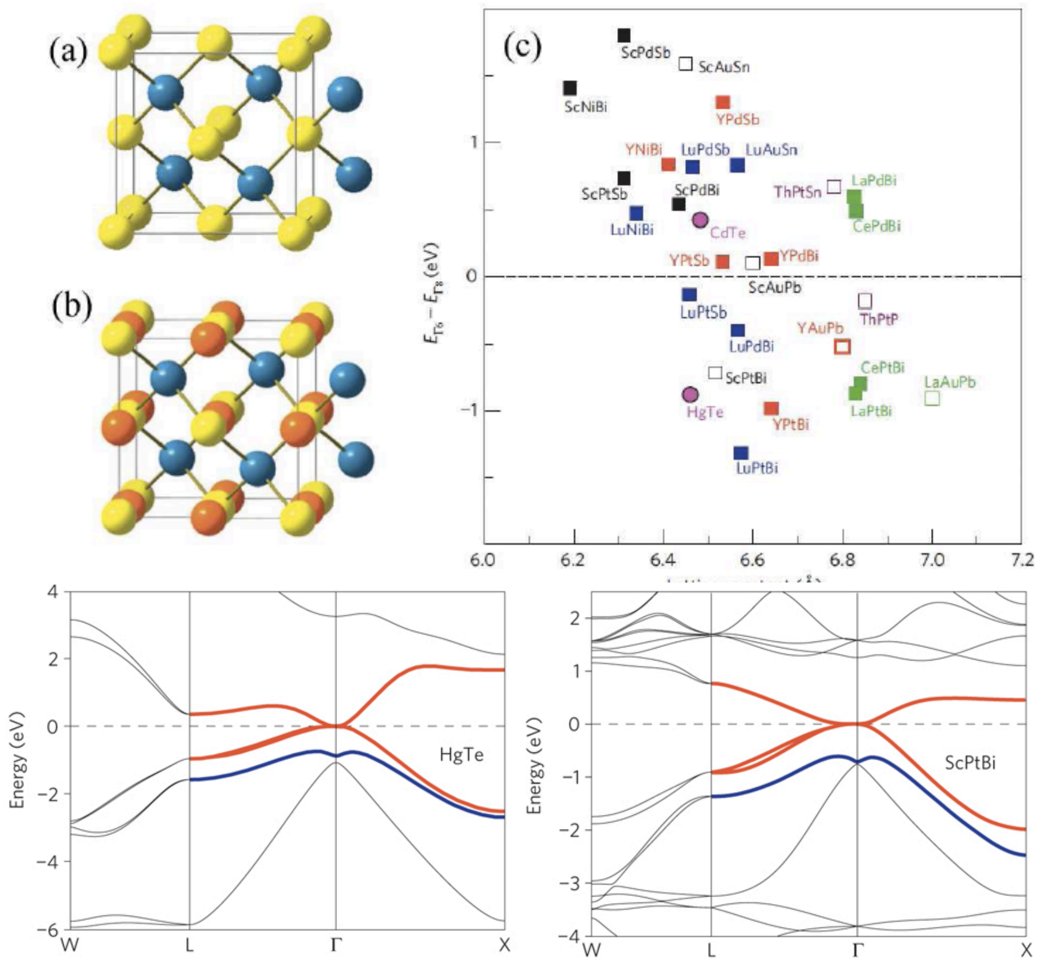
$ZT = TS^2\sigma/\kappa$

Heavy elements(κ,S) → Strong SOC

Smaller gap (σ) → Band inversion

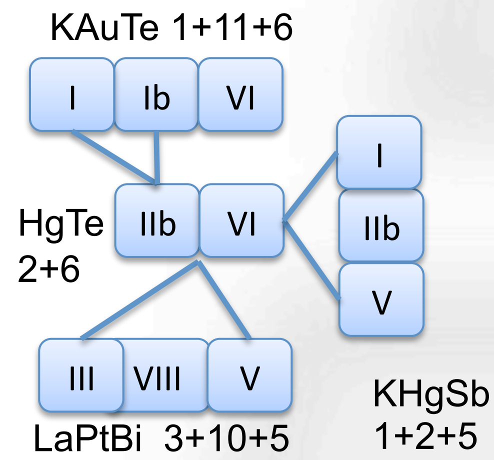
TI

HgTe variation: Heulser compounds



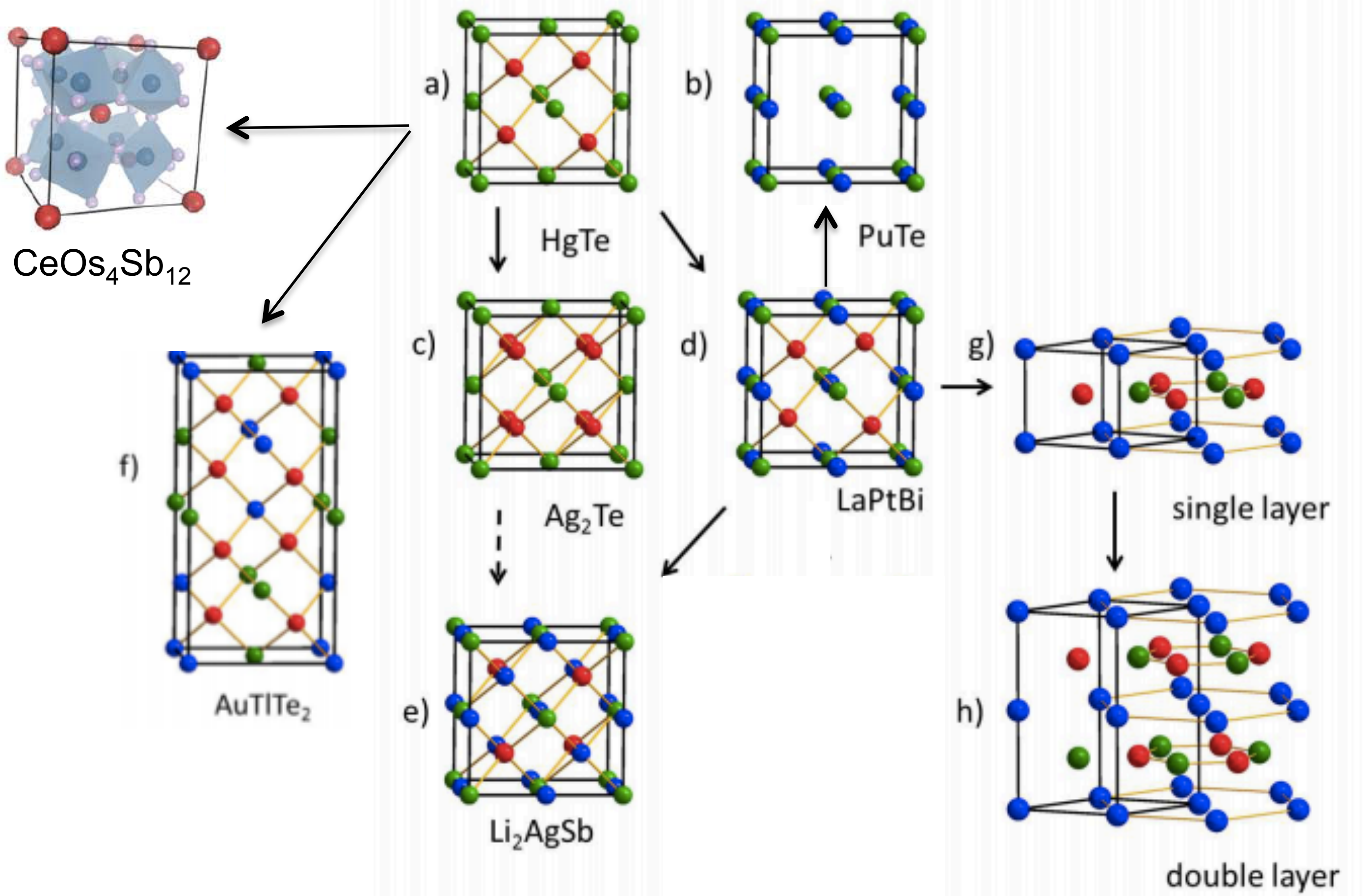
YZ: zincblend lattice
X: stuffed atom

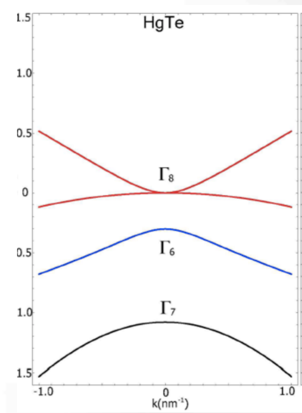
8 or 18 valence electrons.



S. Chadov *et al.* Nature Mater. 9, 541 (2010). H. Lin *et al.* *ibid* 9, 546(2010).

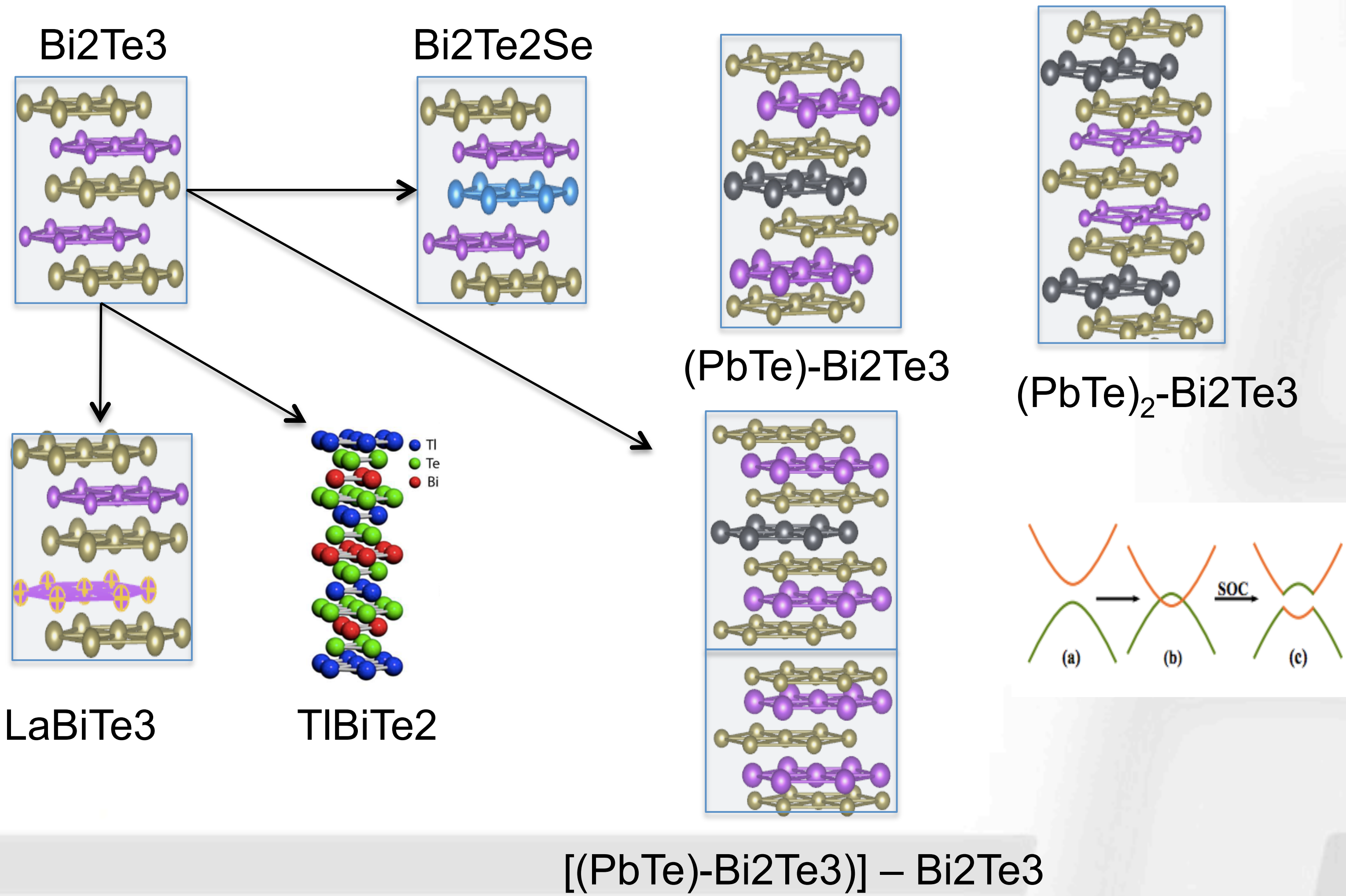
Materials engineering



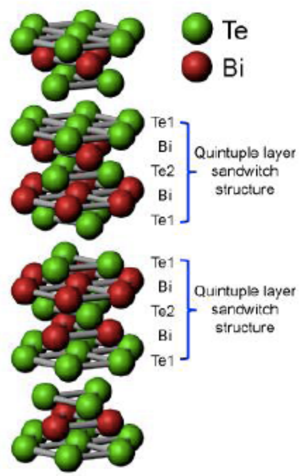


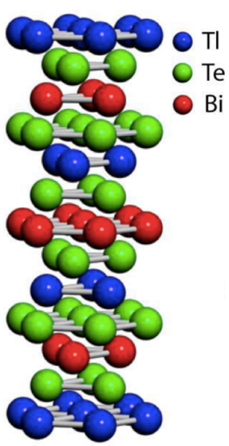
Topological Insulators from a Chemists Perspective
Angew. Chem. Int. Ed. (2012) 51, 7221.

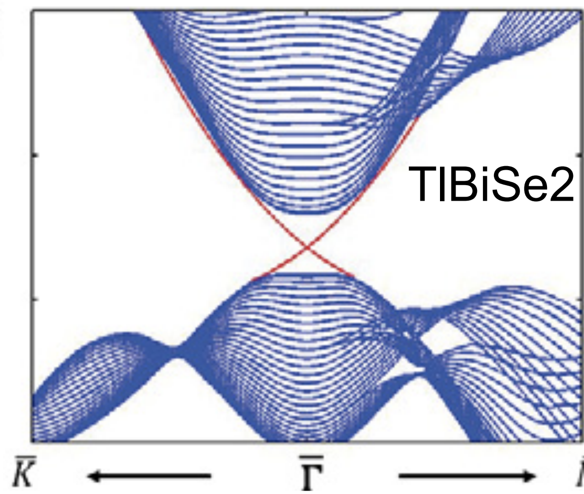
Materials engineering

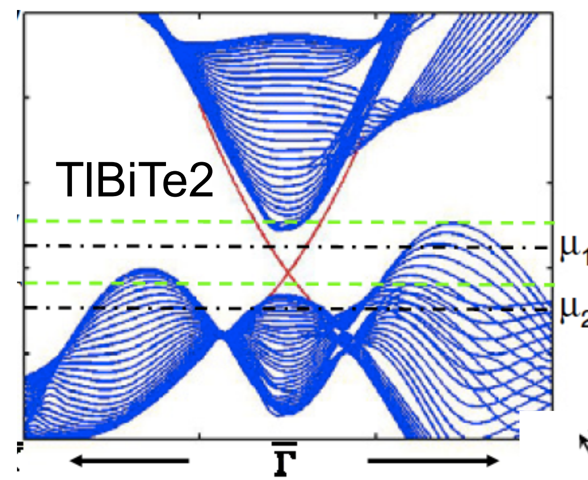


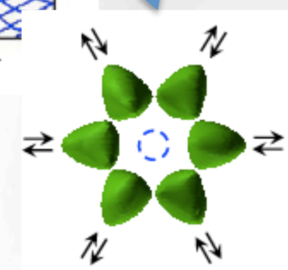
Bi_2Se_3 type: $TlBiSe_2$ and $TlBiTe_2$











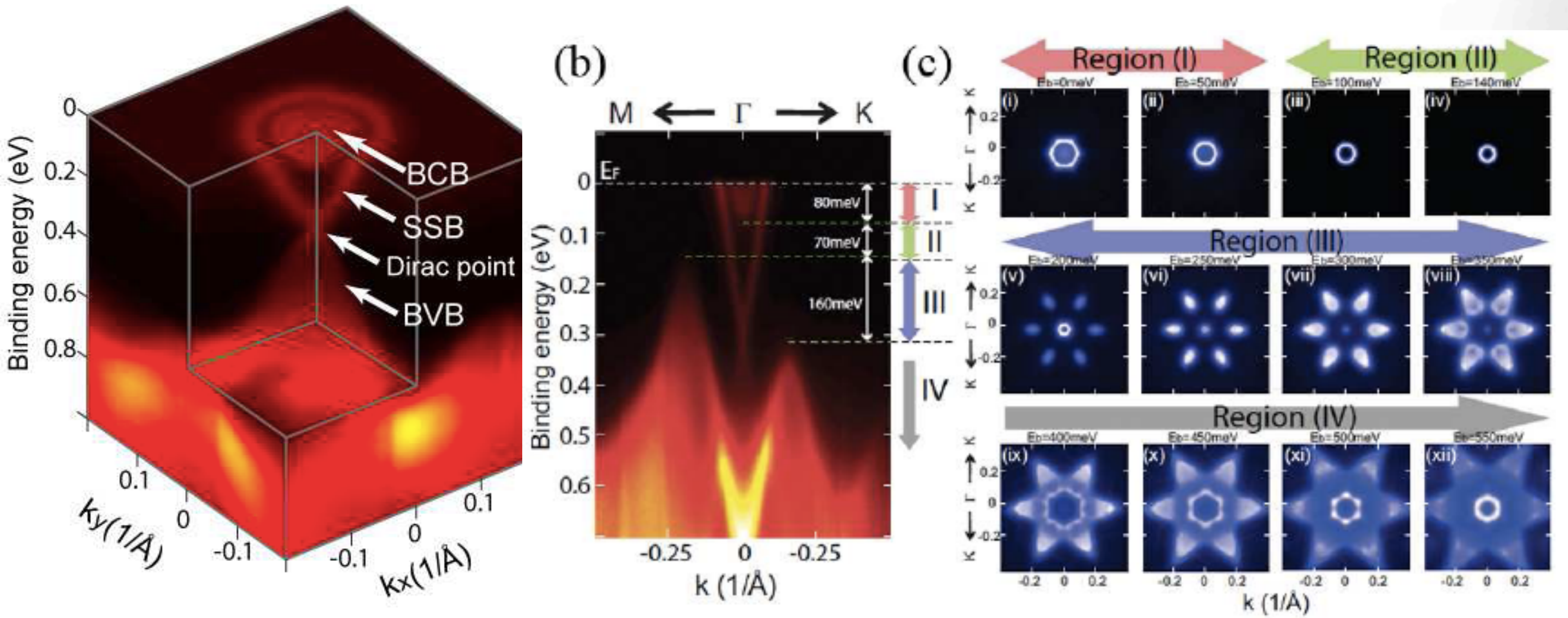
	Parity eigenvalues		Gap at Γ	Bulk gap (eV)
$TlBiTe_2$	+ − + + − − − + + − ; +	(−)	0.16	<0.01*
$TlBiSe_2$	+ − + + − − − + + − ; +	(−)	0.17	0.17
$TlBiS_2$	+ − + + − − − + + − ; +	(−)	0.07	0.07
$TlSbTe_2$	+ − + + − − − + + − ; +	(−)	0.05	0.05
$TlSbSe_2$	+ − + + − − − + + − ; +	(−)	0.19	0.14*
$TlSbS_2$	+ − + + − − − + + + ; −	(+)	0.09	0.04*

* Indirect gap.

Yan et al. EPL 90, 37002 (2010),

Lin et al. PRL105(3) 036404 (2010), Eremeev et al. *JETP Lett.* 91(11) 594 (2010).

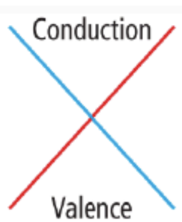
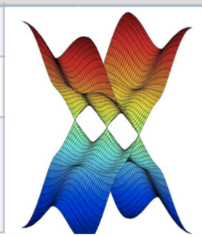
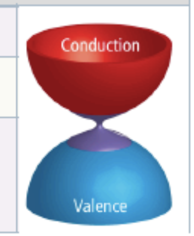
Bi2Se3 type: TlBiSe2 and TlBiTe2

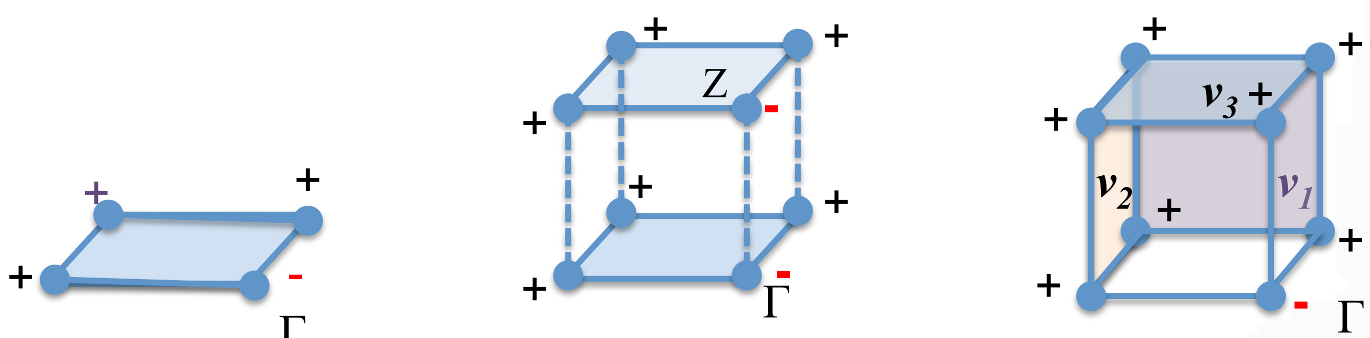


TlBiTe2 :Topological superconductor.
CuxBi2Se3, PdxBi2Te3

Sato et al. *PRL* 105(13) 136802 (2010),
Kuroda et al. ibid, 105(14) 146801 (2010),
Chen et al. ibid, 105(26) 266401 (2010),
Xu et al. *arXiv:1008.3557* (2010).

Search for a weak 3D TI

2D		3D			
QSH		Weak TI		Strong TI	
$\nu = 1$		$\nu = (0; \nu_1\nu_2\nu_3)$		$\nu = (1; \nu_1\nu_2\nu_3)$	
HgTe/CdTe QWs InAs/GaSb/AlSb QWs		?		Bi_2Se_3, Bi_2Te_3, $TlBiSe_2$, Strained HgTe, Ag_2Te …	



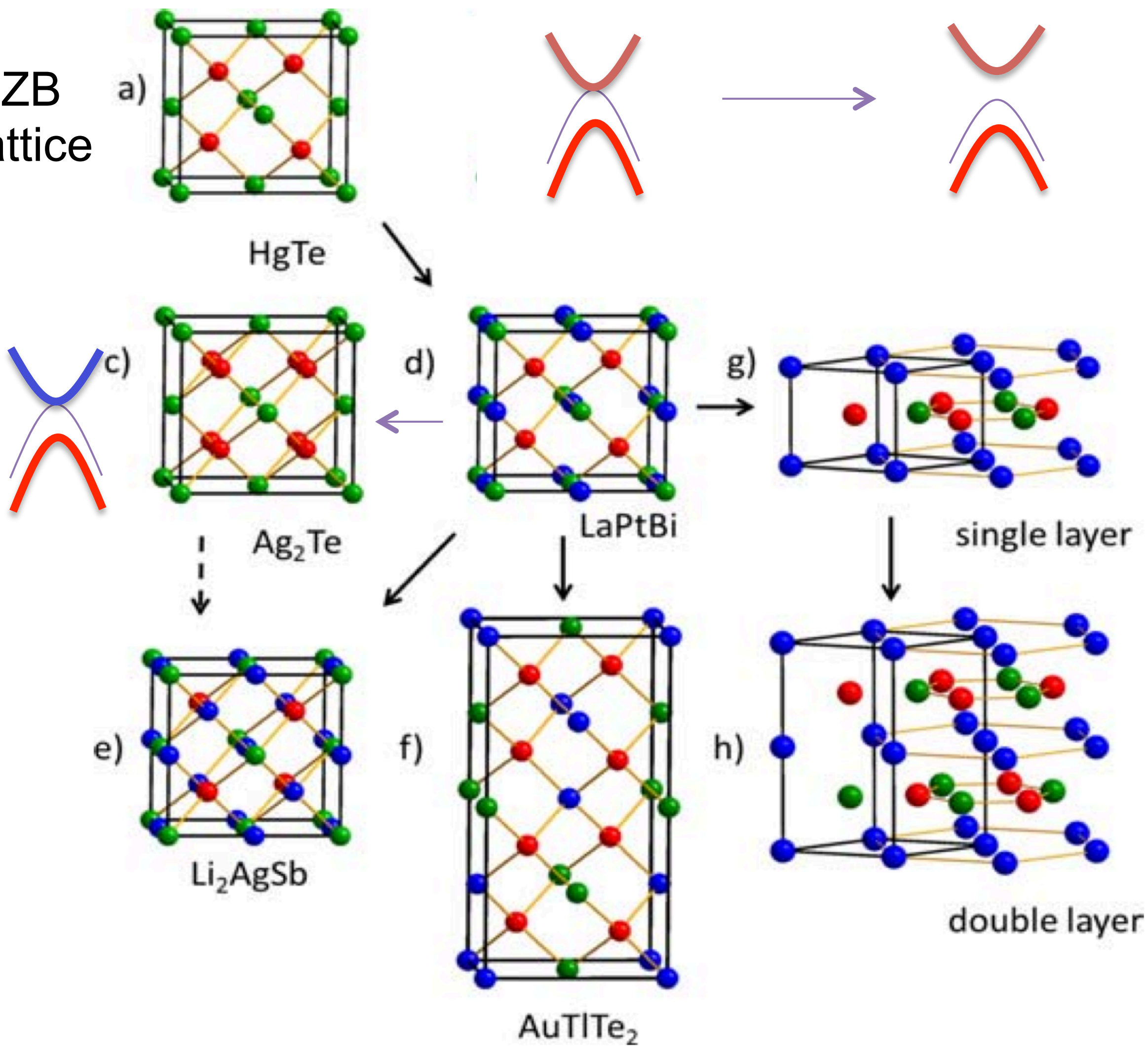
ν=1
2D TI

(0;001)
Weak 3D TI

(1;000)
Strong 3D TI

Generalization of Heusler compounds

ZB lattice



Wurzite lattice

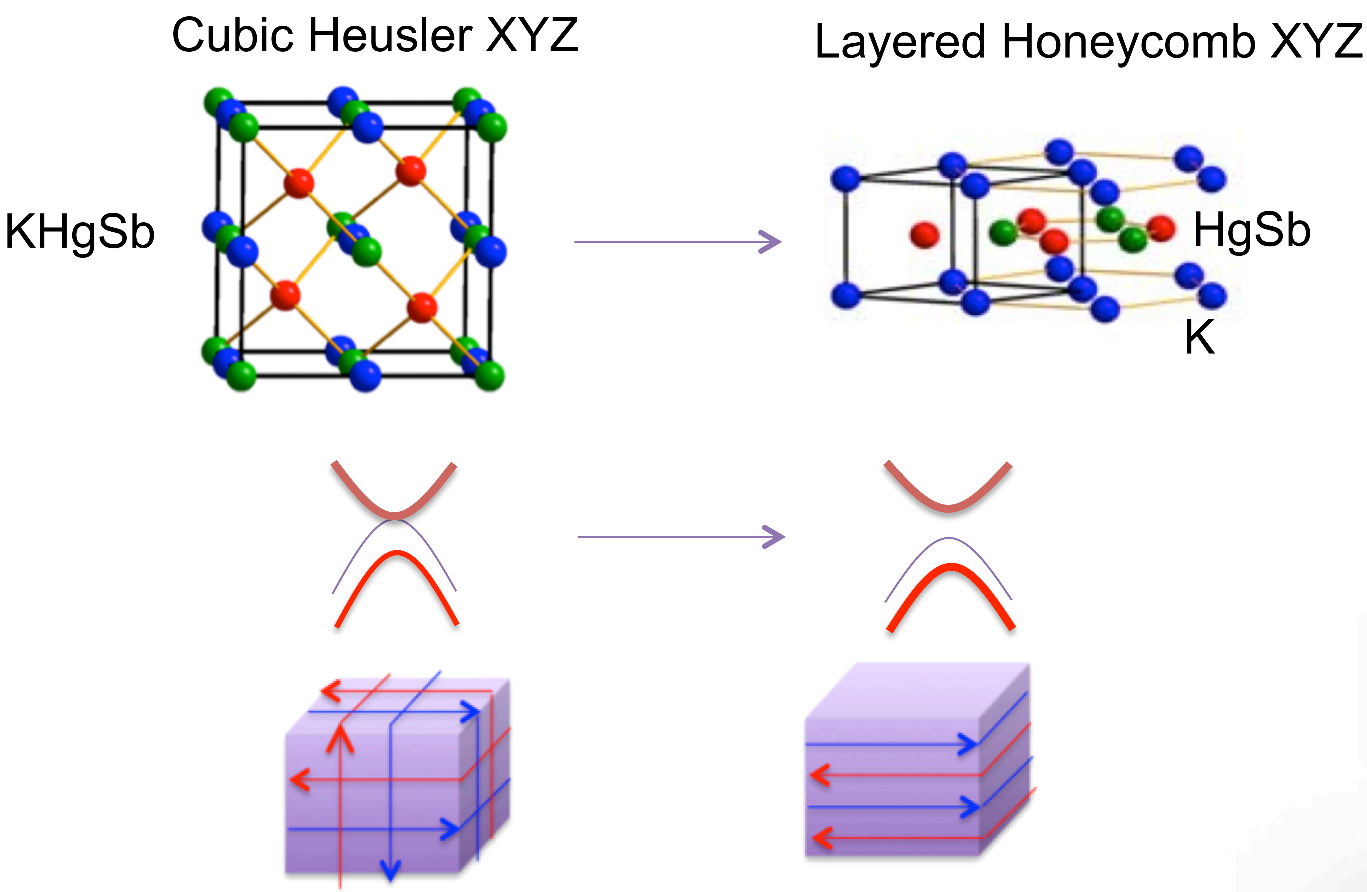
Stacking 2D TI layers

Structure of SrPtAs-type unconventional SC

Biswas et al., PRB 87, 180503(R) (2013);
Fisher et al. PRB 89, 020509 (2014)

Following Heusler's idea to design a weak TI

3D weak TIs

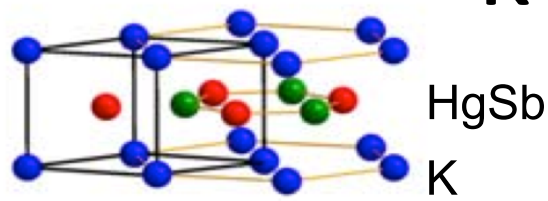


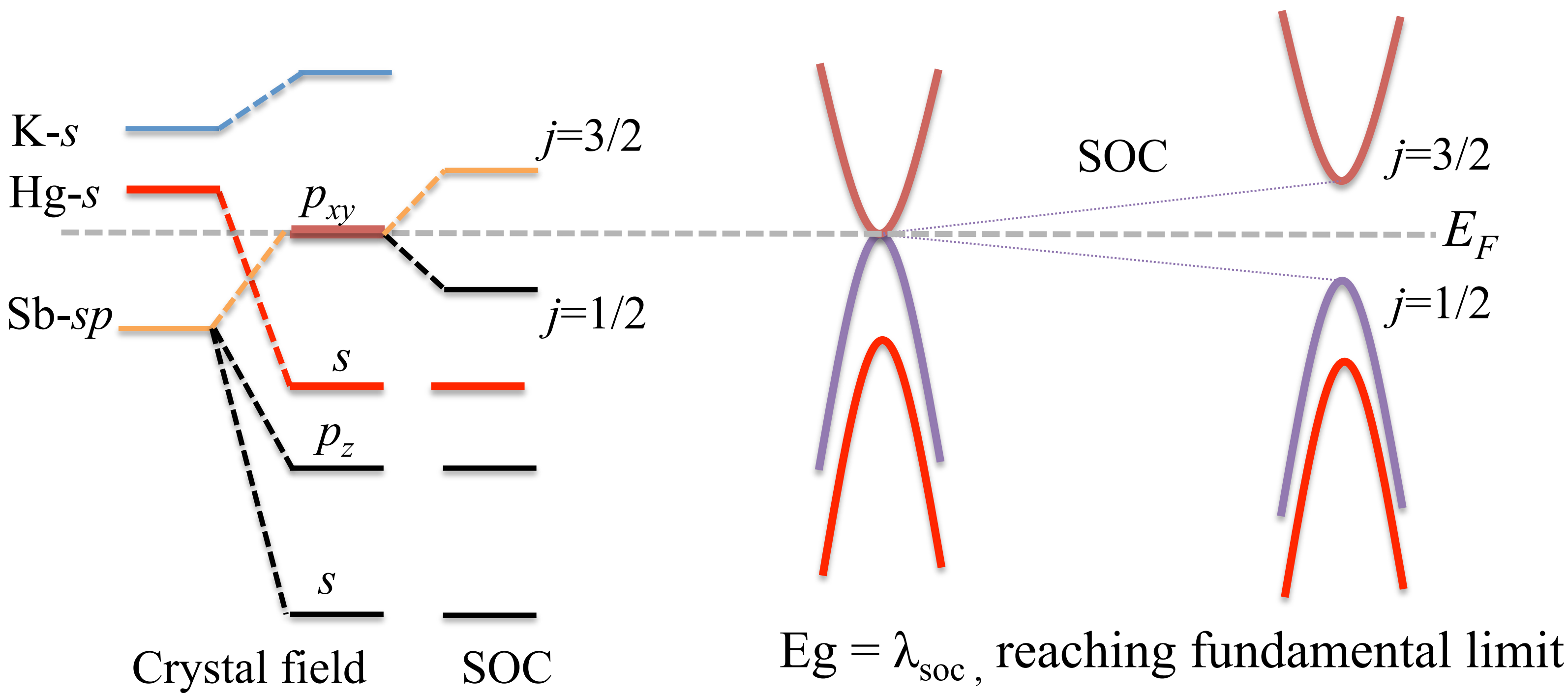
The weak TI has a "*strong*" side.

Z. Ringel, Y. Kraus, and A. Stern, Phys. Rev. B 86, 045102 (2012).

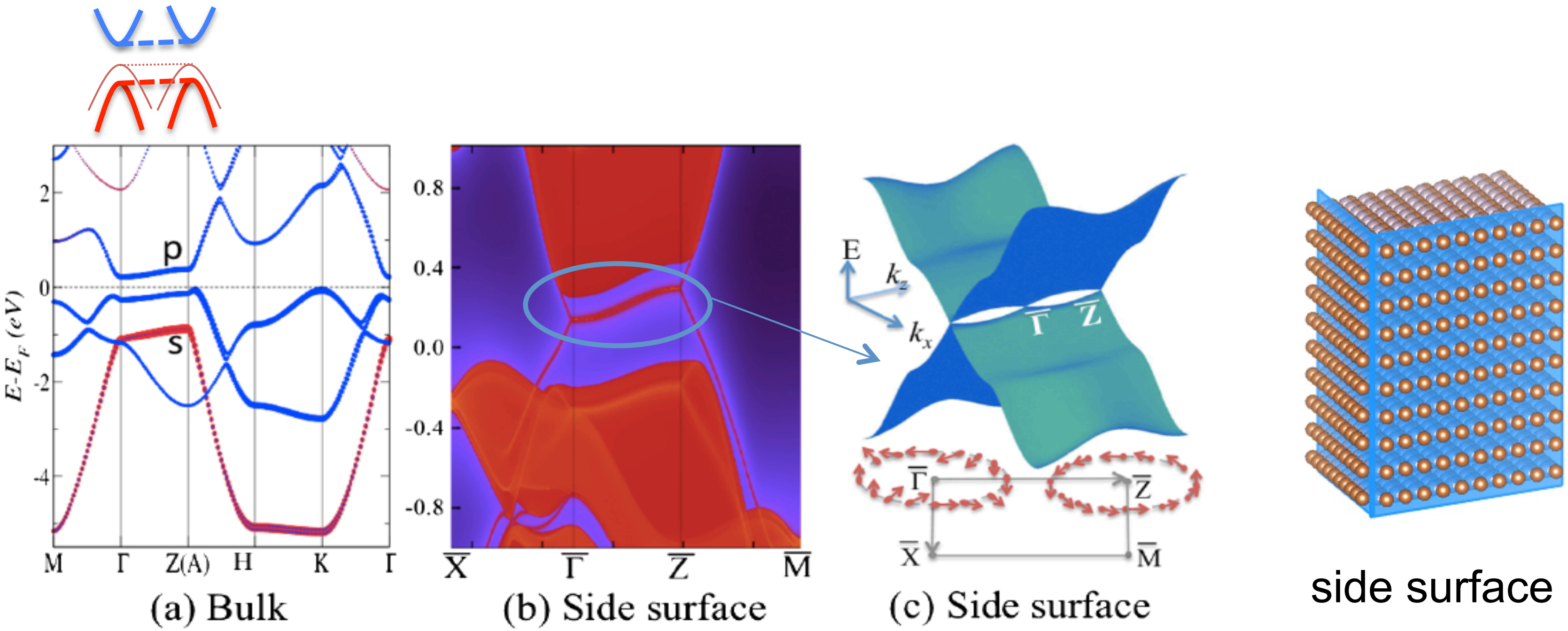
R. S. K. Mong, J. H. Bardarson, and J. E. Moore, Phys. Rev. Lett. 108, 076804 (2012).

Bulk band structure





The first 3D weak TIs



- The first weak TI material, KHgSb
- Surface state with *two* Dirac cones
- Eg ~ 0.2 eV >> RT

KHgSb
(synthesized in 1980)

BY, Mulechler, Felser. PRL 109, 116406 (2012).

3D weak TIs

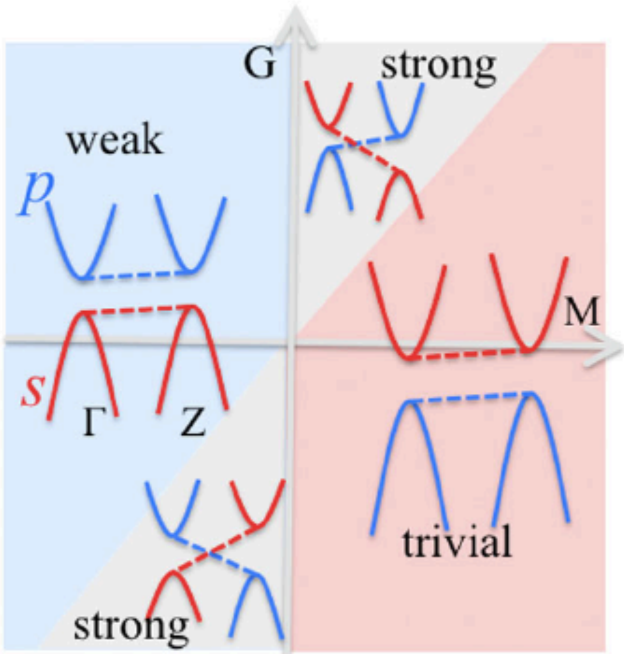
Bernevig-Hughes-Zhang model, minimal Hamiltonian

$$H(k) = \epsilon(k)\mathbb{I}_{4\times4} + \begin{pmatrix} M(k) & Ak_+ & 0 & Ek_z \\ Ak_- & -M(k) & Ek_z & 0 \\ 0 & Ek_z & M(k) & -Ak_- \\ Ek_z & 0 & -Ak_+ & -M(k) \end{pmatrix}$$

Band inversion

$$M(k) = M_0 - B\, k_{//}^2 - G\, k_z^2$$

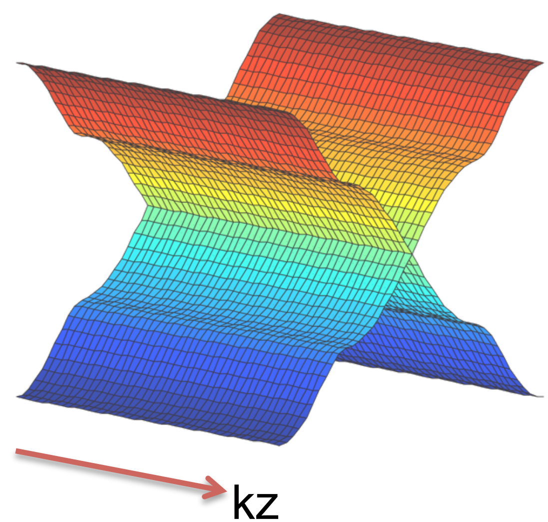
Turning on inter-layer coupling



KHgSb	KHgAs	KHgP
NaHgSb	NaHgAs	NaHgP
LiHgSb	LiHgAs	LiHgP
KCdSb	KCdAs	KCdP
NaCdSb	NaCdAs	NaCdP
LiCdSb	LiCdAs	LiCdP

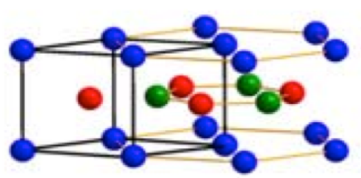
KAuTe	KAuSe
NaAuTe	NaAuSe
LiAuTe	LiAuSe
KAgTe	KAgSe
NaAgTe	NaAgSe
LiAgTe	LiAgSe

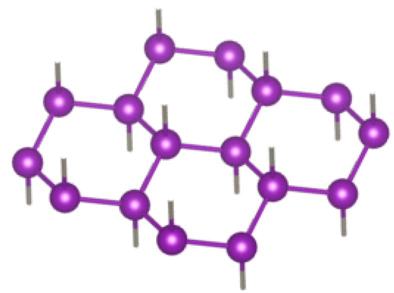
XYZ

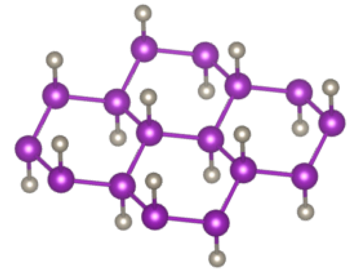


BY, Mulechler, Felser. PRL 109 (2012) 116406.

Extract a QSH layer from the layered weak TI



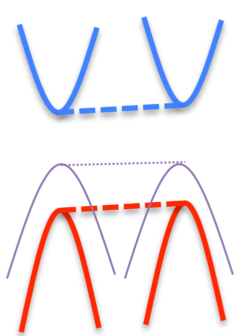


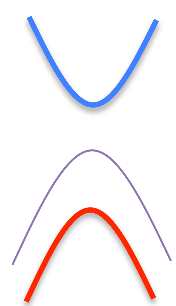


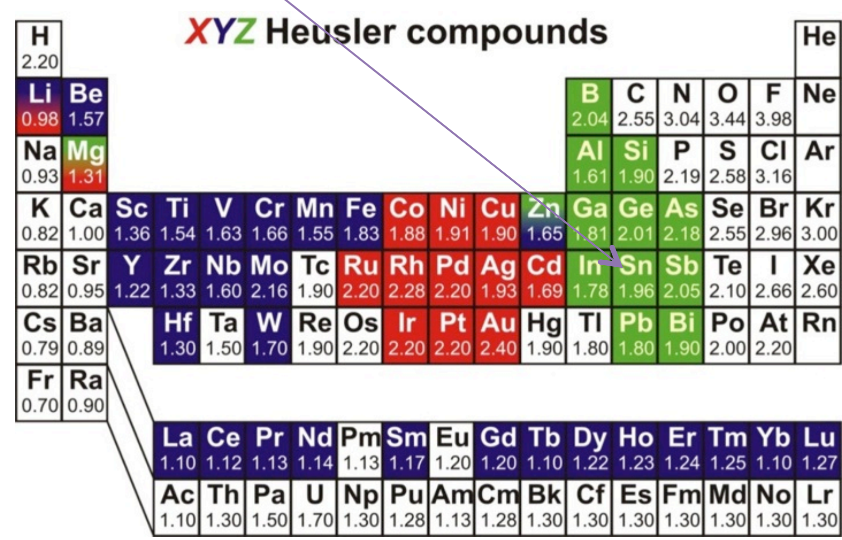
X-Y-Z
8 or 18 electrons

IV-IV
8 electrons

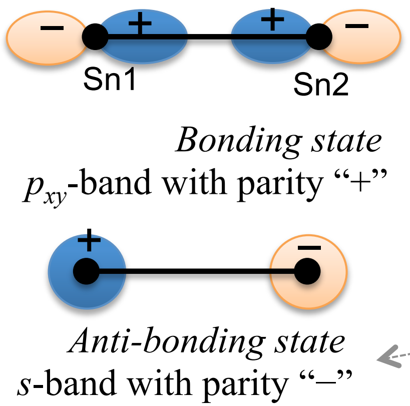
IV2-X2

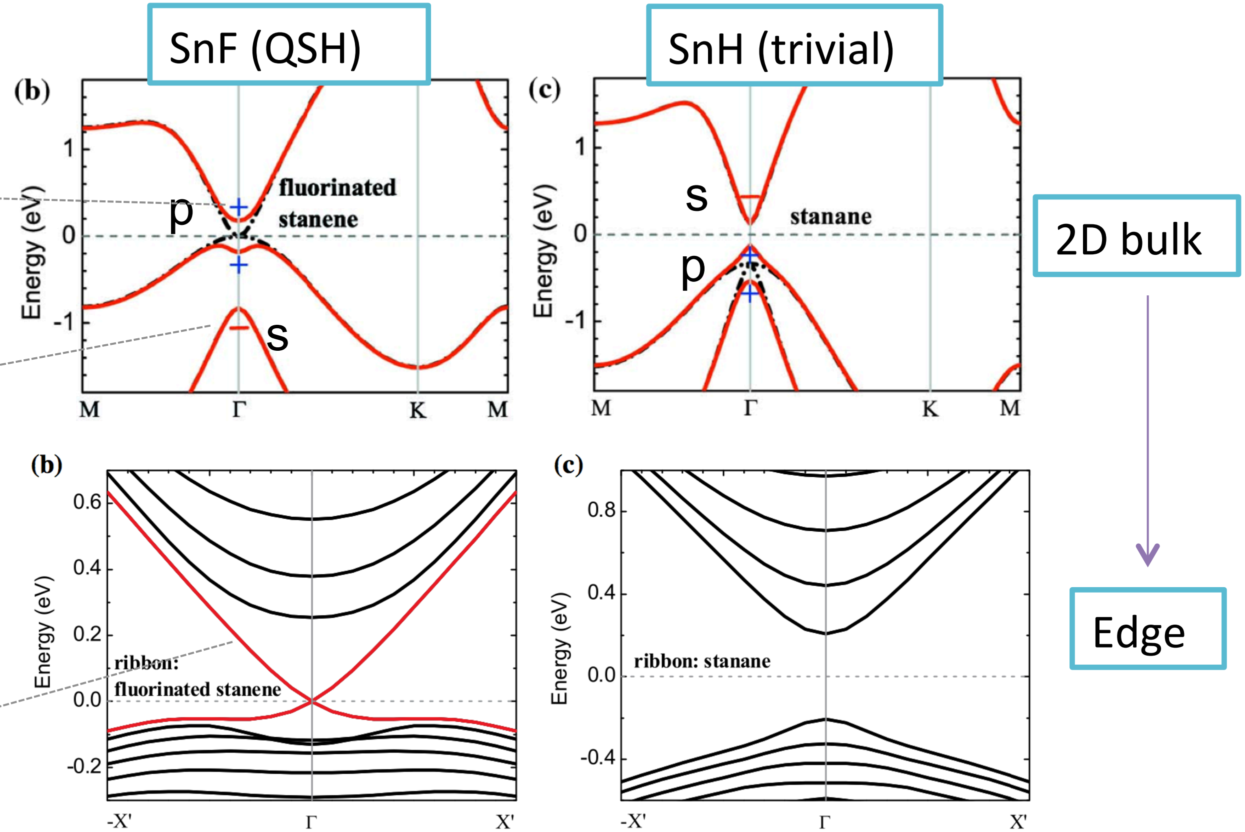


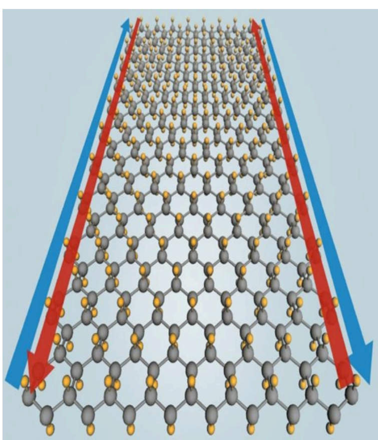




QSH layer





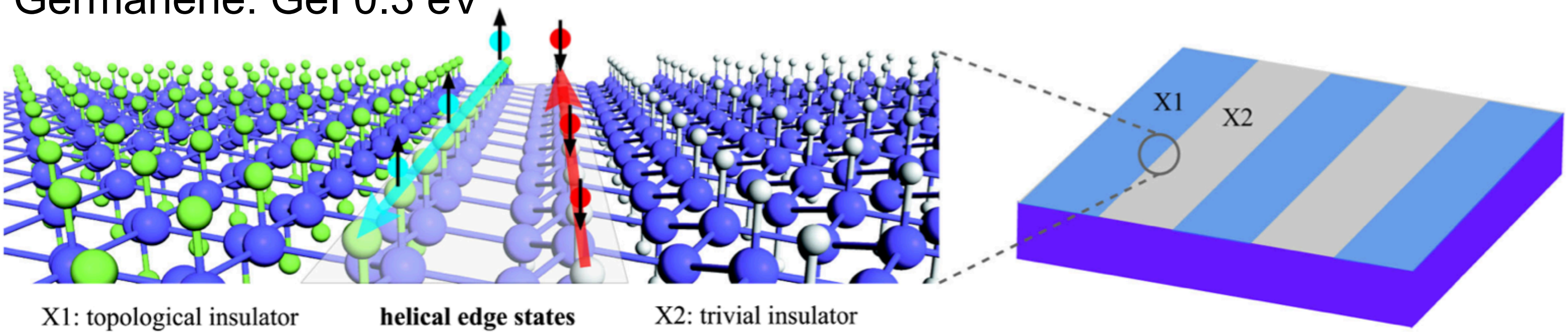


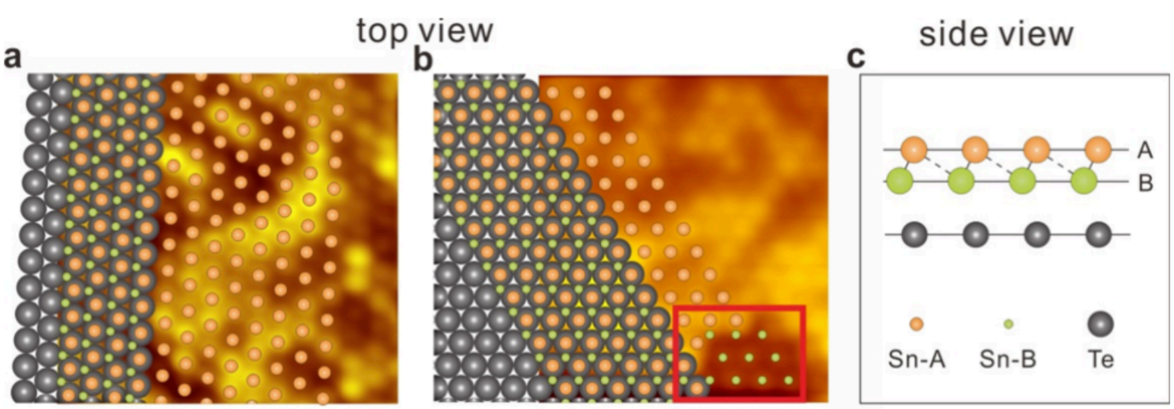
Band inversion at the Γ point, different from graphene.

Y. Xu, **BY**, H.-J. Zhang, J. Wang, G. Xu, P. Tang, W. Duan, and S.-C. Zhang, PRL 111, 136804(2013).

QSH layer with large energy gap

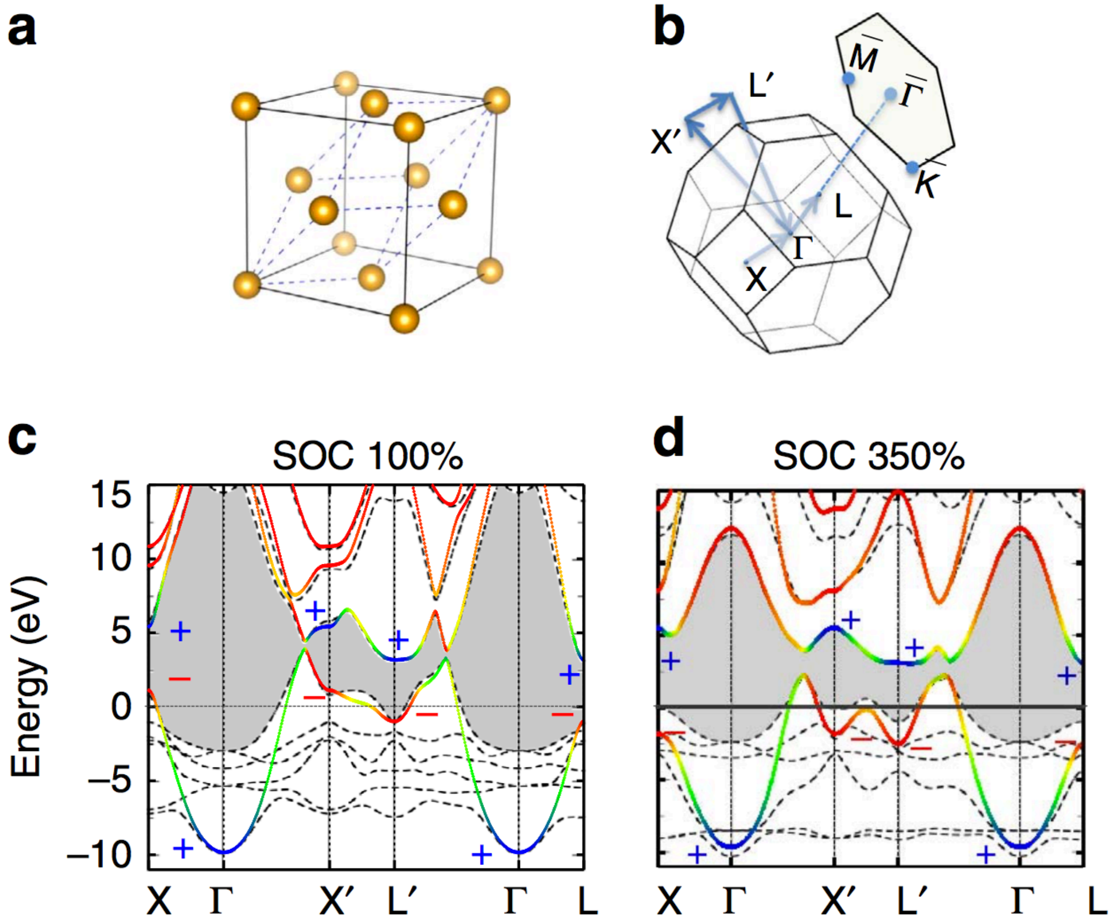
Stanene: SnI 0.4 eV
Germanene: GeI 0.3 eV



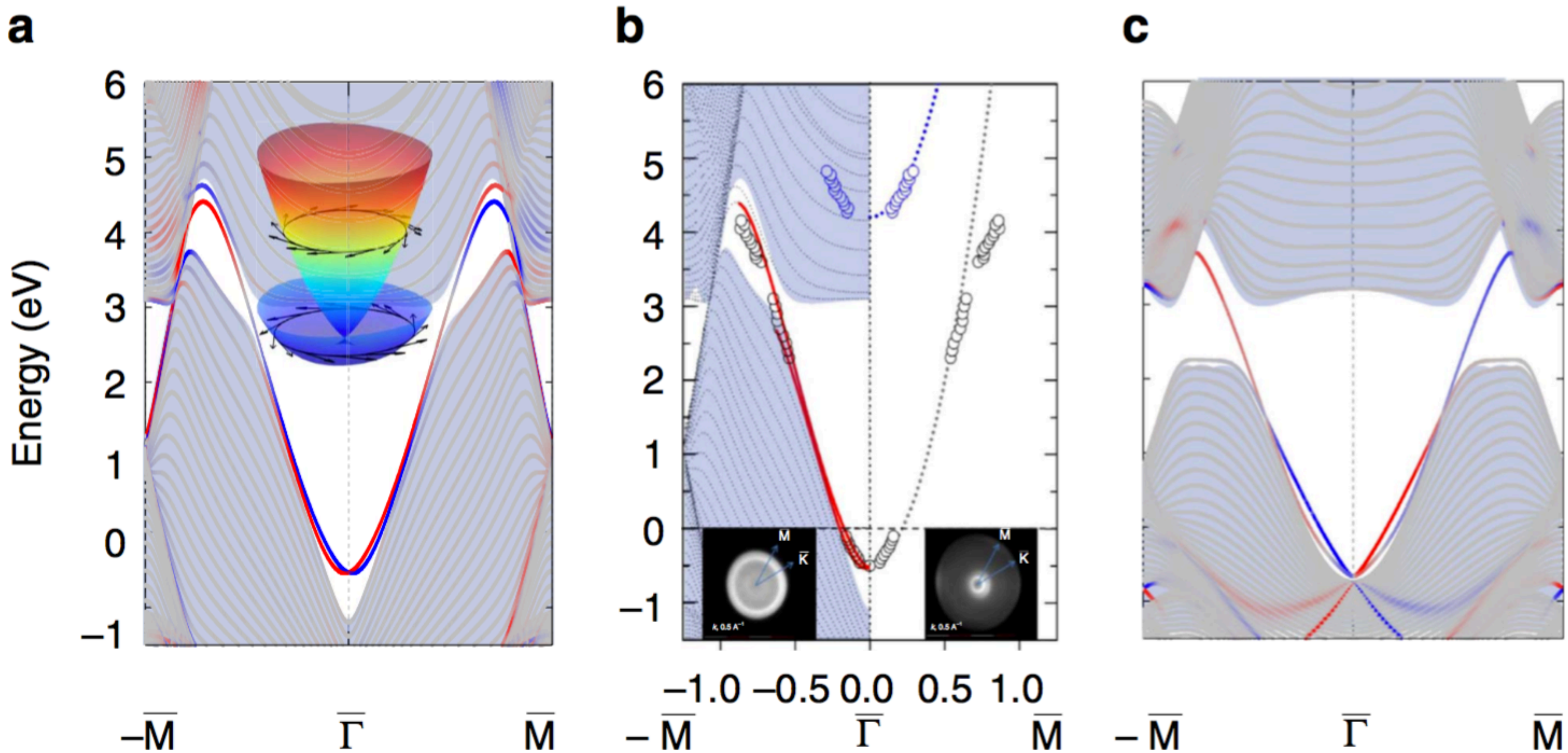


Recent MBE growth
Zhu et al.
arXiv:1506.01601 (2015)

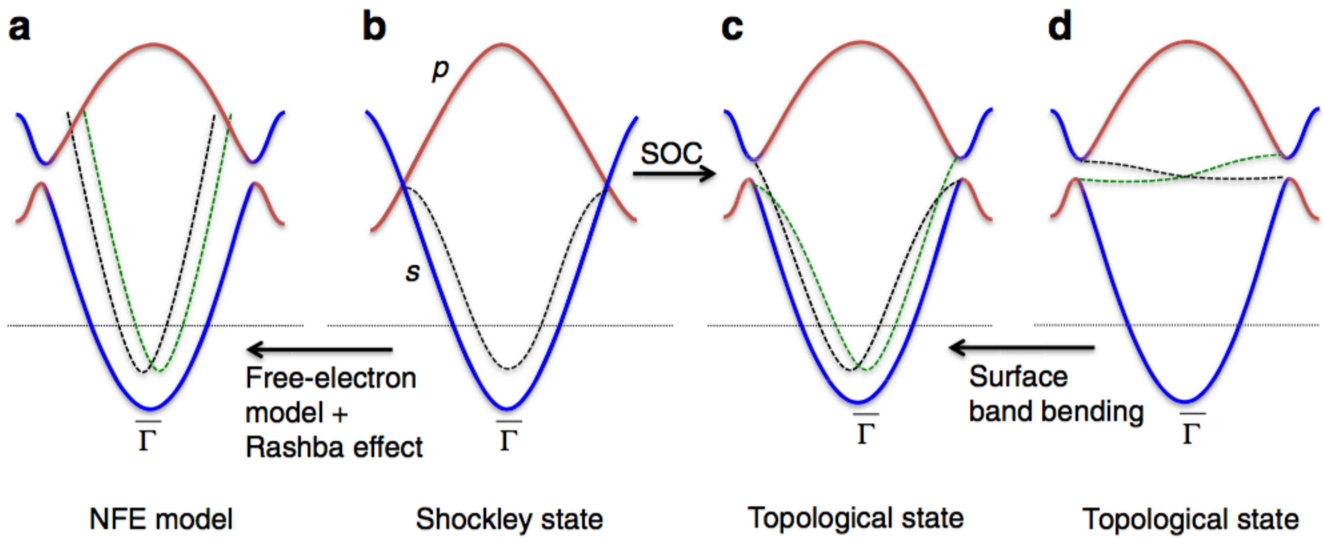
Gold surface



Gold surface



Gold surface



B. Yan et al. Nature Communications **6**, 10167 (2015).

Topological mirror insulator

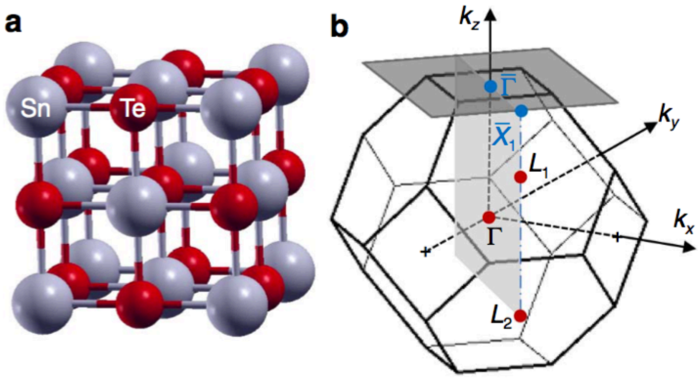
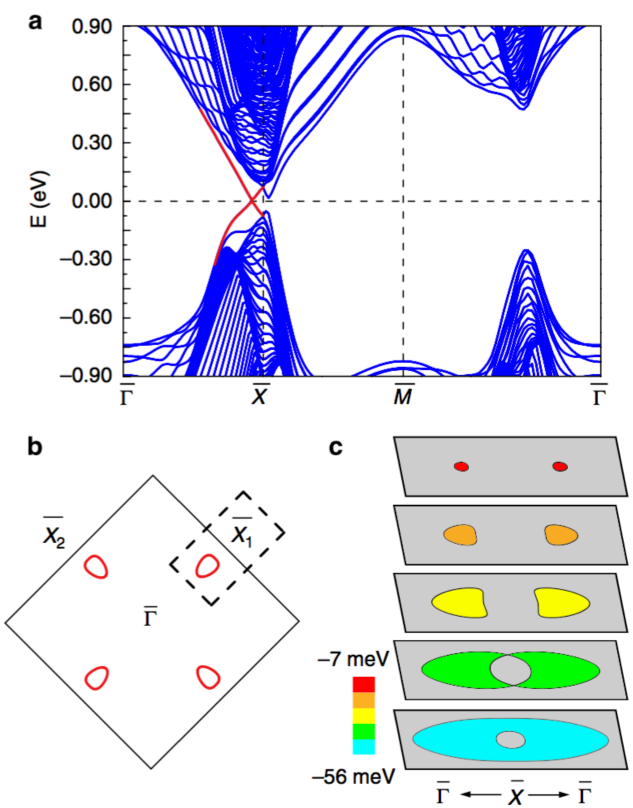
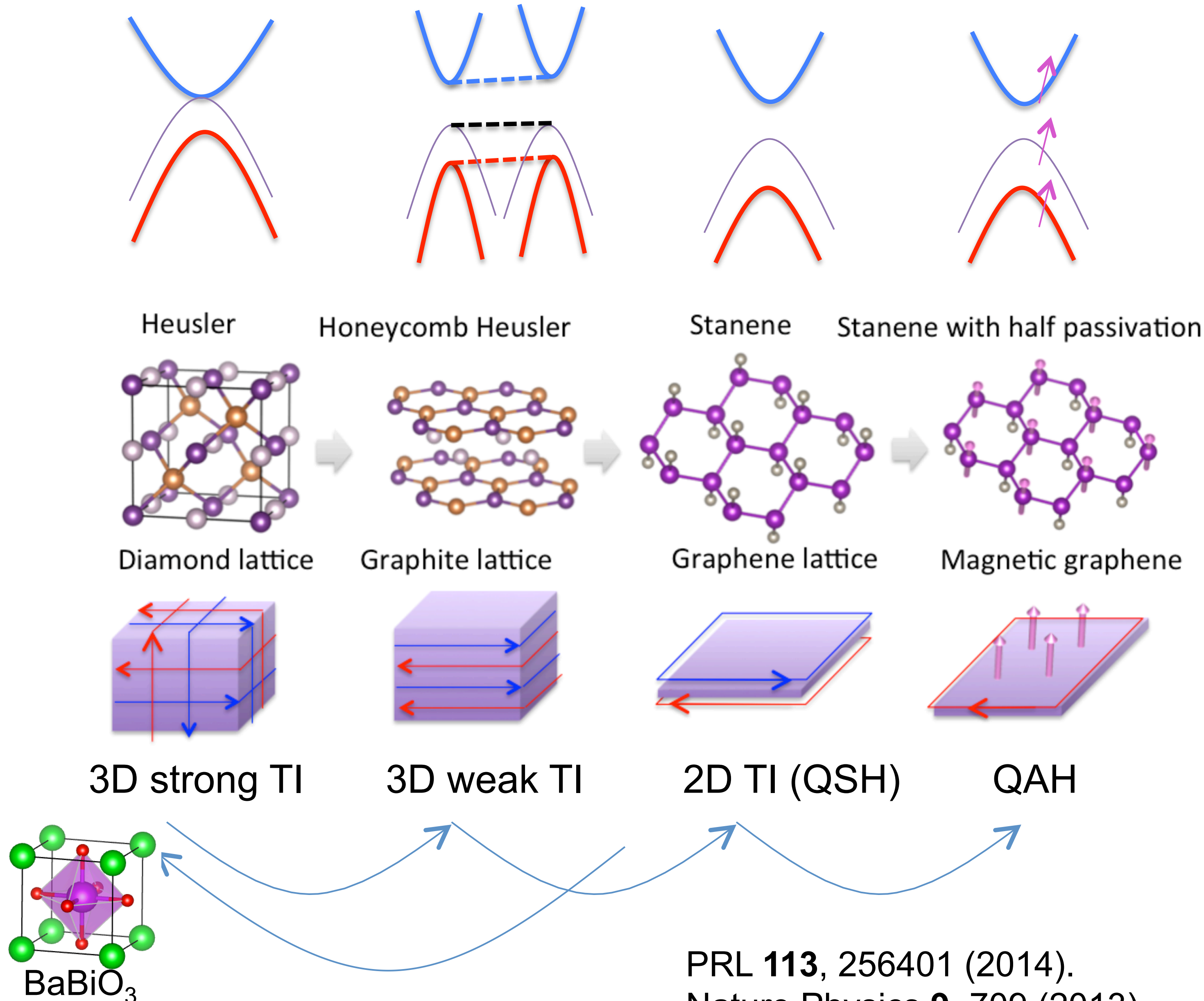


Figure 1 | SnTe lattice and Brillouin zone. (**a**) the crystal structure of SnTe; (**b**) the face-centered-cubic (FCC) Brillouin zone showing the plane $\Gamma L_1 L_2$, which is invariant under reflection about the (110) axis and projects onto the $\bar{\Gamma}\bar{X}_1$ line in the [001] surface.



Fu 2012'

Materials design for TIs

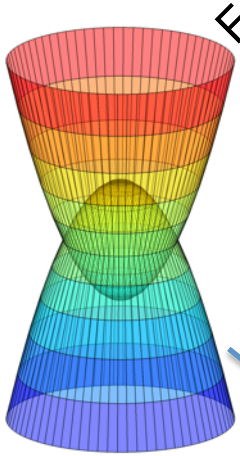


PRL **113**, 256401 (2014).
Nature Physics **9**, 709 (2013).

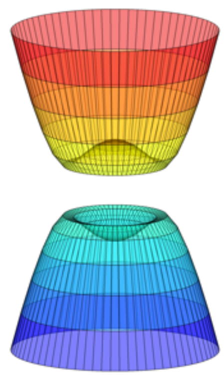
Topological insulators and topological metals

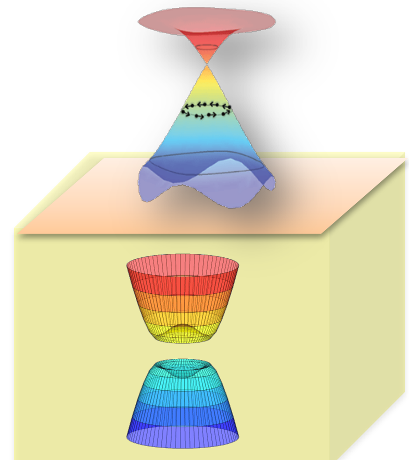
3D bulk

2D Surface



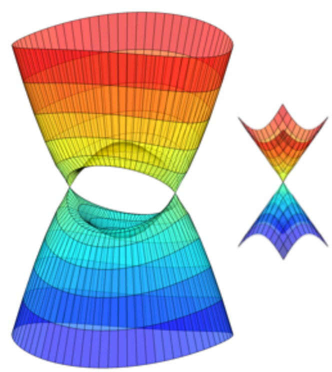
Full gap

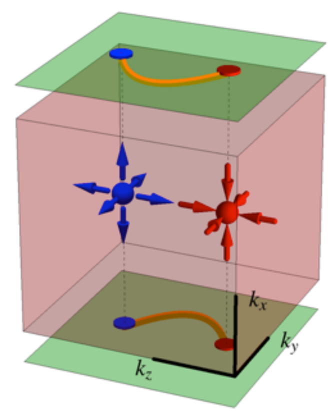




Topological insulator
Time reversal symmetry (TRS)x

Partial gap





Weyl Semimetal
Non spin degenerate
TRS and/or IS breaking

Band inversion

3D analoge of graphene

Fermi arcs

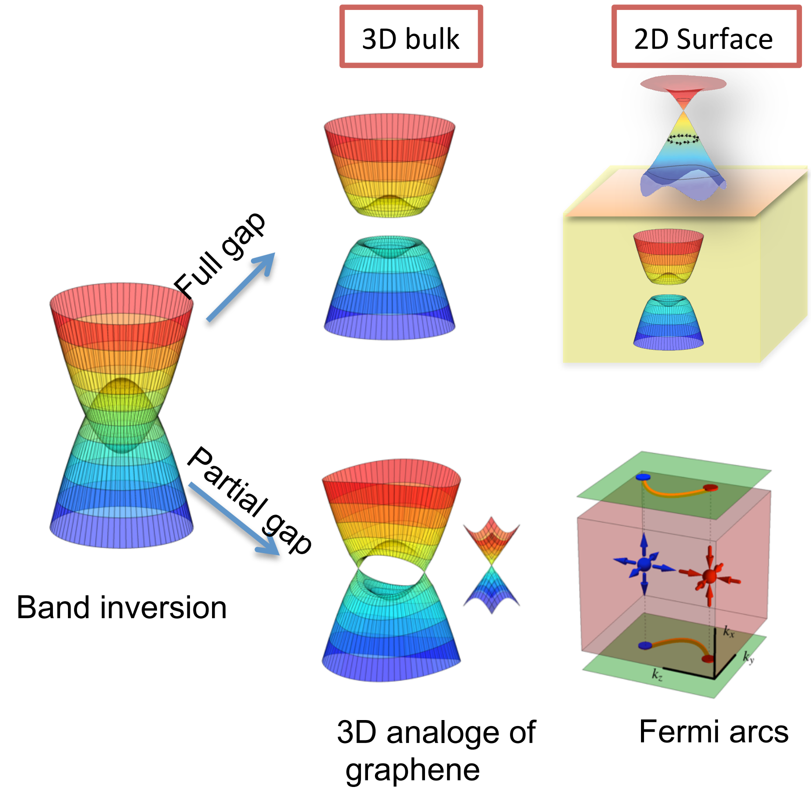
Summary

Topological insulators

- Topological surface states, Dirac cone
- 2D TI, 3D strong and weak TIs

Topological metals (3D graphene)

- Topological surface states, Fermi arcs
- Chiral anomaly, MR, high mobility



Thanks for your attention!