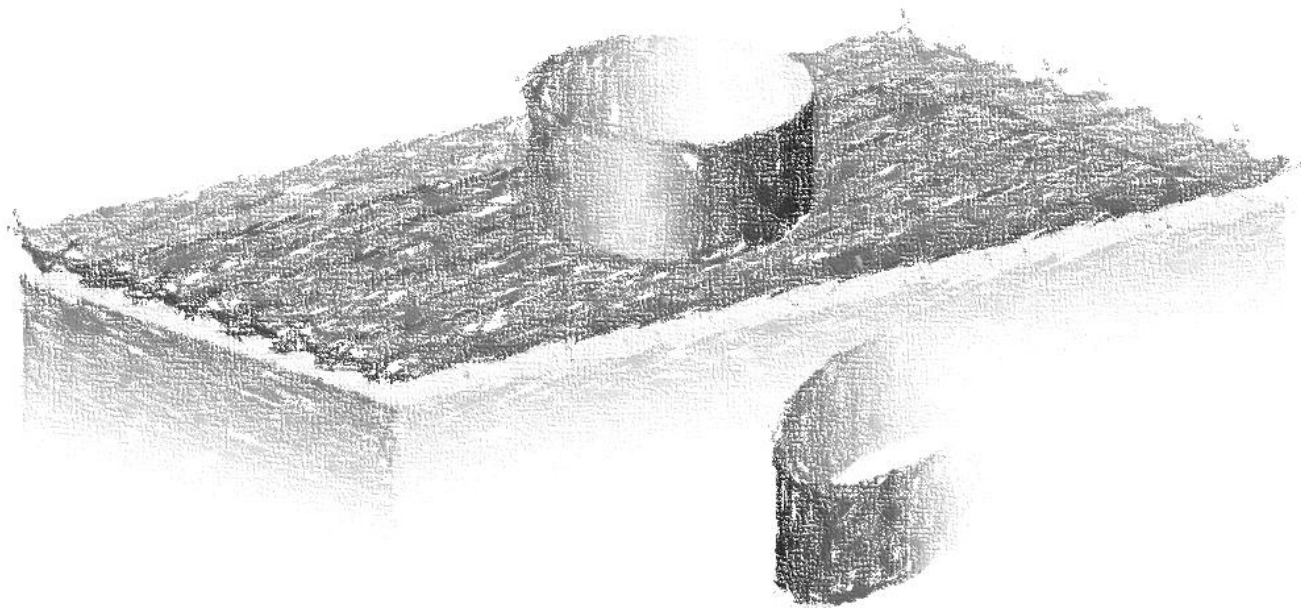




Topological insulators



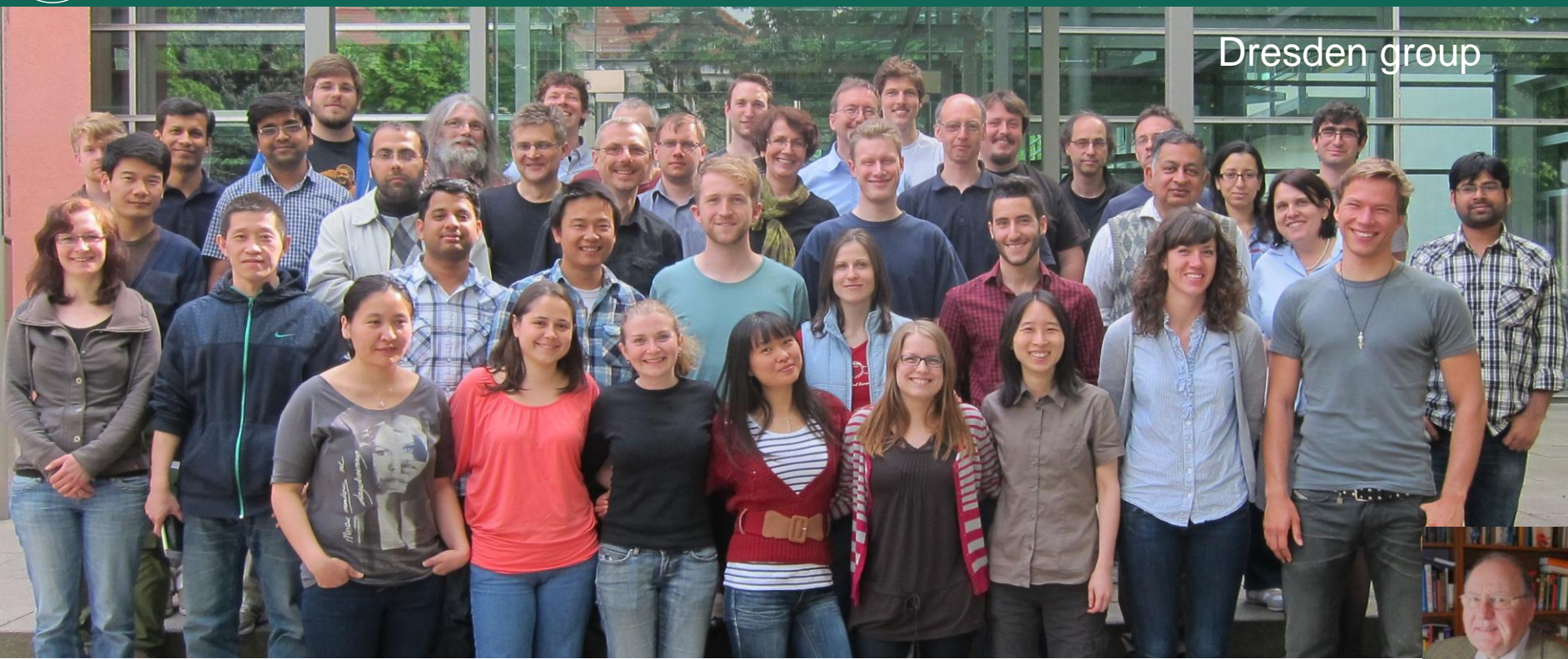
Claudia FELSER, Binghai YAN,

Shekhar Chandra, Stas Chadov, Lukas MÜCHLER, Martin Jansen, Jürgen Kübler,
Shou-Chen Zhang, Xiaoliang Qi, Yulin Chen

www.superconductivity.de



Co-workers in Dresden and elsewhere



Dresden group

Shou-Cheng Zhang et al., Stanford

Yulin Chen et al. Oxford

Stuart Parkin et al. IBM Almaden

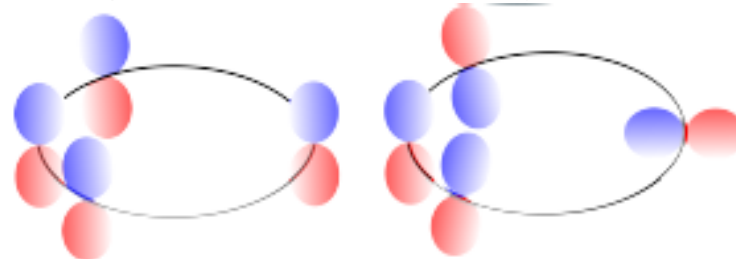
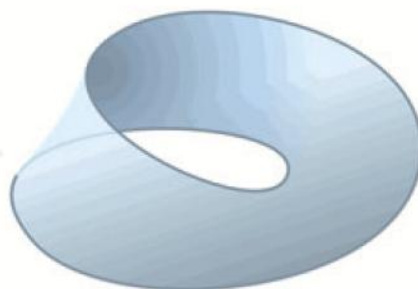
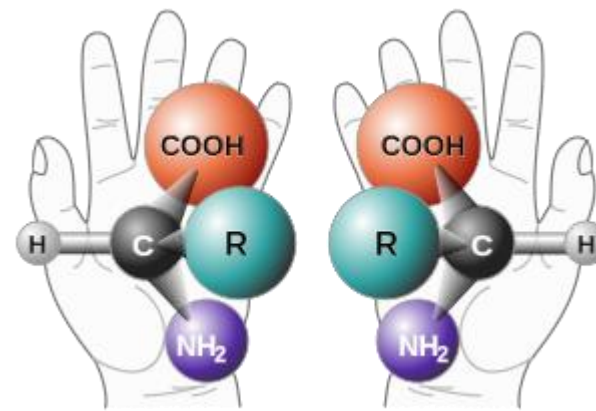
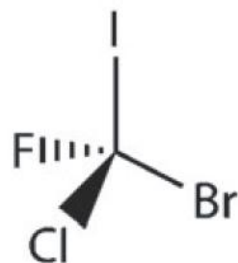
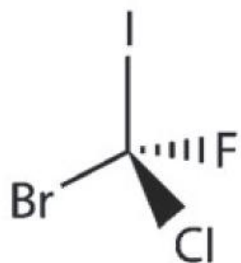
Paul Canfield, Ames Lab.





Topology in chemistry

Molecules with different chiralities can have different physical and chemical properties



Topologically interesting compounds are $4n$ aromatics with Möbius geometry, whereas normal $4n$ compounds are anti-aromatic



Hückel and Möbius aromaticity

secular equation

$$\begin{vmatrix} \alpha-E & \beta & \dots & \beta \\ \beta & \alpha-E & \beta & \vdots \\ \vdots & \beta & \ddots & \beta \\ \beta & \dots & \beta & \alpha-E \end{vmatrix}$$

N: number p-orbitals
 E_j : π MO energies
 $j = 0, 1, 2, 3 \dots (N-1)$
 α : Coulomb integral
 β : Resonance integral

Magic electron numbers

Hückel:

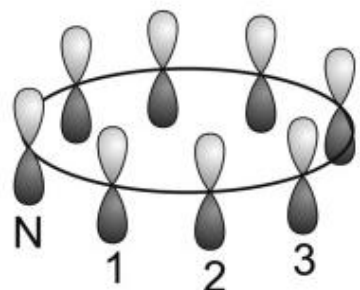
4n+2 aromatic

4n antiaromatic

Möbius

4n aromatic

4n+2 antiaromatic

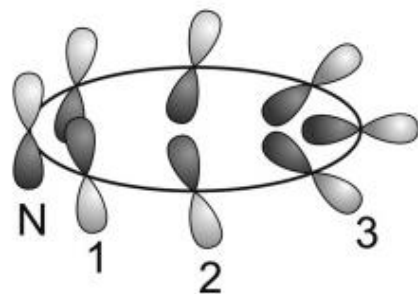


$$E_j = \alpha + 2\beta \cos \frac{2\pi j}{N}$$

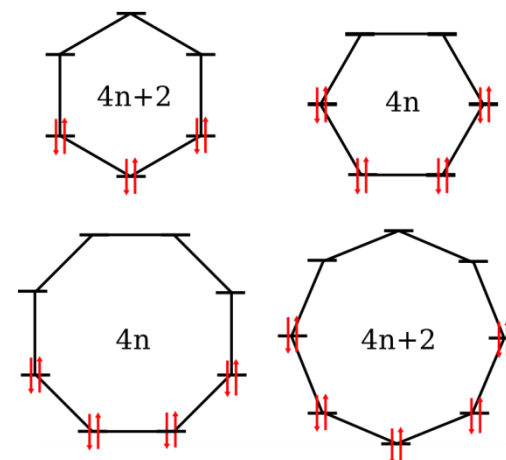
Möbius Annulenes

secular equation

$$\begin{vmatrix} \alpha-E & \beta & \dots & -\beta \\ \beta & \alpha-E & \beta & \vdots \\ \vdots & \beta & \ddots & \beta \\ -\beta & \dots & \beta & \alpha-E \end{vmatrix}$$



$$E_j = \alpha + 2\beta \cos \frac{\pi(2j+1)}{N}$$





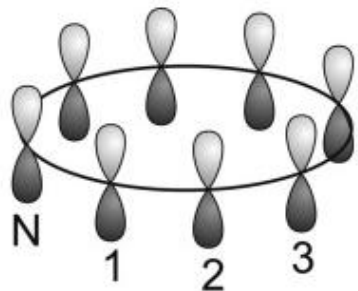
Hückel and Möbius aromaticity

ORGANIC CHEMISTRY

Aromatics with a twist

Rainer Herges

The properties of flat aromatic molecules are well known to chemists, but some non-planar aromatics remain a mystery. A molecule that can twist into a Möbius band on command might shed light on their features.



Möbius Annulenes

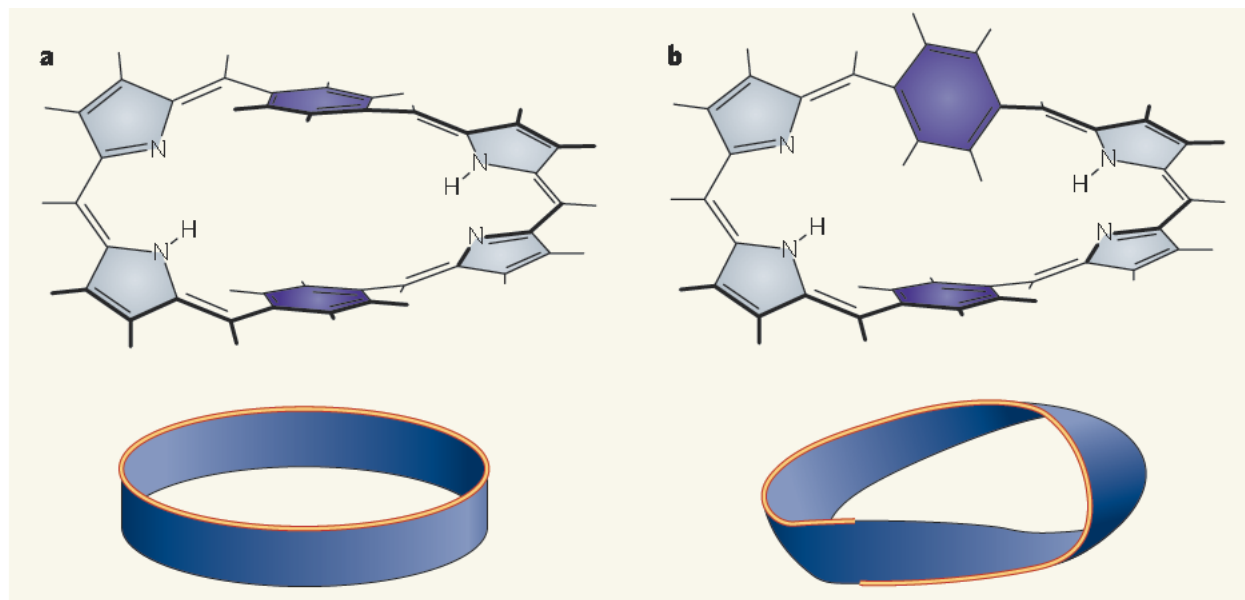
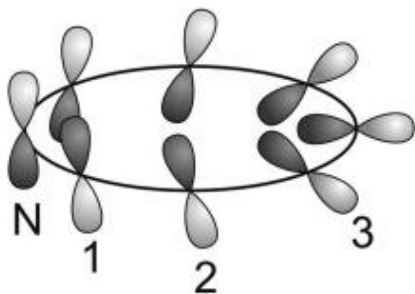
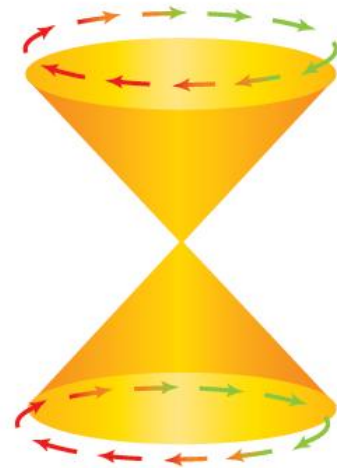
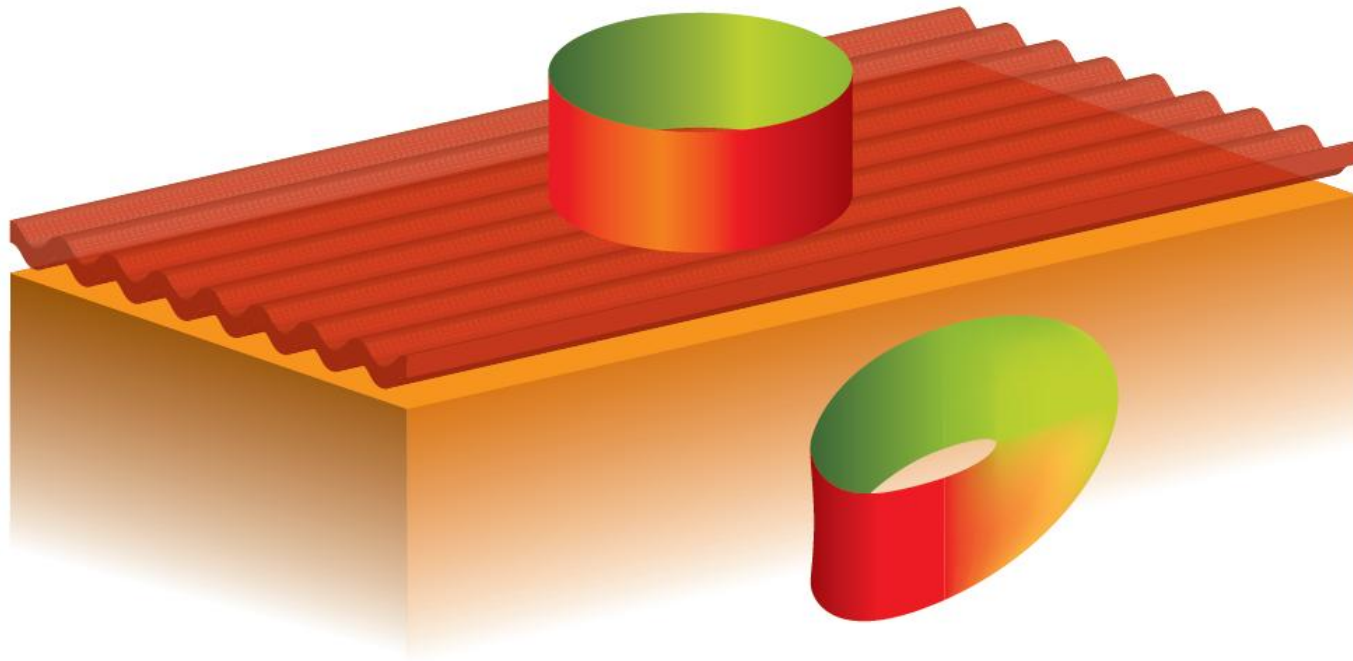


Figure 2 | A molecular topological switch. Latos-Grażyński and colleagues¹ have made a compound that is antiaromatic in nonpolar solvents, but not in polar solvents. **a**, In nonpolar solvents, the two benzene rings (purple) in the molecule are parallel, and the molecule is a two-sided, non-twisted band. **b**, In polar solvents, the upper benzene ring twists by 90°, so that the molecule becomes a one-sided, Möbius structure. This conformational change alters the aromaticity of the molecule.

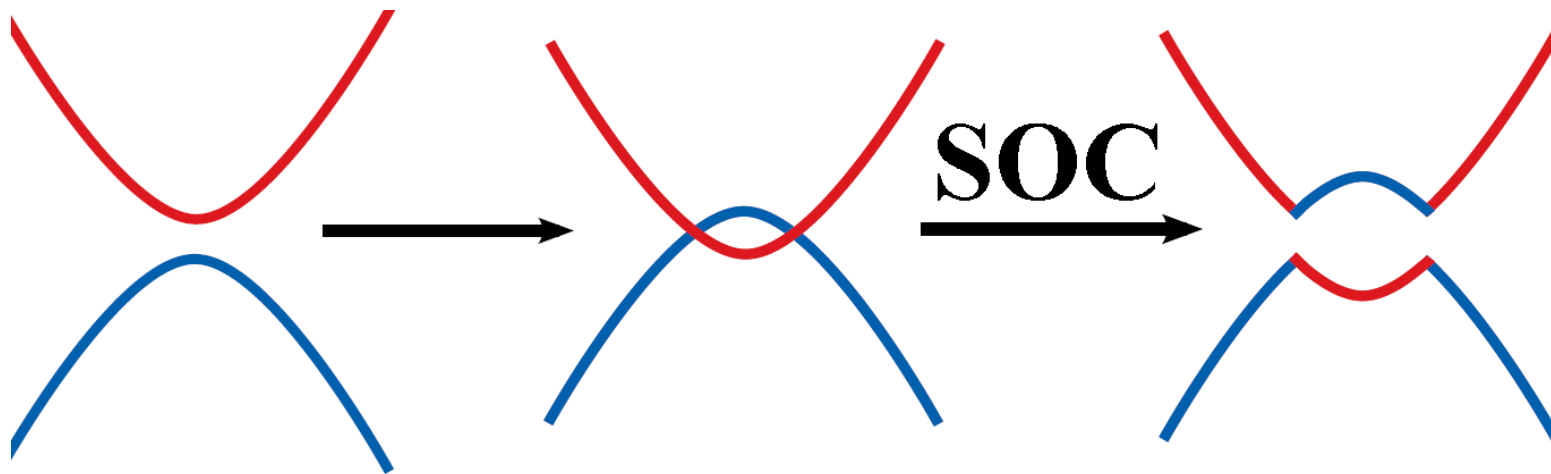
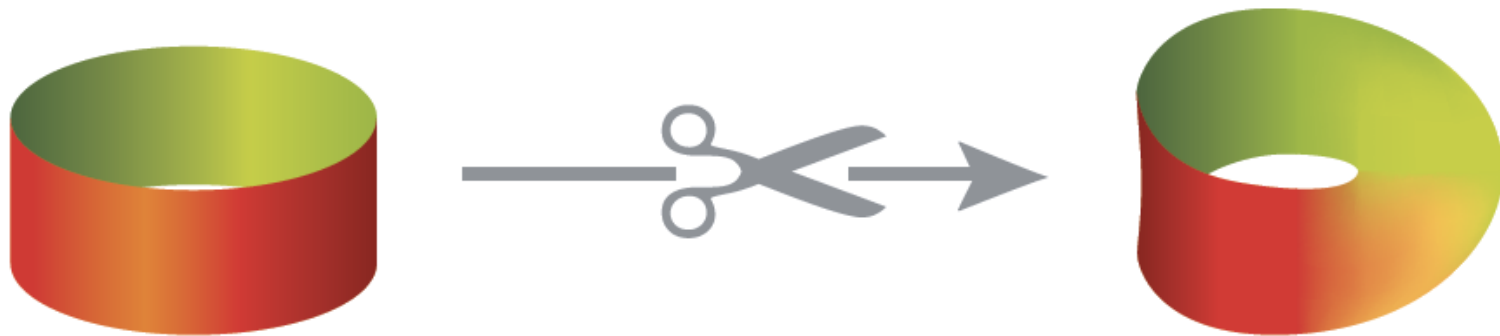


Topological Insulator





Topological Insulator



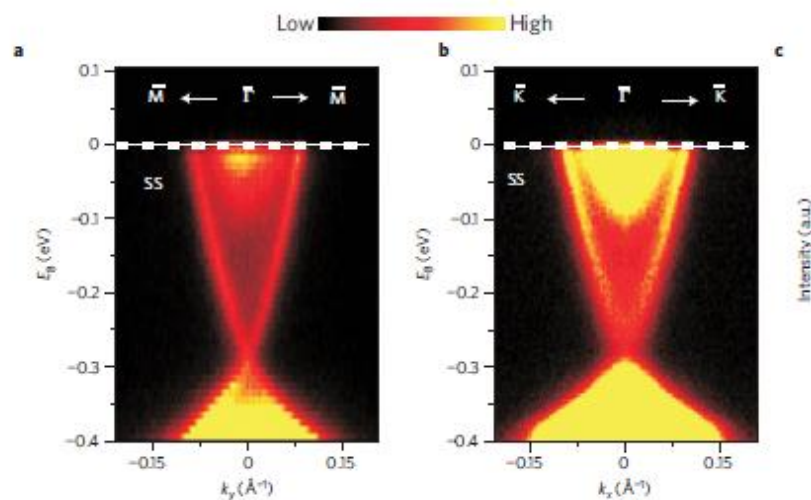
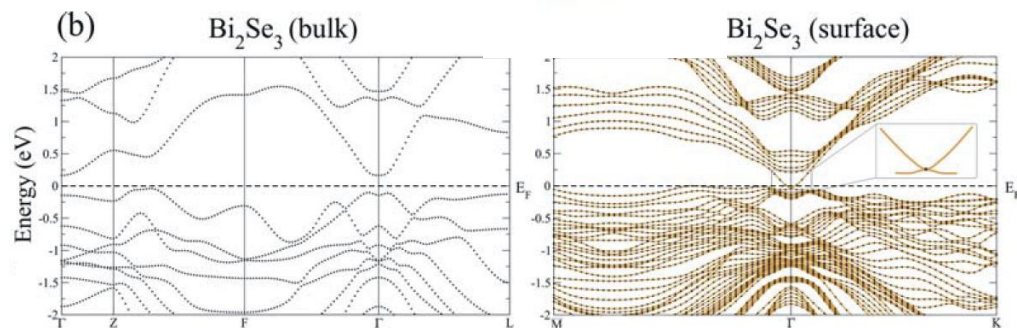
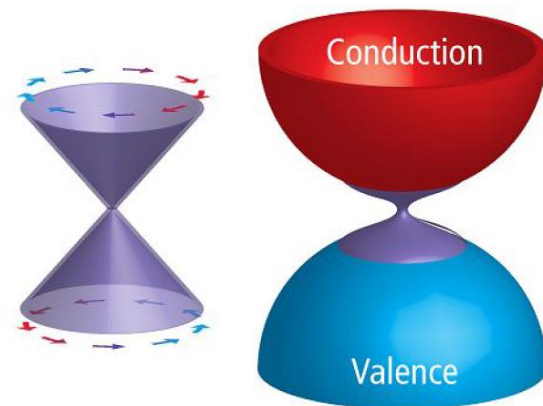
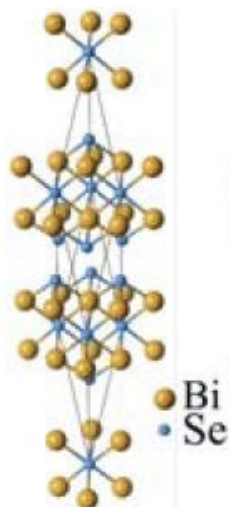


Topological insulators

3D Topological Insulators

Bi-Sb alloys

Bi_2Se_3 and relatives



Moore and Balents, PRB 75, 121306(R) (2007)

Fu and Kane, PRB 76, 045302 (2007)

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

Hsieh, et al., Science 323, 919 (2009)

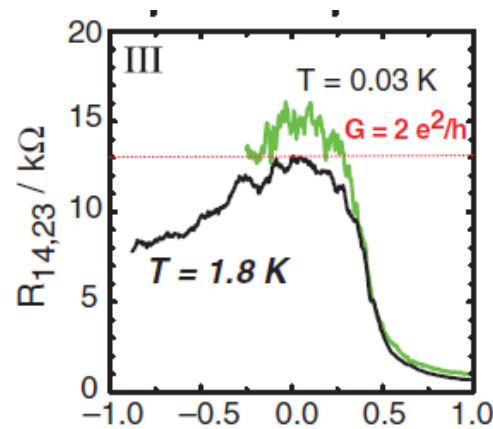
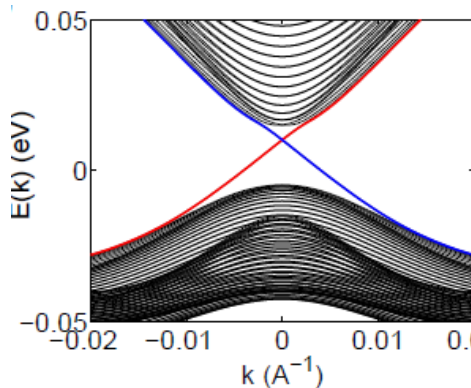
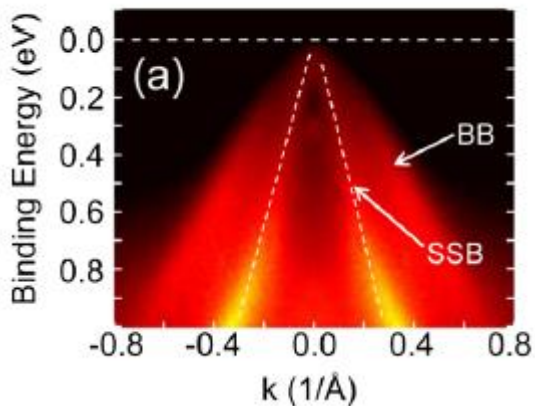
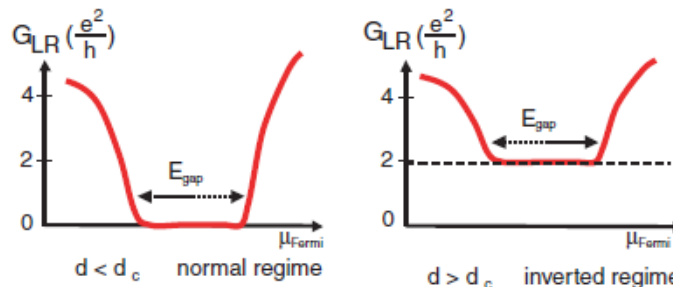
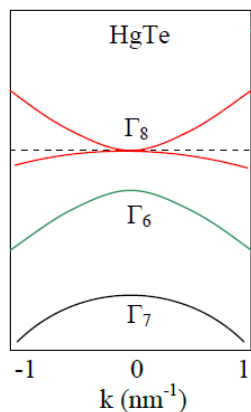
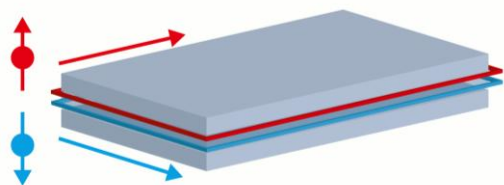
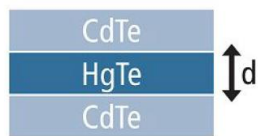
Xia, et al., Nature Phys. 5, 398 (2009); Zhang, et al., Nature Phys. 5, 438 (2009)



Topological insulators

2D TI ... prediction and realization

- HgTe and relatives
- Quantum well structure

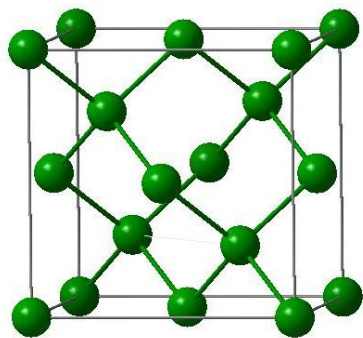


Kane and Mele, PRL 95, 146802 (2005)
 Bernevig, et al., Science 314, 1757 (2006)
 Bernevig, S.C. Zhang, PRL 96, 106802 (2006)
 König, et al. Science 318, 766 (2007)

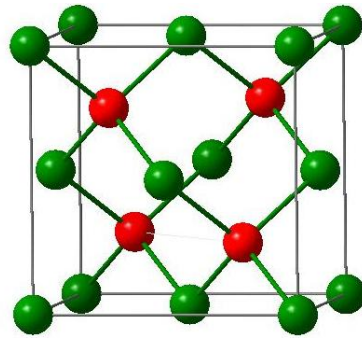


Heusler compounds

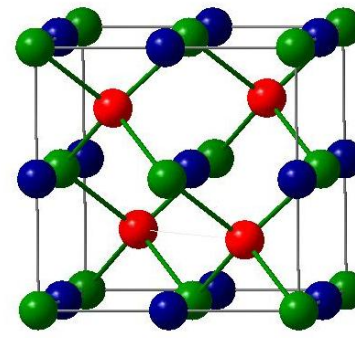
Diamond



ZnS



Heusler XYZ C1_b



C 2.55	N 3.04
Si 1.90	P 2.19
Ge 2.01	As 2.18
Sn 1.96	Sb 2.05

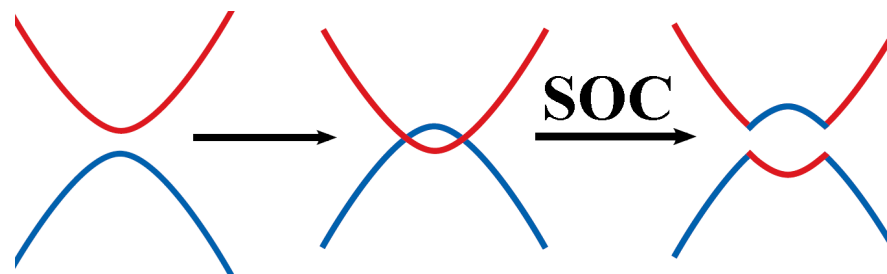
H 2.20																	He	
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne	
Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar	
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00	
Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.60	Mo 2.16	Tc 1.90	Ru 2.20	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.10	I 2.66	Xe 2.60	
Cs 0.79	Ba 0.89			Hf 1.30	Ta 1.50	W 1.70	Re 1.90	Os 2.20	Ir 2.20	Pt 2.20	Au 2.40	Hg 1.90	Tl 1.80	Pb 1.80	Bi 1.90	Po 2.00	At 2.20	Rn
Fr 0.70	Ra 0.90																	
		La 1.10	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.20	Gd 1.20	Tb 1.10	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.10	Lu 1.27		
		Ac 1.10	Th 1.30	Pa 1.50	U 1.70	Np 1.30	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.30	Cf 1.30	Es 1.30	Fm 1.30	Md 1.30	No 1.30	Lr 1.30		

Graf, Felser, Parkin, IEEE TRANSACTIONS ON MAGNETICS 47 (2011) 367

Graf, Felser, Parkin, Progress in Solid State Chemistry 39 (2011) 1



spin orbital coupling counts



XYZ Heusler compounds

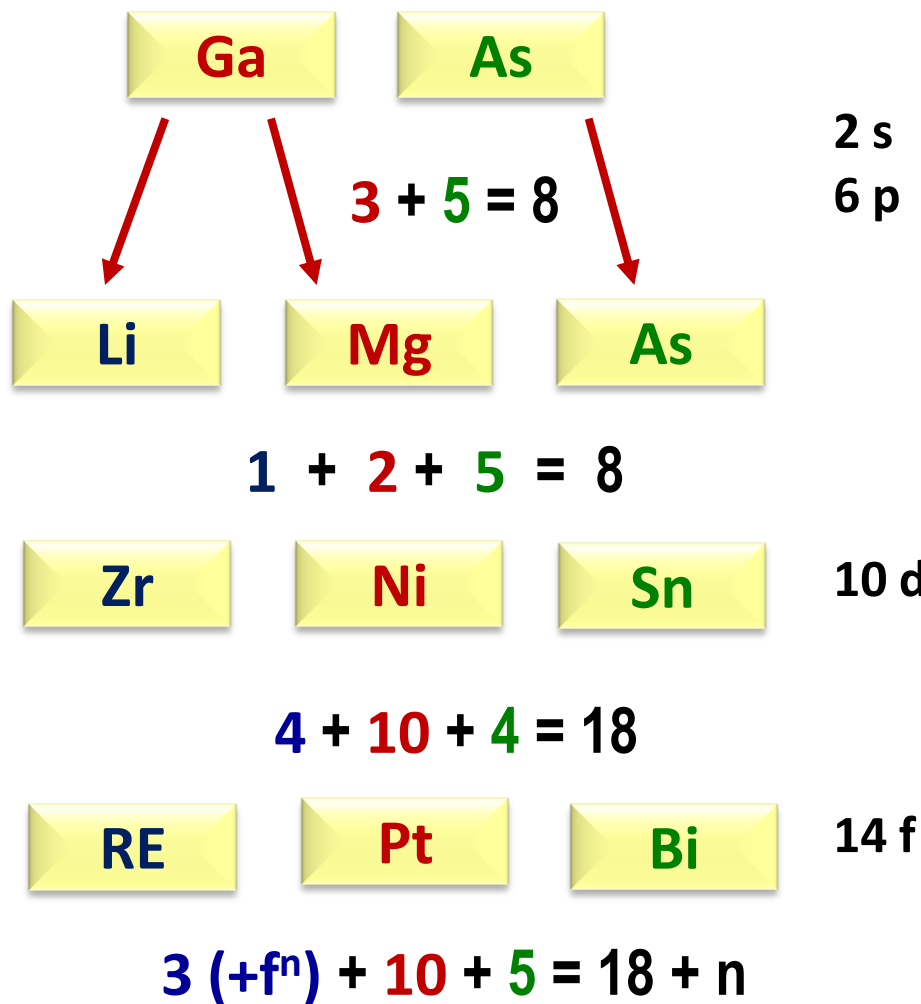
H 2.20																	He	
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne	
Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar	
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00	
Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.60	Mo 2.16	Tc 1.90	Ru 2.20	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.10	I 2.66	Xe 2.60	
Cs 0.79	Ba 0.89		Hf 1.30	Ta 1.50	W 1.70	Re 1.90	Os 2.20	Ir 2.20	Pt 2.20	Au 2.40	Hg 1.90	Tl 1.80	Pb 1.80	Bi 1.90	Po 2.00	At 2.20	Rn	
Fr 0.70	Ra 0.90																	
		La 1.10	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.20	Gd 1.20	Tb 1.10	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.10	Lu 1.27		
		Ac 1.10	Th 1.30	Pa 1.50	U 1.70	Np 1.30	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.30	Cf 1.30	Es 1.30	Fm 1.30	Md 1.30	No 1.30	Lr 1.30		

$$\lambda_{\text{SOC}} \sim Z^2 \text{ for valence shells}$$

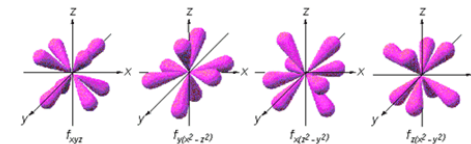
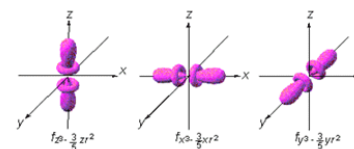
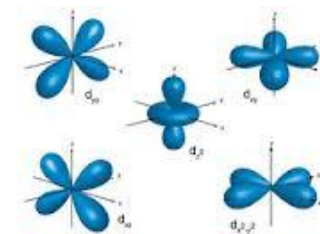
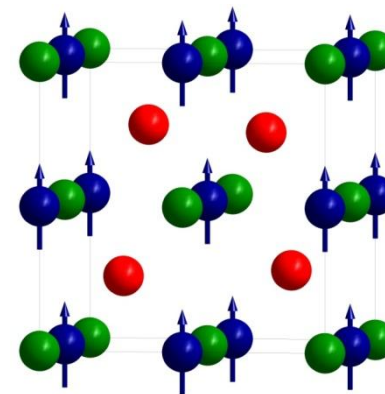


Counting Electrons

From wide to low band gap semiconductor

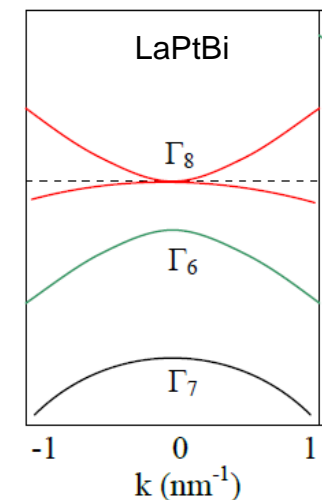
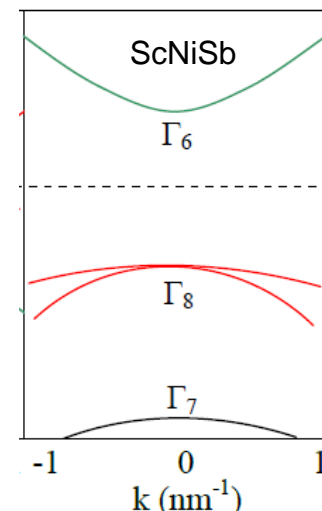
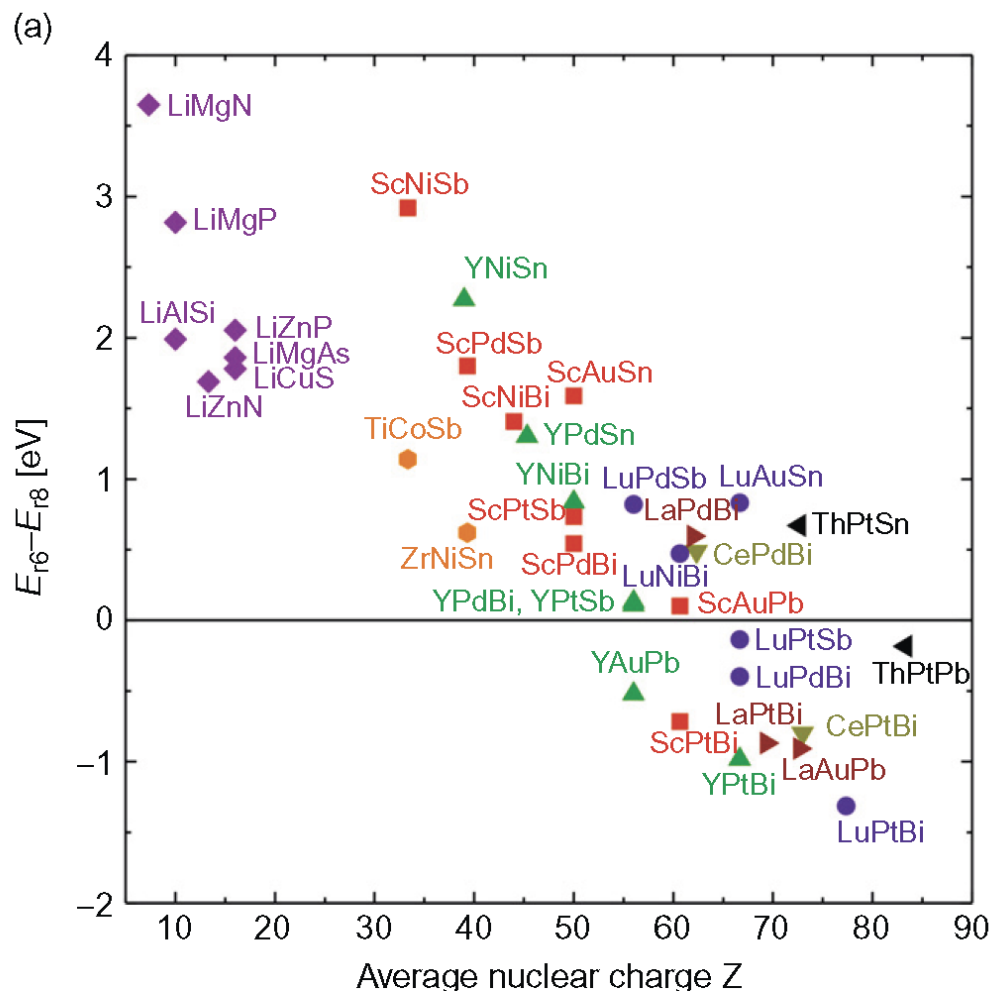
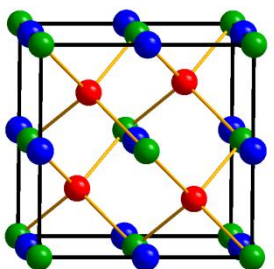
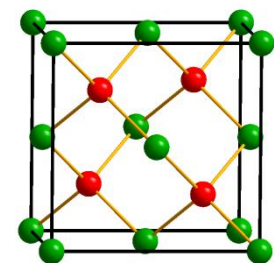


2 s
6 p





Predicting new Compounds



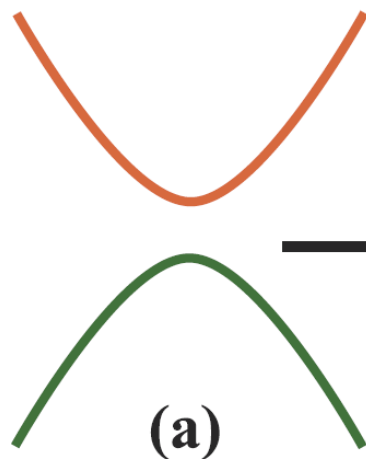
Graf, Felser, Parkin, Progress in Solid State Chemistry (2011)

Chadov, Qi, Kübler, Zhang, Felser Nature Mat. 9 (2010) 541, arXiv:1003.0193

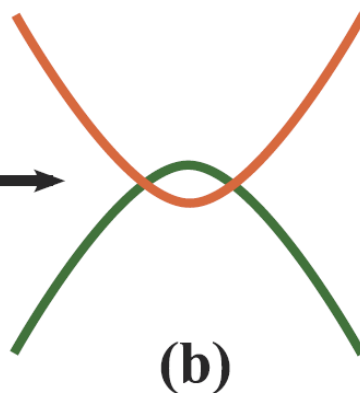


Trivial and topological insulators

Trivial semiconductor
CdS

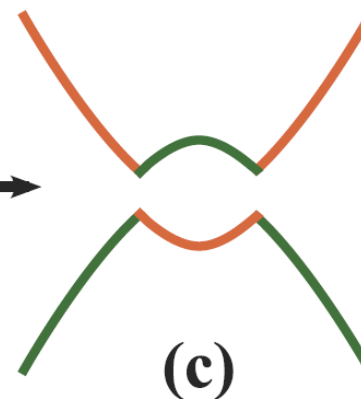


Topological Insulator
Without spin orbit coupling



SOC

Topological Insulator
With spin orbit coupling

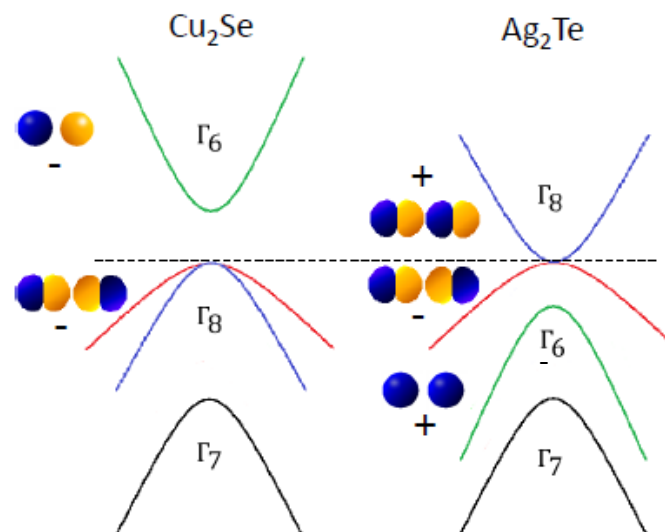


Sufficient condition:

Parity change

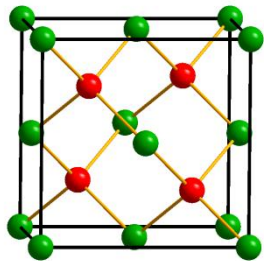
Centro symmetric \rightarrow Eigenvalues

Noncentro sym. \rightarrow Z2 classification



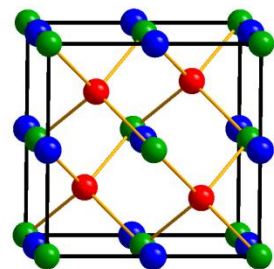


Structure to Property



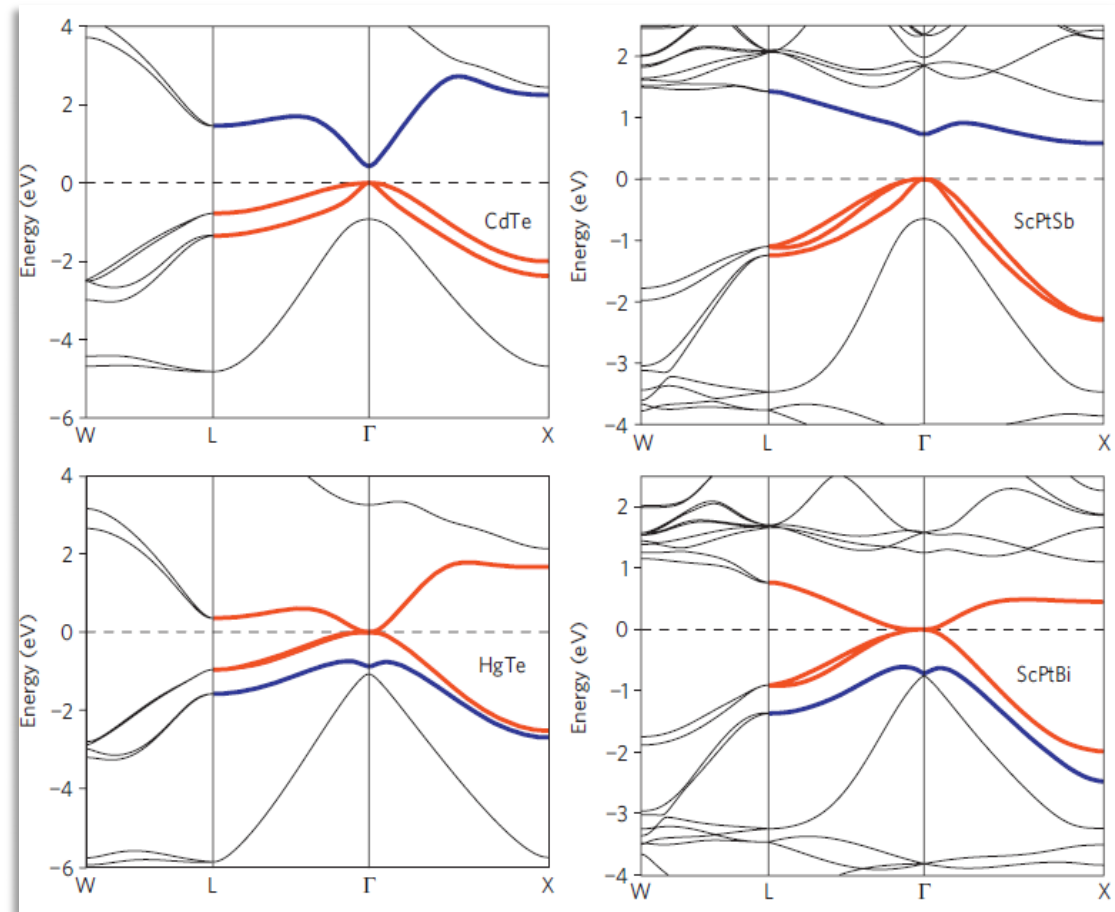
CdTe

HgTe



ScPtSb

ScPtBi





Multifunctional topologic insulators

Magnetism and heavy fermion-like behavior in the RBiPt series

P. C. Canfield, J. D. Thompson, W. P. Beyermann, A. Lacerda, M. F. Hundley,
E. Peterson, and Z. Fisk
Los Alamos National Laboratory, Los Alamos, New Mexico 87545

H. R. Ott
ETH, Zurich, Switzerland

J. Appl. Phys. **70** (10), 15 November 1991

Multifunctional properties

- RE: Gd Magnetism and TI
 - Antiferromagnetism with GdPtBi
- RE: Ce
 - complex behaviour of the Fermi surface
- RE: Yb Kondo insulator and TI
 - YbPtBi is a super heavy fermion with the highest γ value



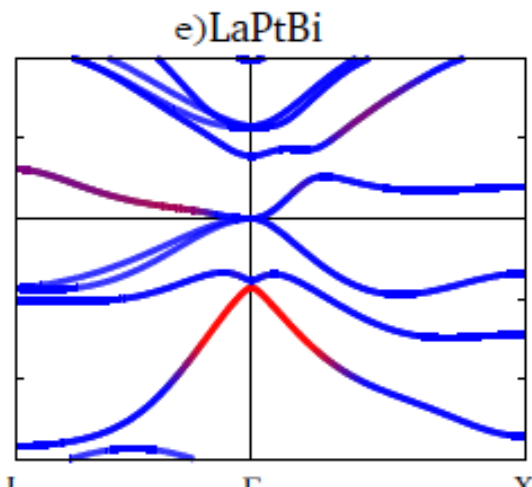
$$10 + 3 (+f^n) + 5 = 18$$



Non centro symmetric Superconductor

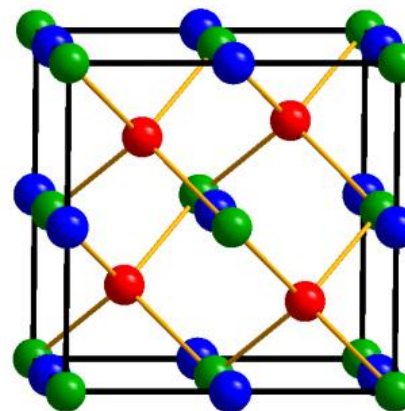
Multifunctional properties

- RE: La Superconductivity and TI
 - LaPtBi is superconductor
 - p-type semiconductors
 - with a band inversion
 - without inversion symmetry and
 - low charge carrier concentration $n = 6 \cdot 10^{18} \text{cm}^{-3}$



$$10 + 3 (+f^n) + 5 = 18$$

Goll *et al.* Physica B 403 1065 (2008)

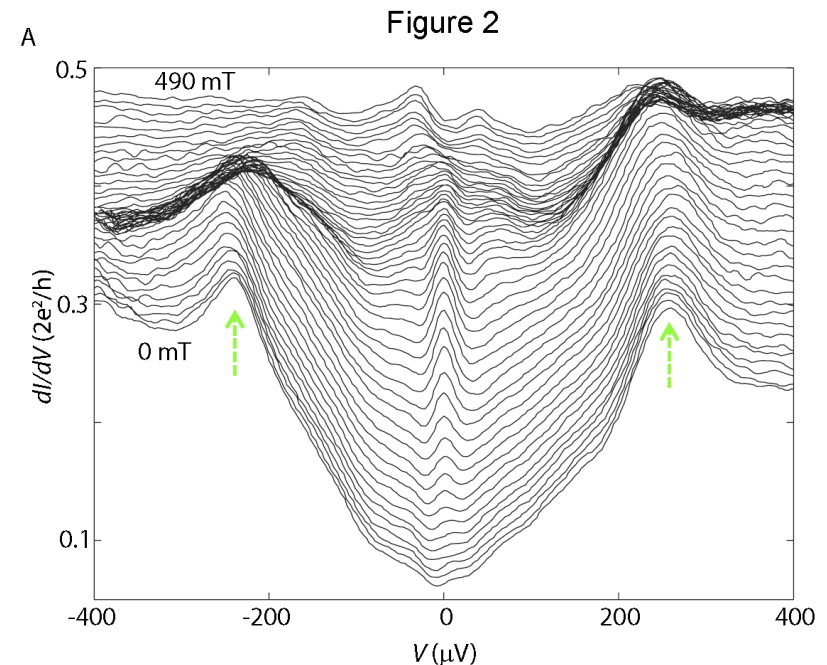
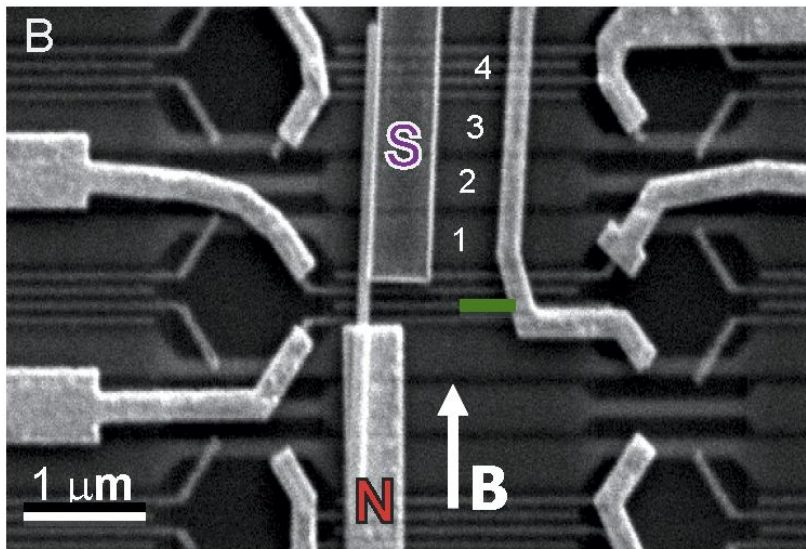




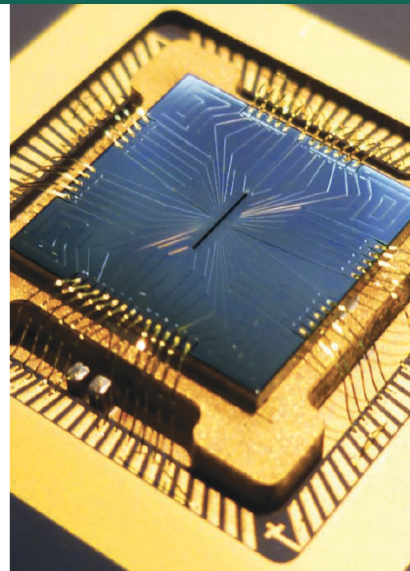
Hunting Majorana



Wikipedia: A Majorana fermion, also referred to as a Majorana particle, is a **fermion that is its own antiparticle**. They were hypothesised by Ettore Majorana in 1937. The term is sometimes used in opposition to a Dirac fermion, which describes fermions that are not their own antiparticles. No elementary fermions are known to be their own antiparticle, though the nature of the neutrino is not settled and it might be a Majorana fermion.



Mourik et al. Science 336 (2012) 1003



SPECIAL SECTION

INTRODUCTION

The Future of Quantum Information Processing

Topological phenomena

topological structure in the physical system, which are thus usually universal and robust against perturbations.

- flux quantization in superconductors
- Hall conductance quantization in the Quantum Hall states
- topological insulators and topological superconductors

Quantum entanglement

essential for quantum information and quantum computation

The understanding of quantum entanglement provides a *new probe to the physical properties of the many-body systems* compared to the conventional response properties such as conductivity, spin susceptibility, etc.

What is the relation between quantum entanglement and topological states of matter?

Xiaoliang Qi

Quantum Information Processing

CONTENTS

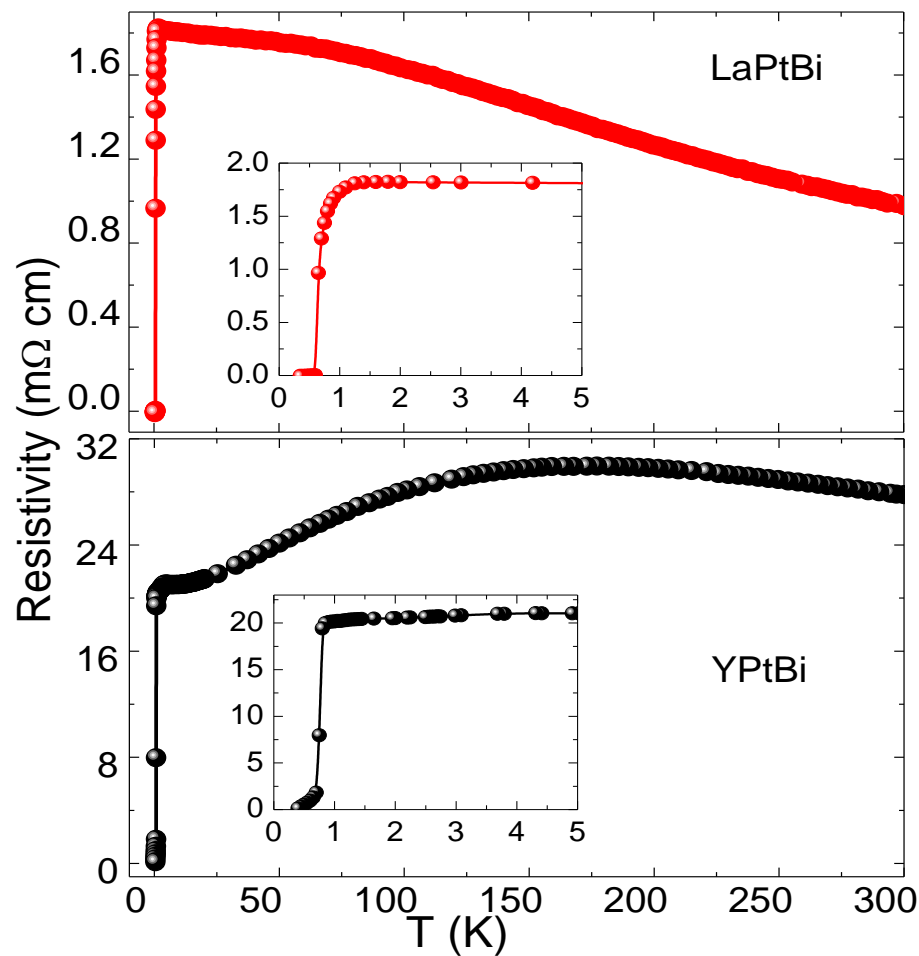
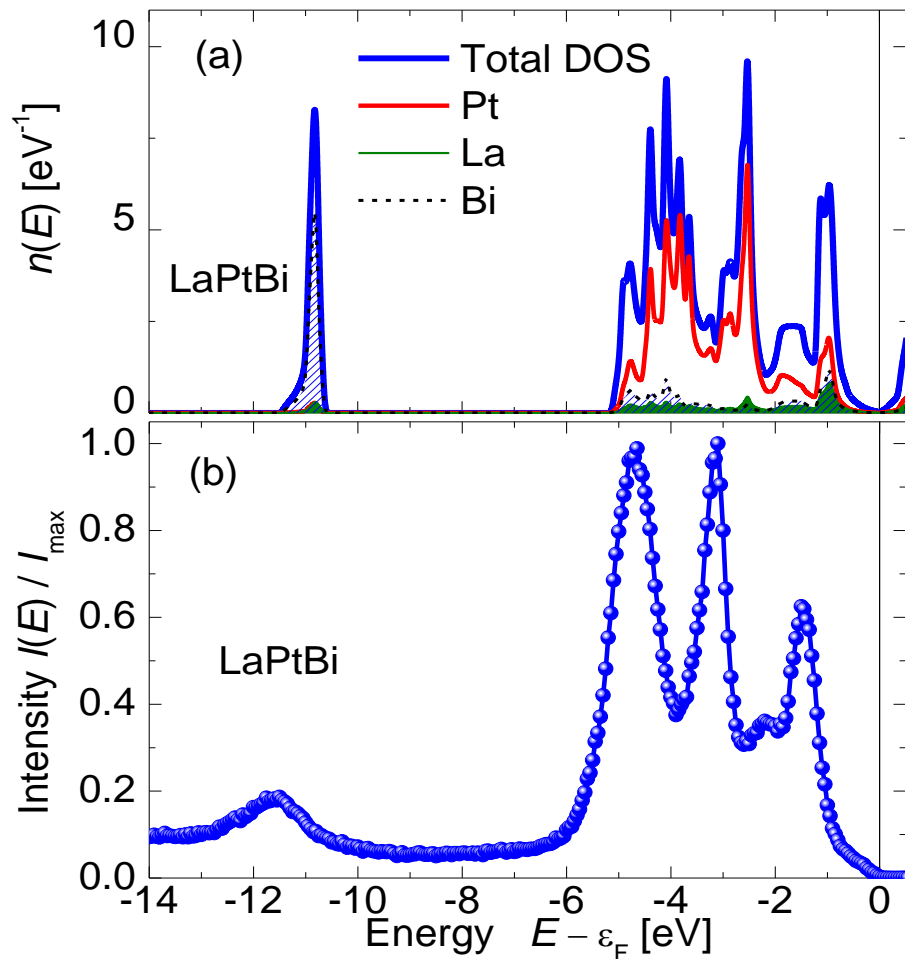
Reviews

- | | |
|------|--|
| 1164 | Scaling the Ion Trap Quantum Processor
<i>C. Monroe and J. Kim</i> |
| 1169 | Superconducting Circuits for Quantum Information: An Outlook
<i>M. H. Devoret and R. J. Schoelkopf</i> |
| 1174 | Quantum Spintronics: Engineering and Manipulating Atom-Like Spins in Semiconductors
<i>D. D. Awschalom et al.</i> |
| 1179 | Topological Quantum Computation—From Basic Concepts to First Experiments
<i>A. Stern and N. H. Lindner</i> |



Topological Insulator + Superconductor

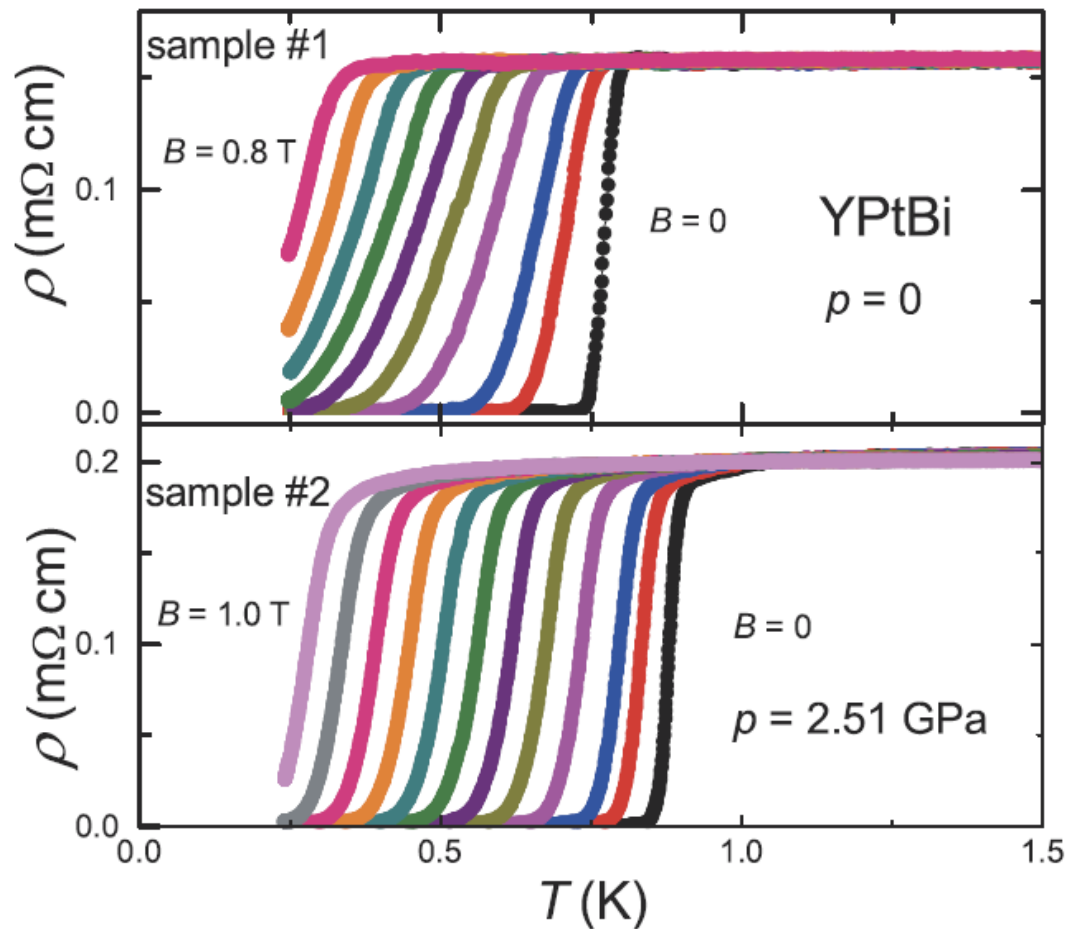
Hard X-ray Photoemission





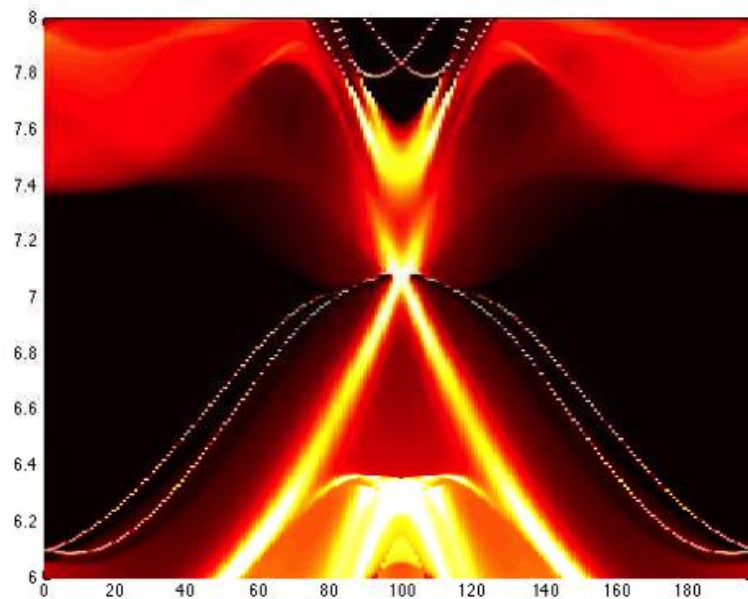
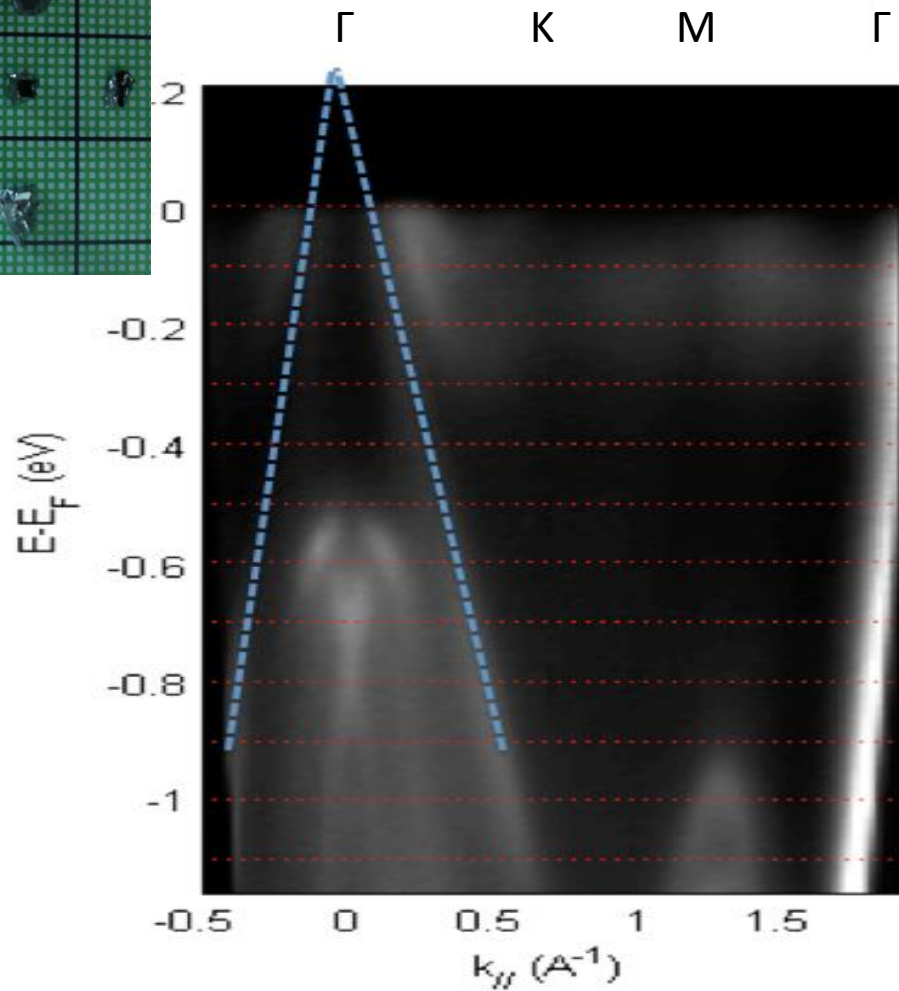
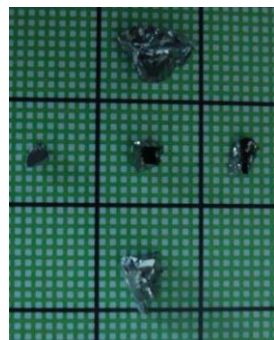
Superconductivity in noncentrosymmetric YPtBi under pressure

T. V. Bay,¹ T. Naka,² Y. K. Huang,¹ and A. de Visser^{1,*}



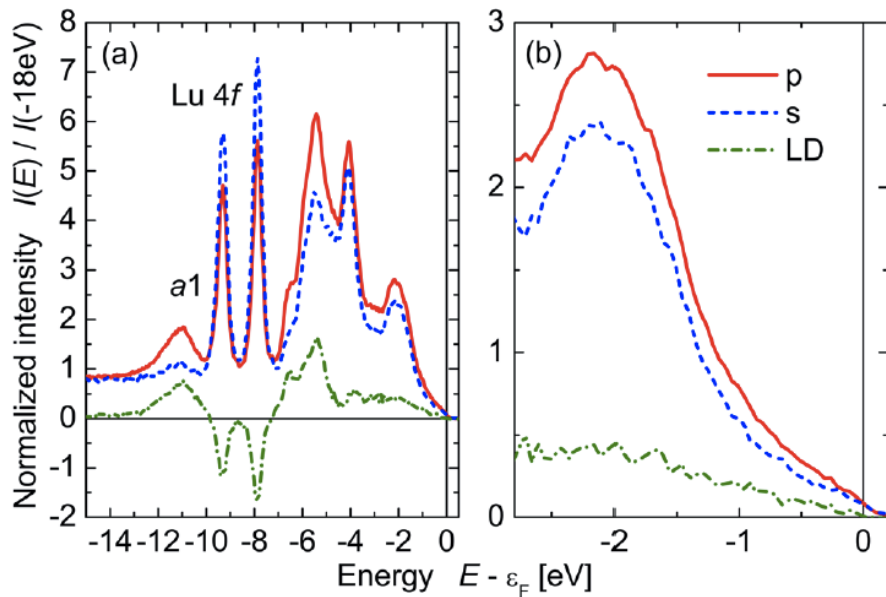


YPtBi ARPES and Theory

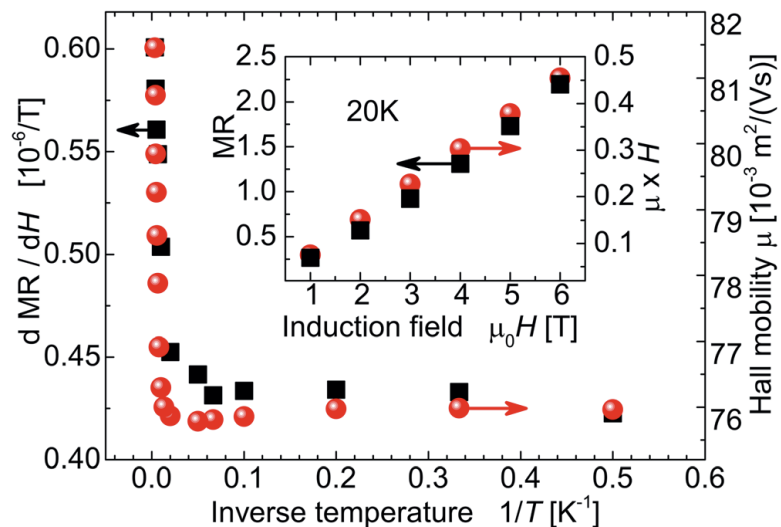
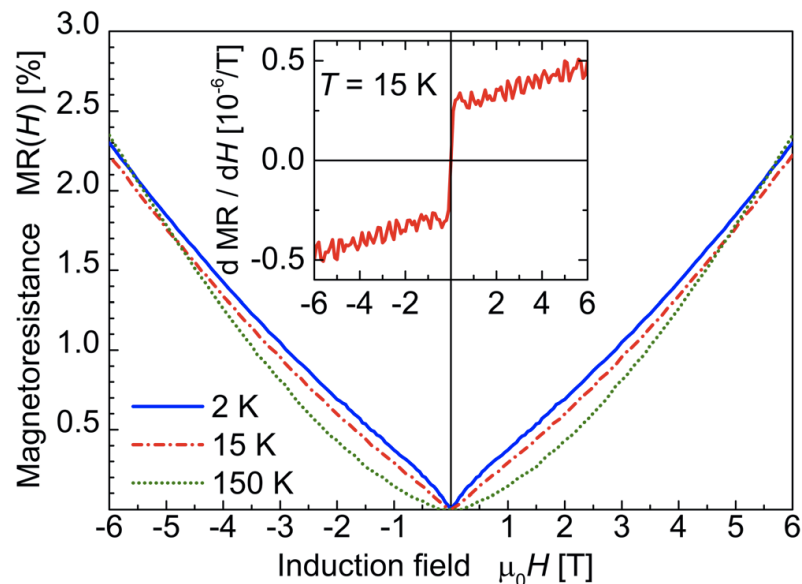




Zero band gap



Polarization dependent valence band spectra and linear MR of PtLuSb



Ouardi et. al. Appl. Phys. Lett. 99, 211904 (2011).

Ouardi et. al. Appl. Phys. Lett. 98, 211901 (2011).

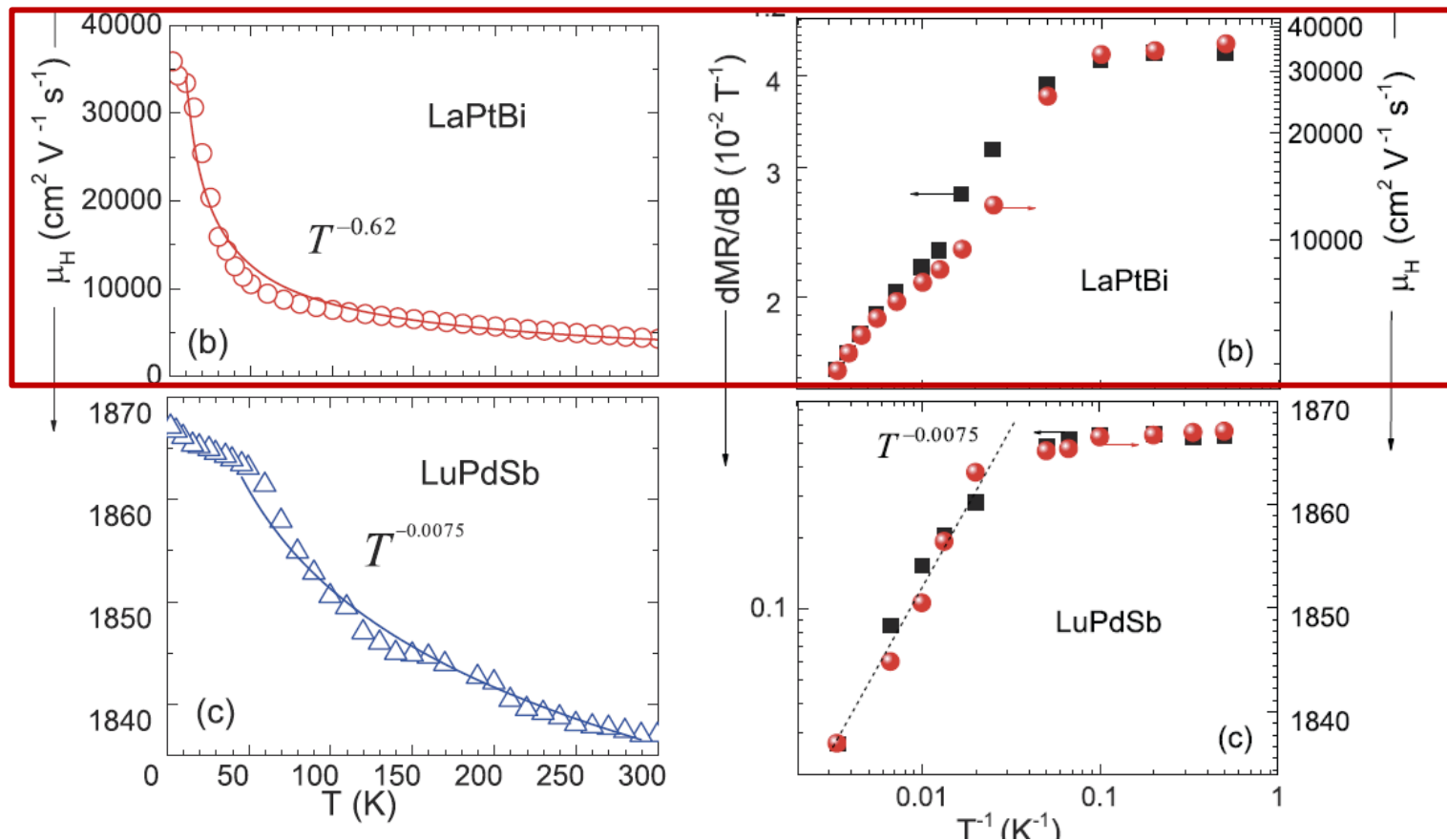
Shekhar, C. et. al. Appl. Phys. Lett. 100, 2152109 (2012).



Linear MR and ultrahigh mobility

Weak localisation

A close relation between the linear MR and the Hall mobility for this class of materials



Ouardi et. al. Appl. Phys. Lett. 99, 211904 (2011).

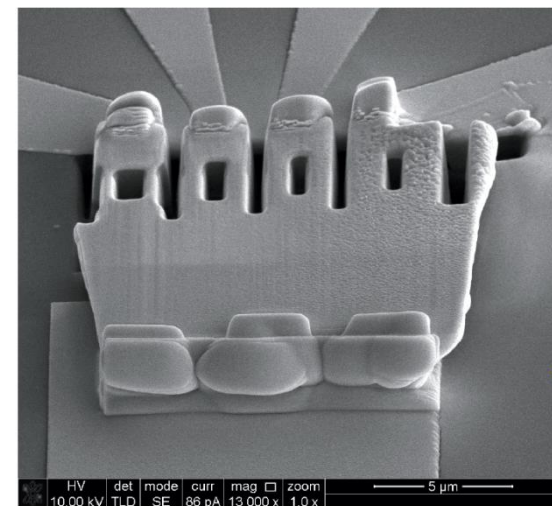
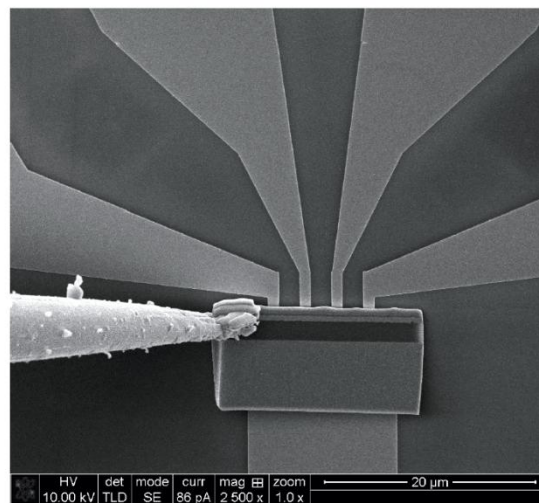
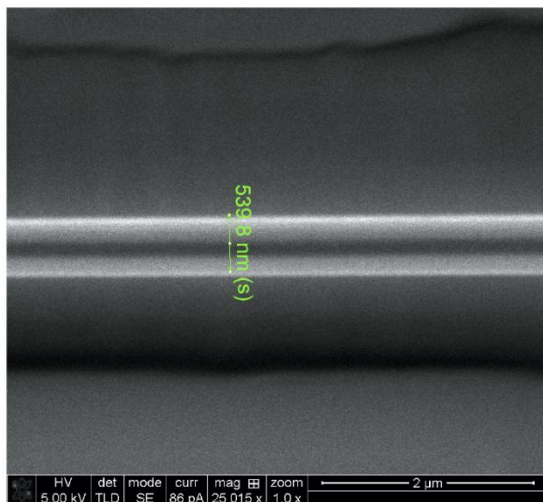
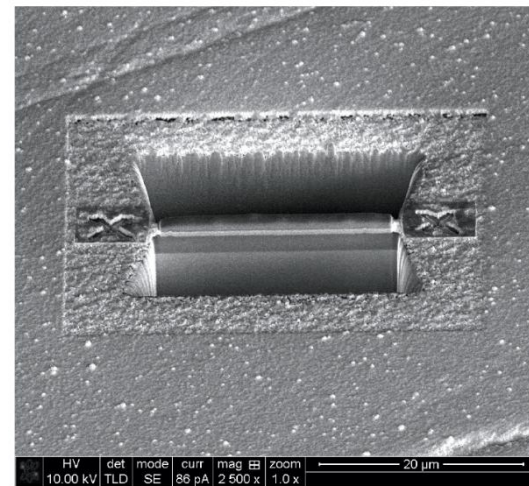
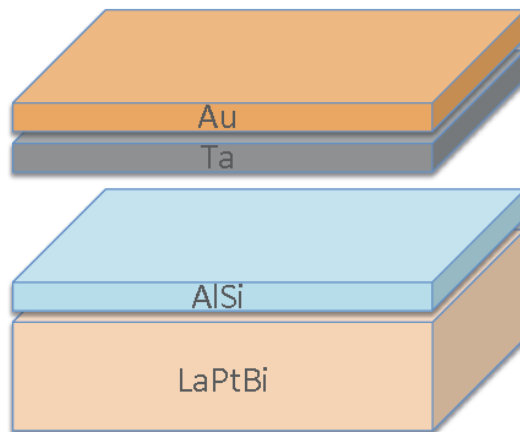
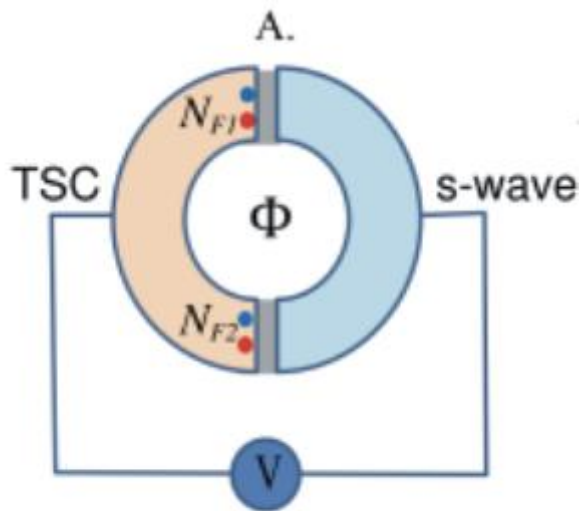
Ouardi et. al. Appl. Phys. Lett. 98, 211901 (2011).

Shekhar, C. et. al. Appl. Phys. Lett. 100, 2152109 (2012).

Shekhar et al. PRB 86, 155314 (2012)



Hunting Majorana



Ebke, Reiss, Wernsdorfer, Felser et al. unpublished

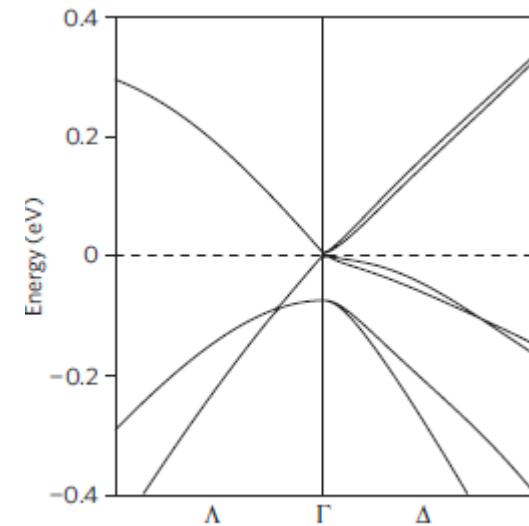
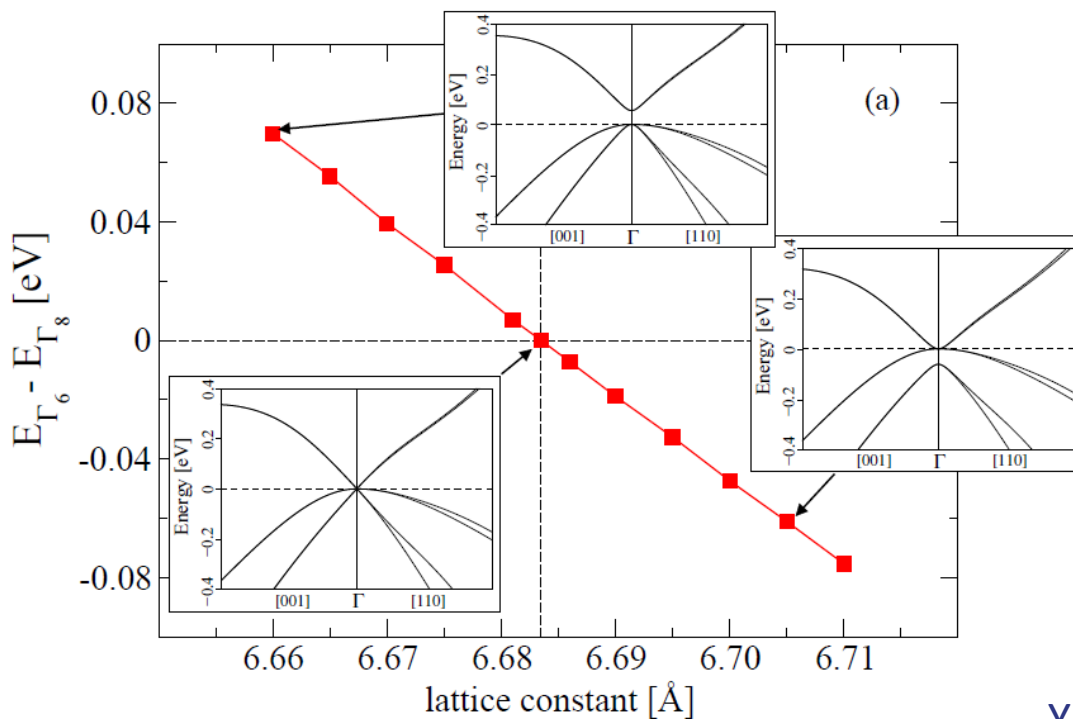
October, 13-17, 2013

Sino-German Workshop on Kondo and Mott



Quantum phase transition

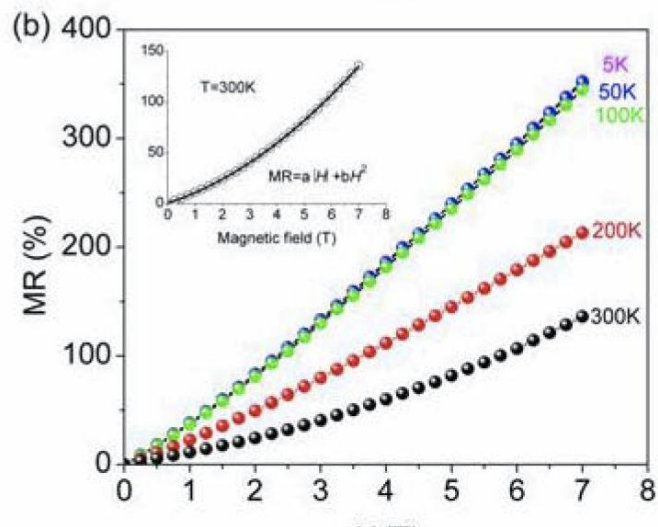
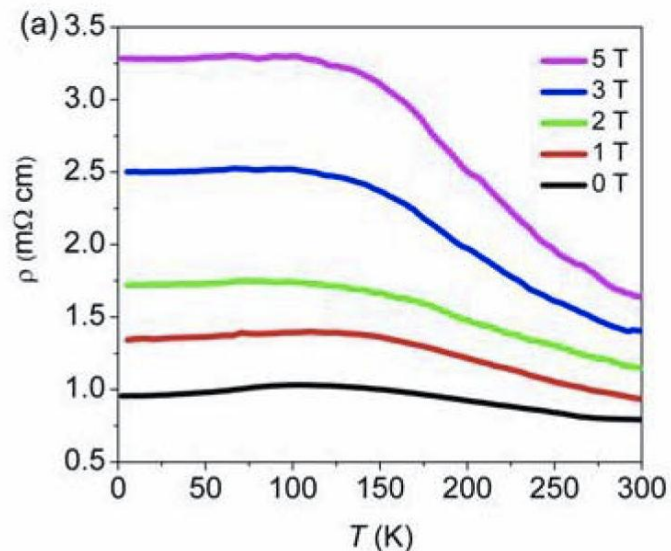
- Taking the borderline compound **YPtSb** at a quantum critical line/point
- Applying strain: A gap will be opened and the Dirac cone stays in the gap
- Critical thickness for the quantum well structure



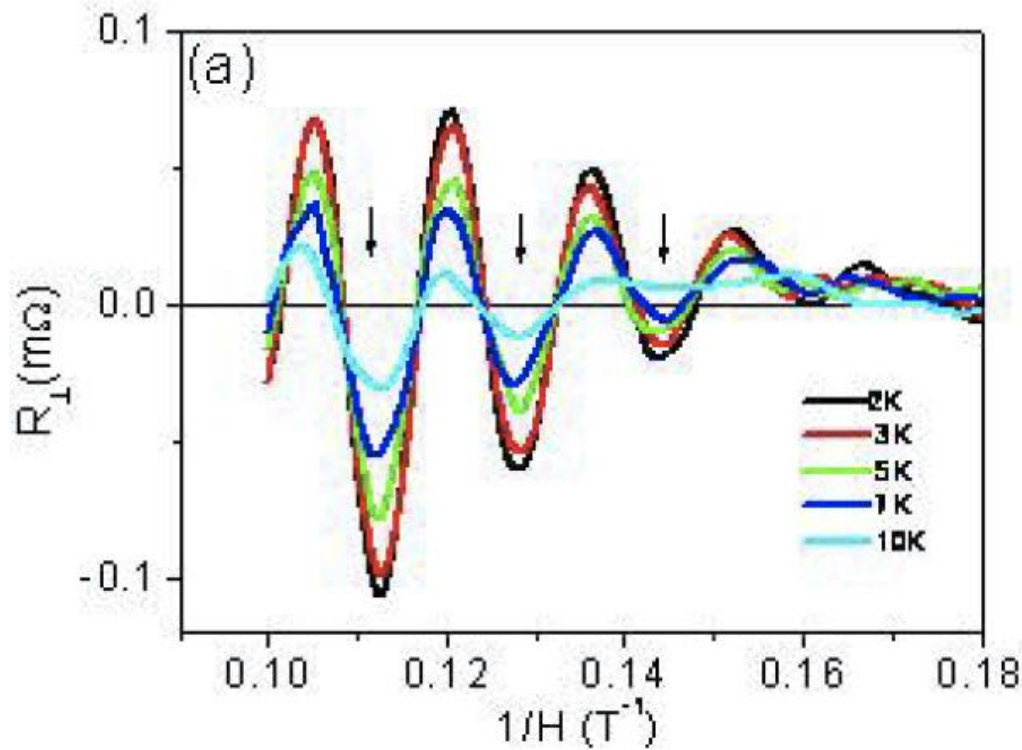
YPtSb is an excellent piezoelectric
arXiv:1107.5078 (Vanderbilt, Rabe)



Zero band gap

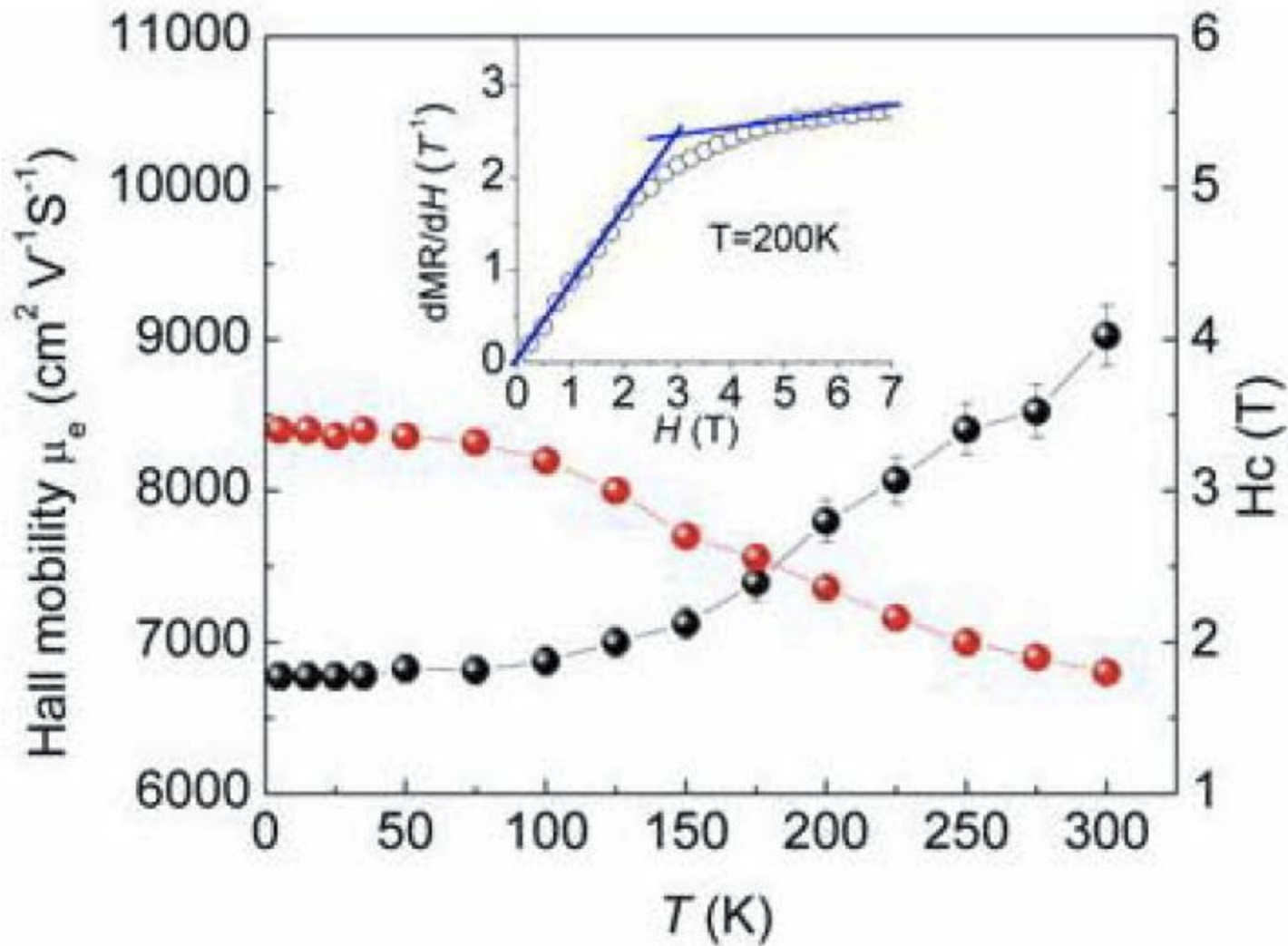


Large Linear Magnetoresistance and Shubnikov-de Hass Oscillations in Single Crystals of YPdBi Heusler Topological Insulators





Zero band gap

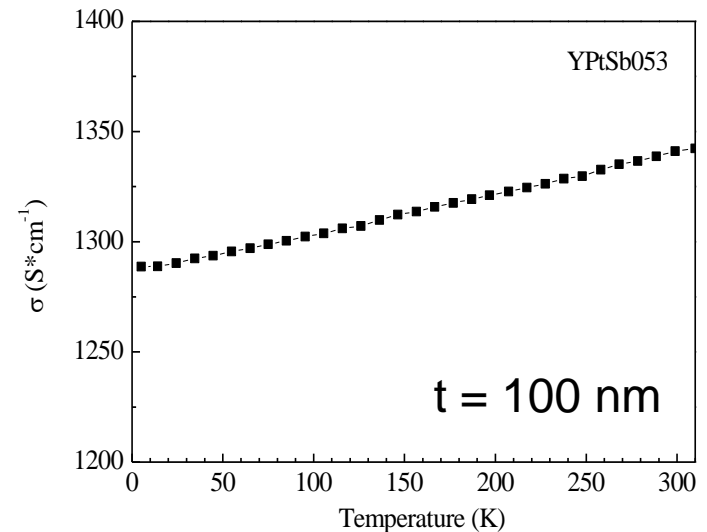
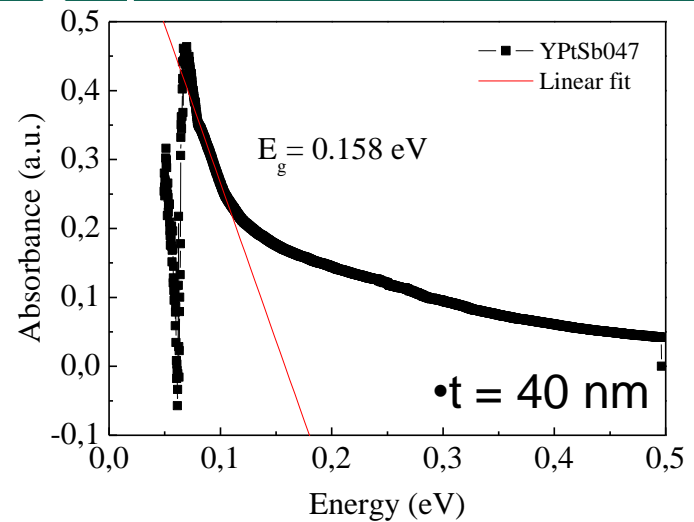




Small Bandgap in YPtSb

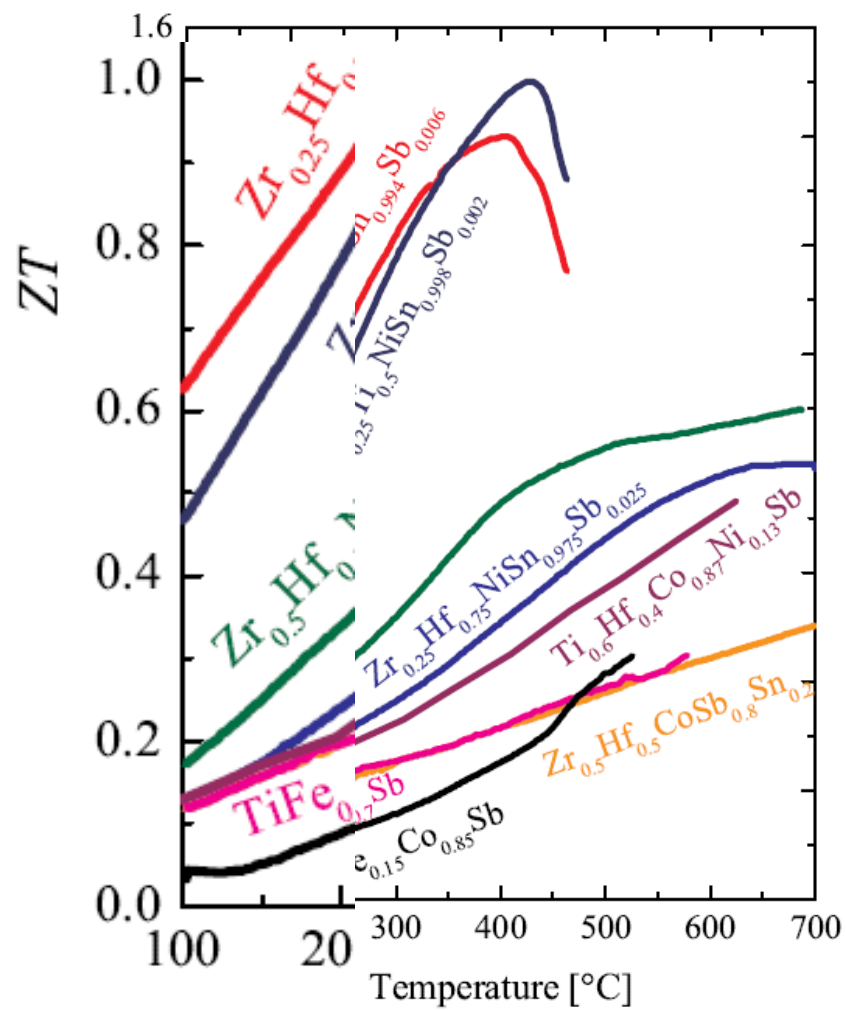
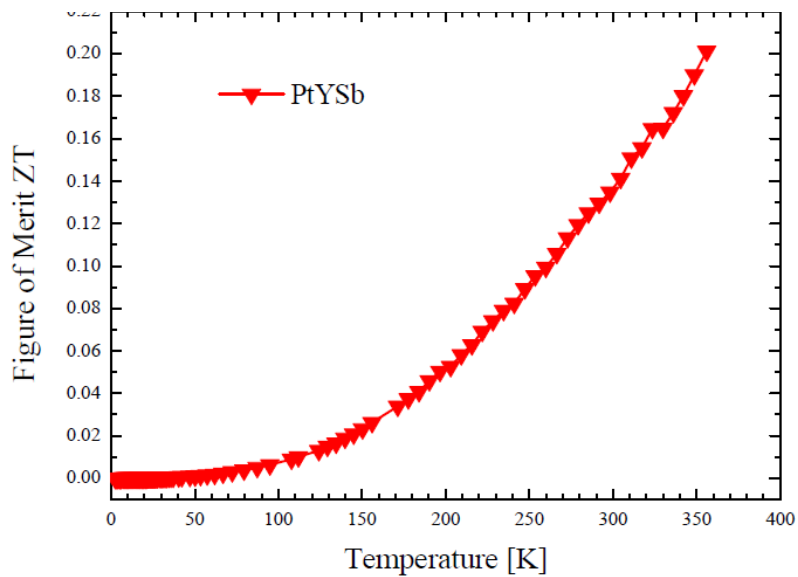
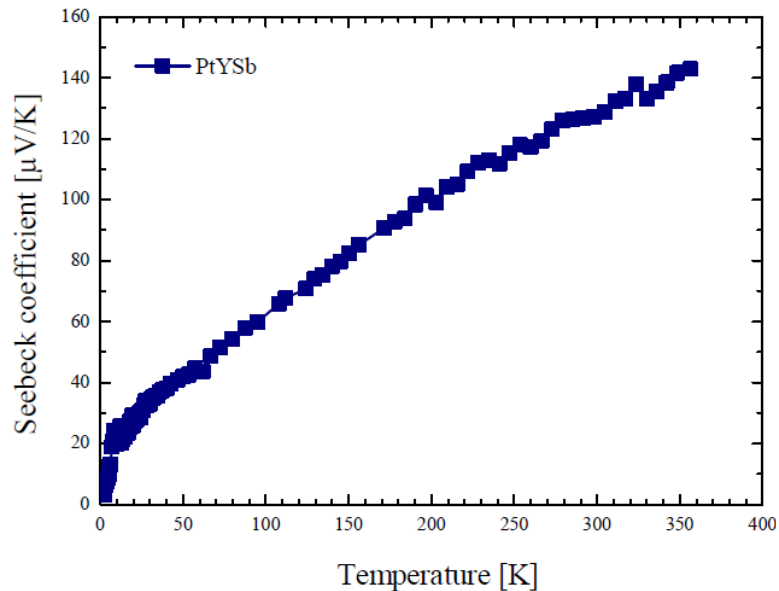
Infrared spectroscopy. band gap predicted theoretically and observed from bulk material (0.16 eV).

Temperature dependence of the conductance indicates a semiconducting behavior. Hall effect shows a carrier concentration is in the order of 10^{19} cm^{-3} and the mobility is around $380 \text{ cm}^2/\text{Vs}$.



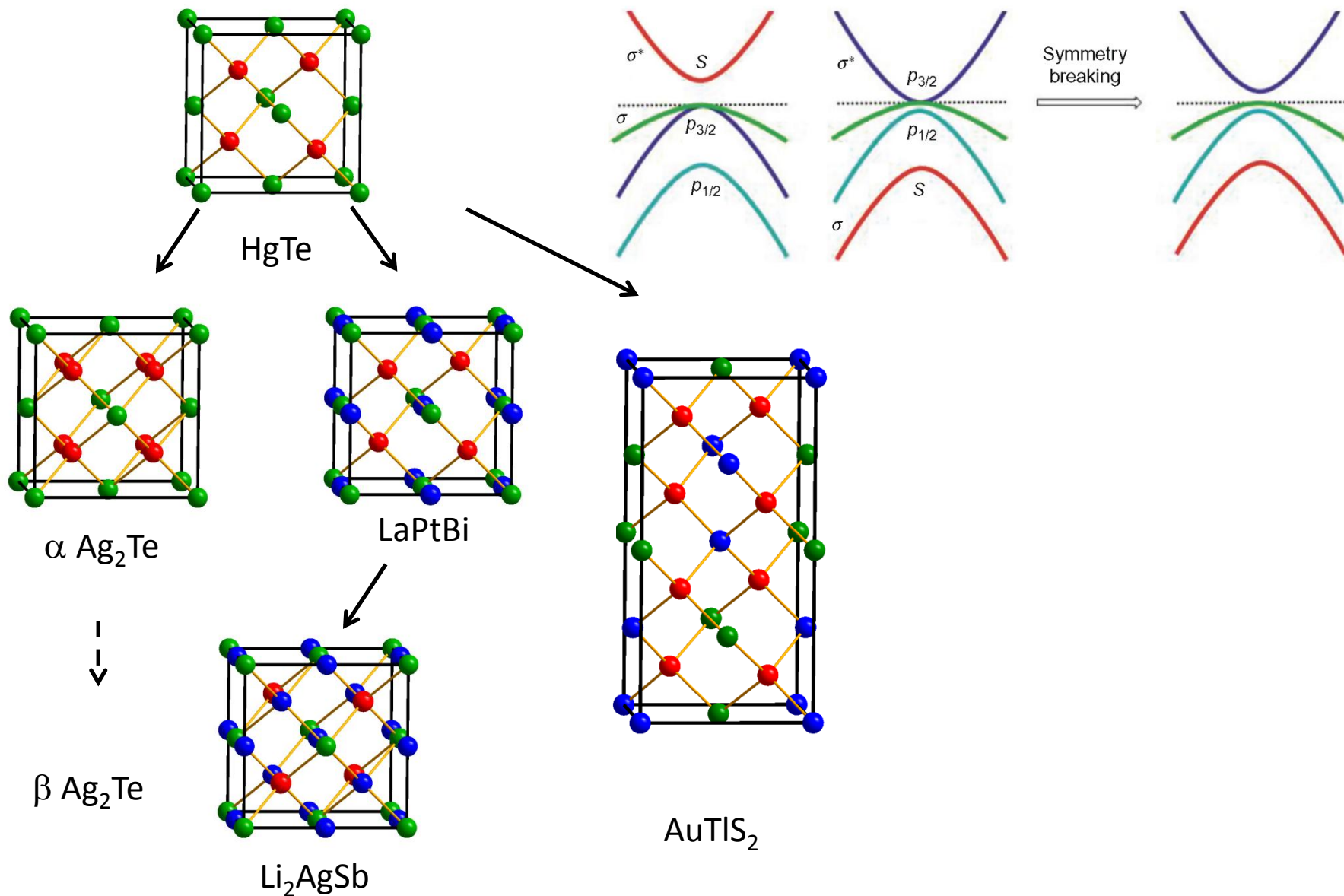


Good TI are good thermoelectrics





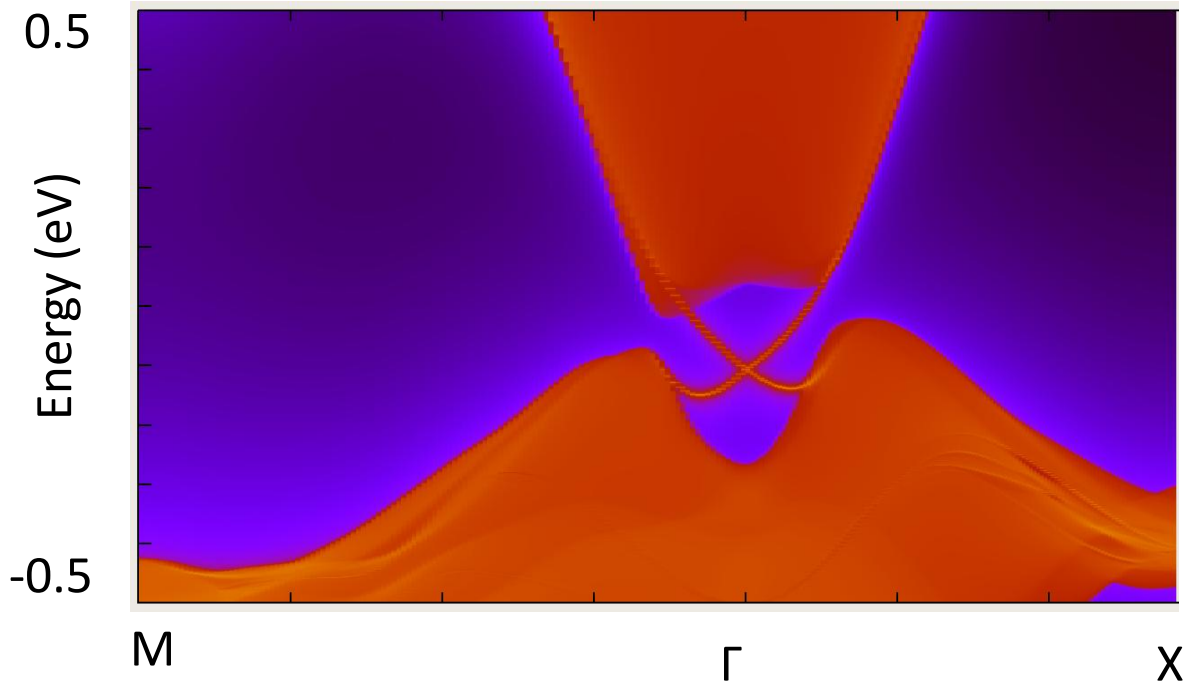
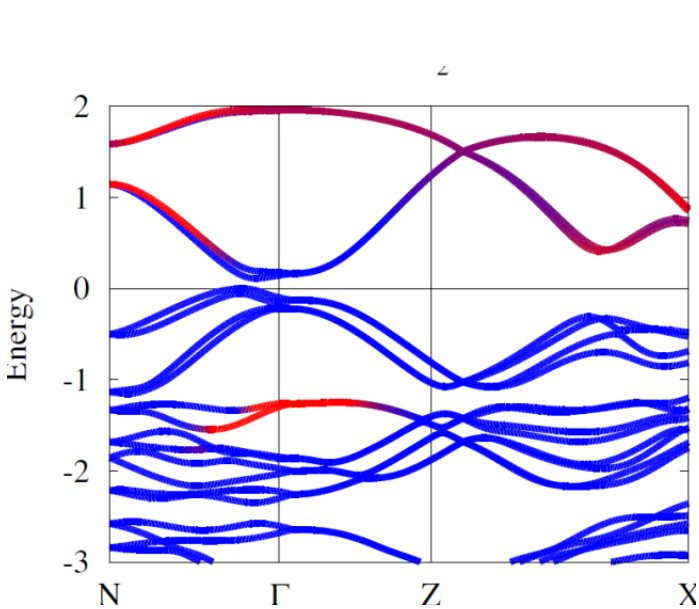
Distorted Structure to Property





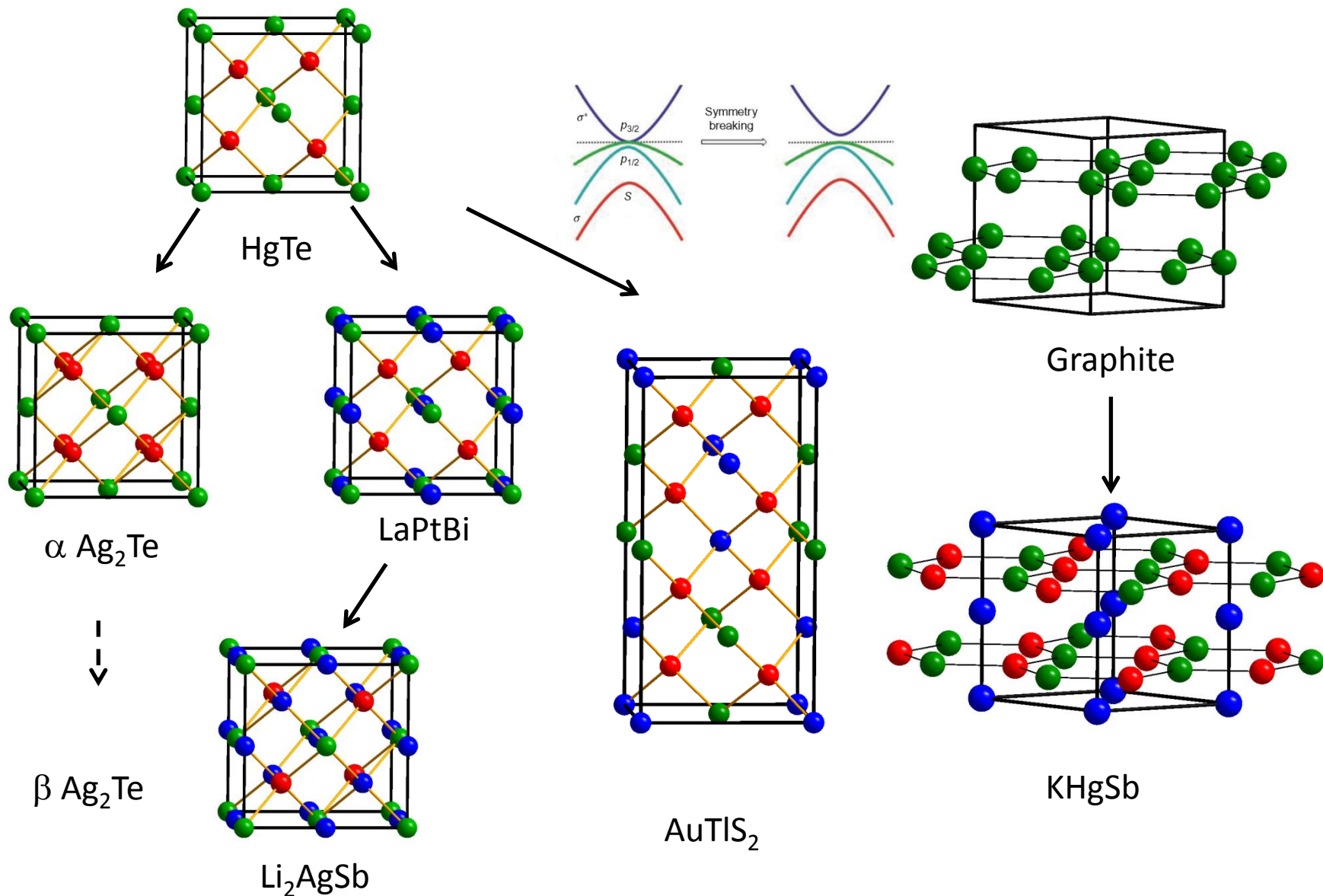
Surface states

AuTlS₂



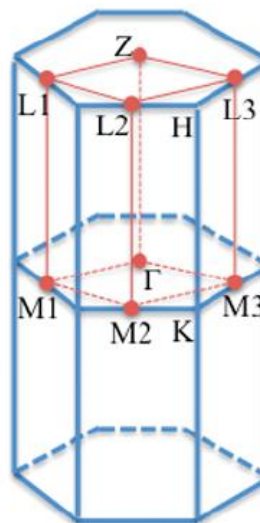
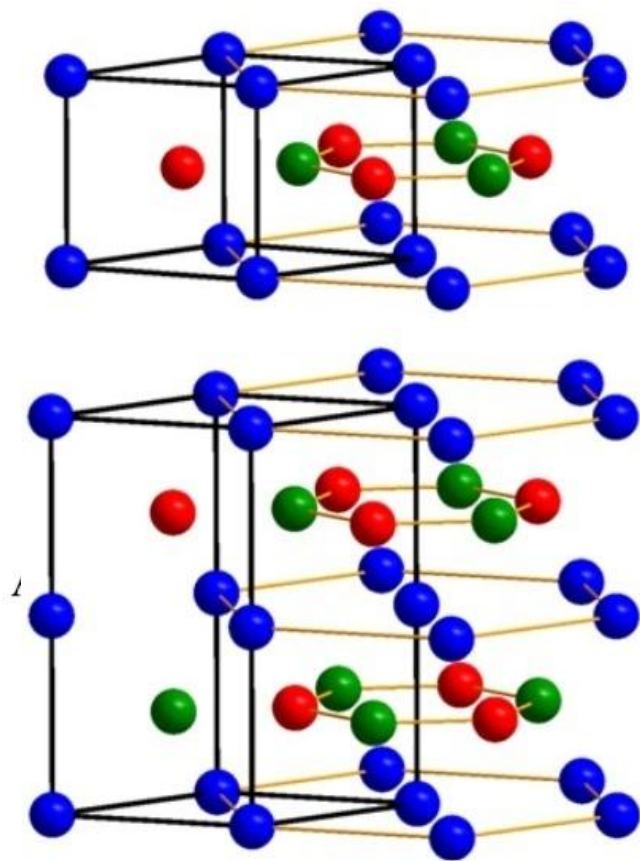


structure to property

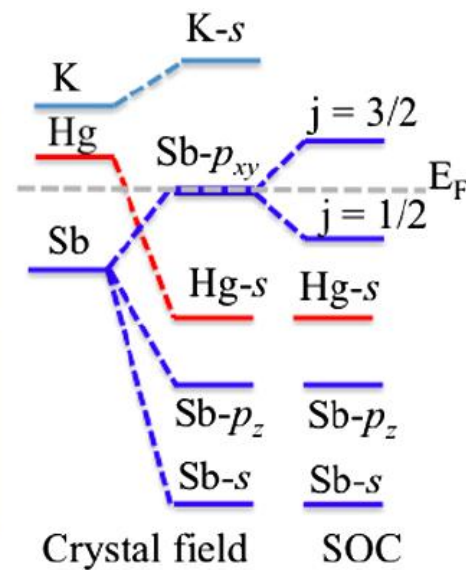




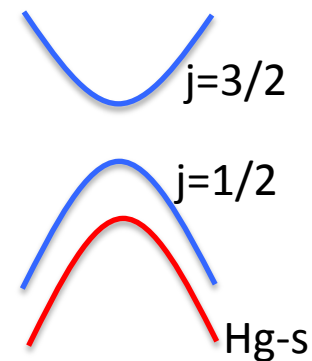
Honeycomb: Weak TI



(c)

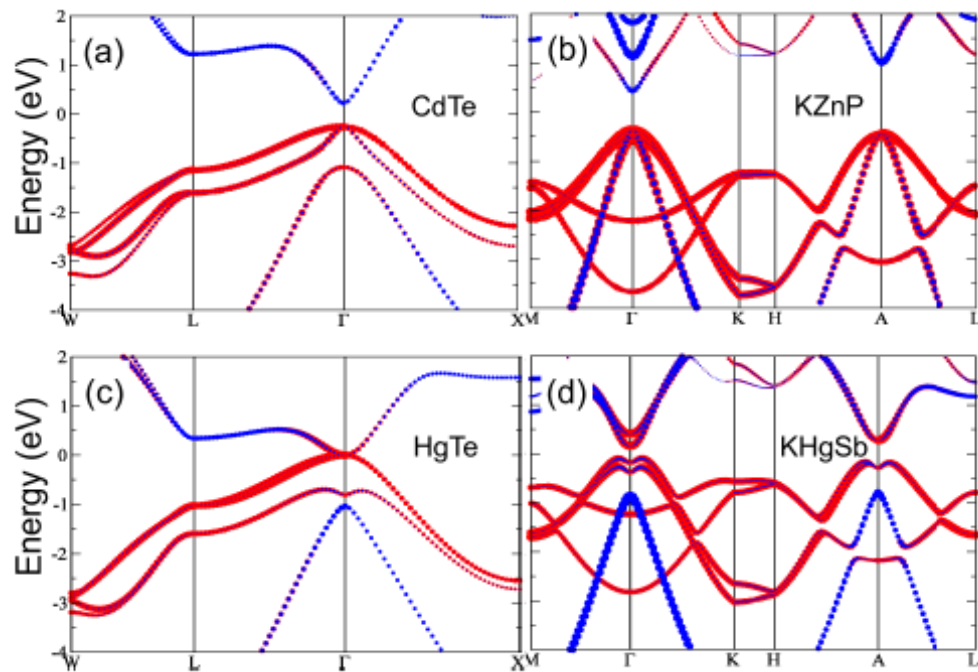
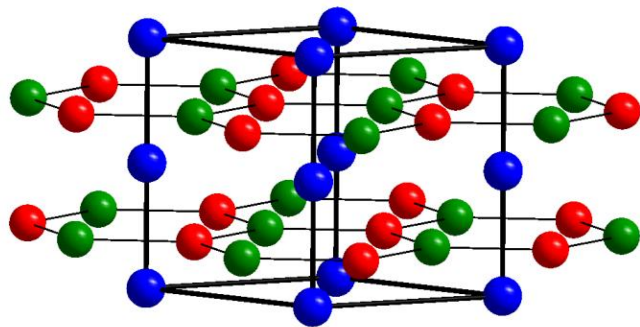


(d)





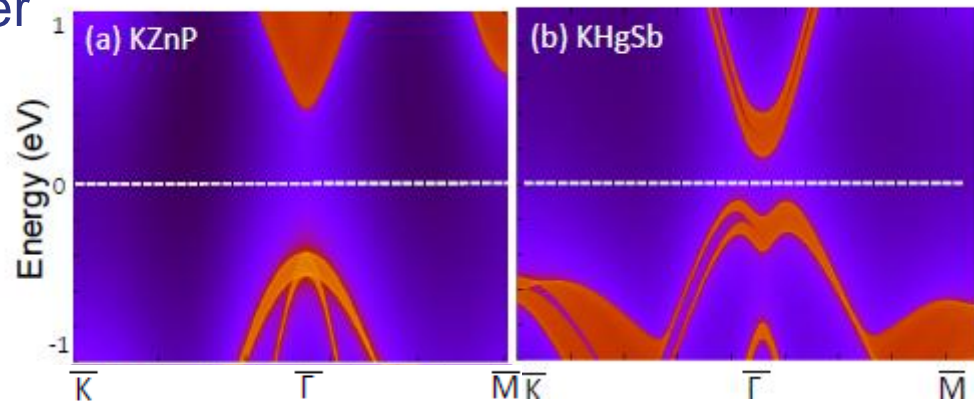
Honeycomb from sp^3 to sp^2



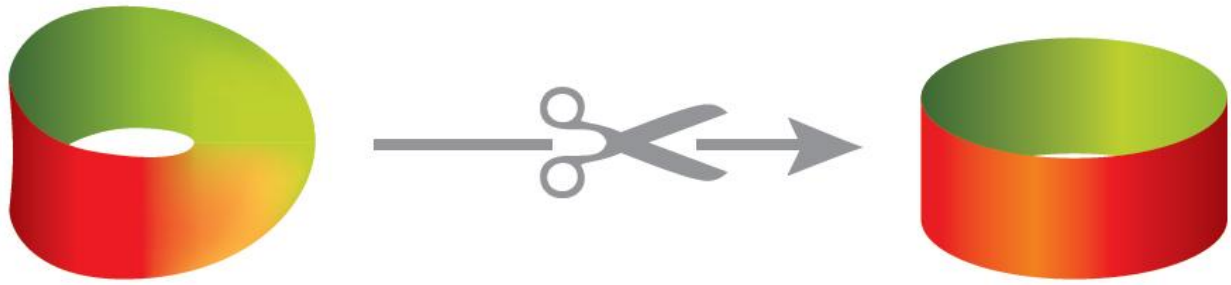
Band inversion is found in the heavier compounds

No surface state? Why ?

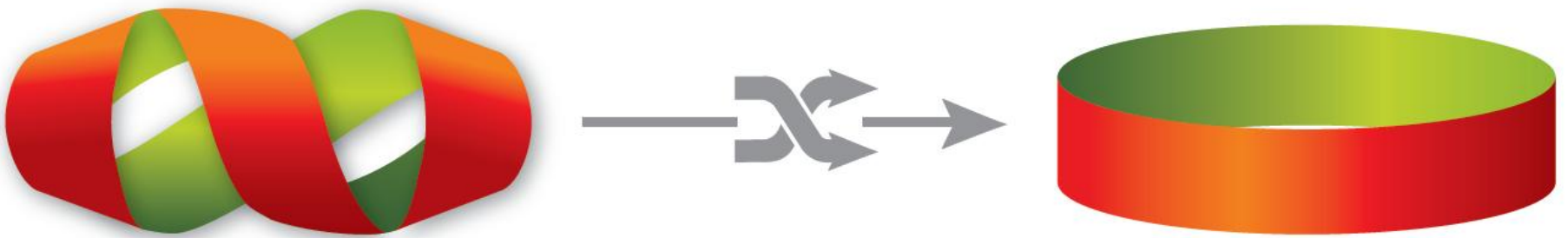
➔ Interaction between the two layers in the unit cell and two Dirac Cones



a)

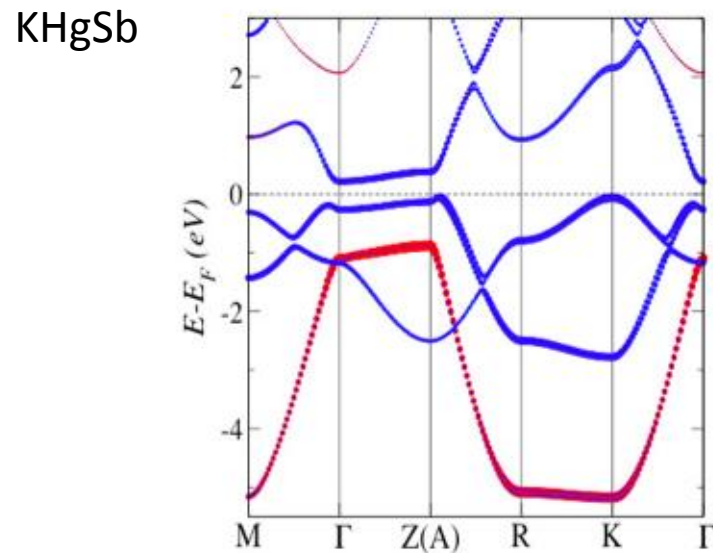
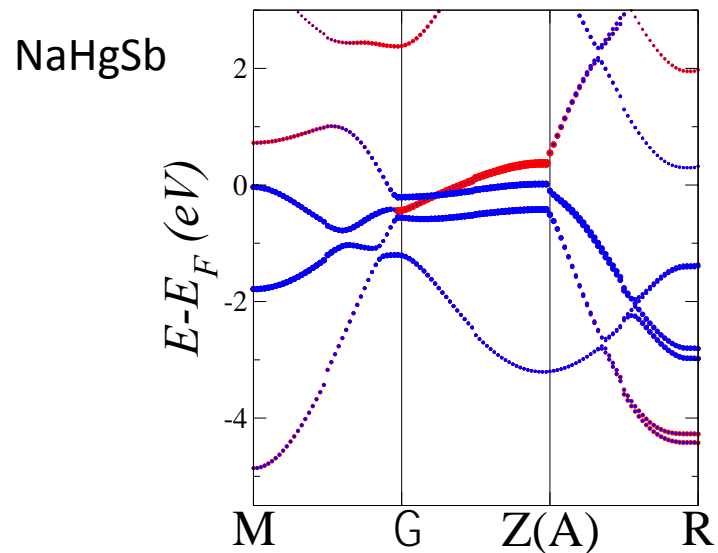
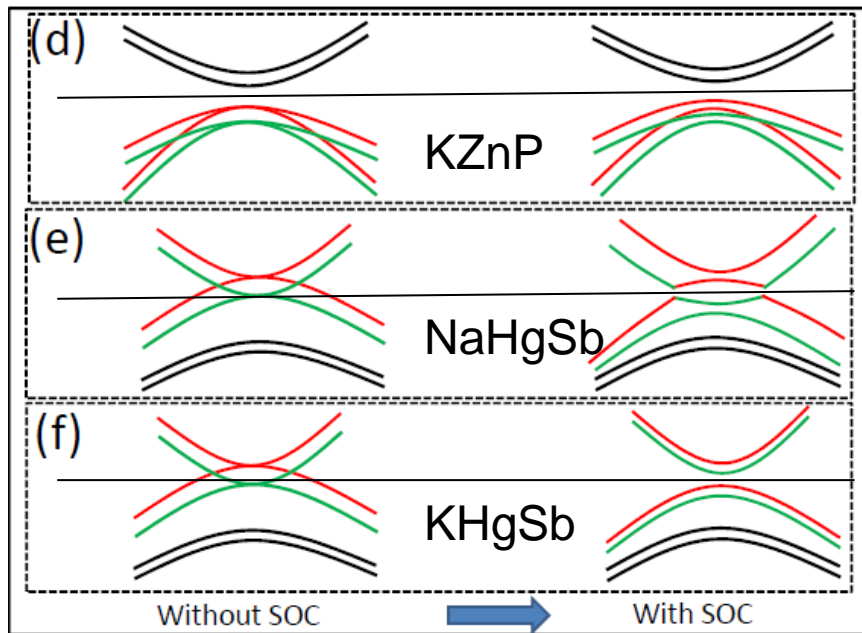


b)



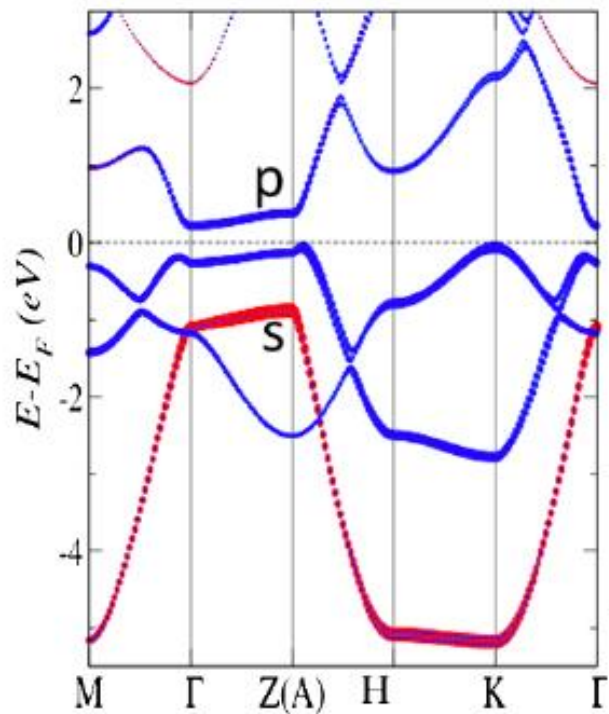


Honeycomb from sp^3 to sp^2

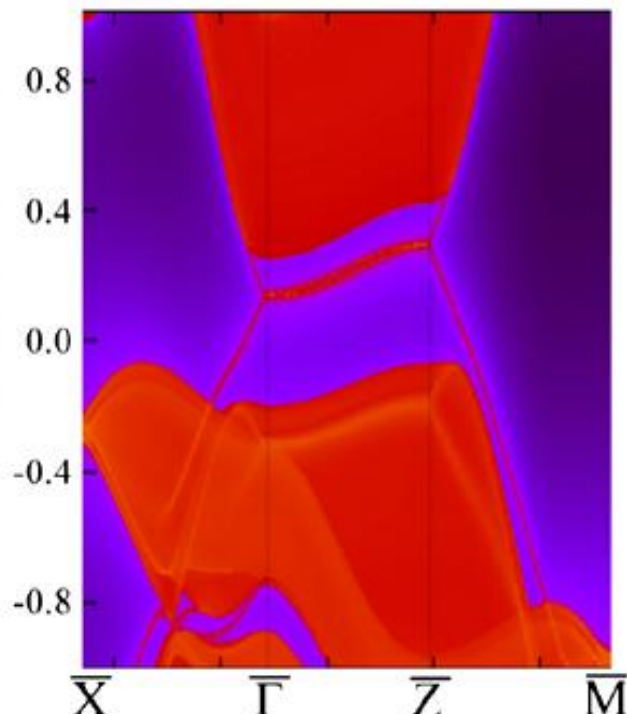




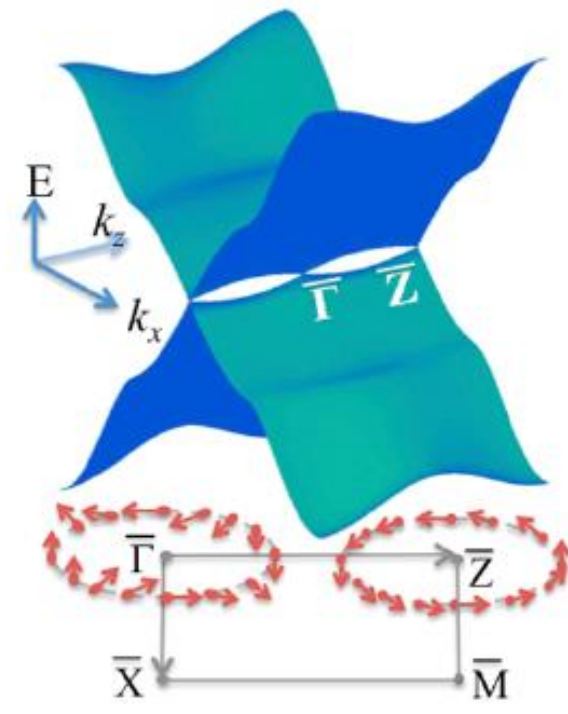
Honeycomb: weak TI



(a) Bulk



(b) Side surface



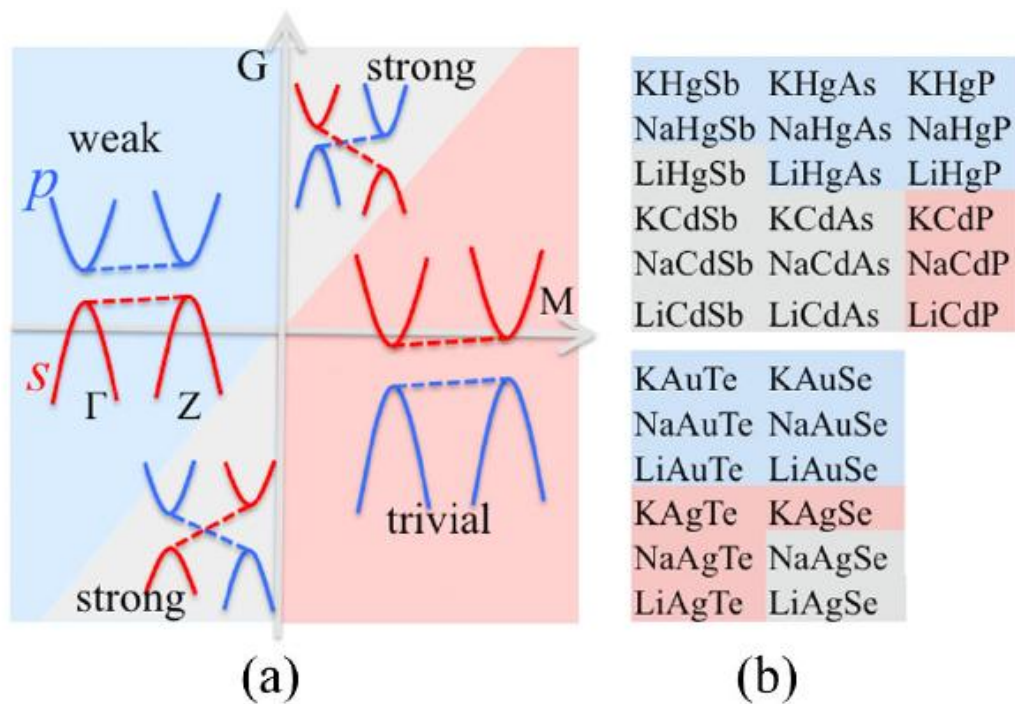
(c) Side surface



a large family of weak and strong TIs

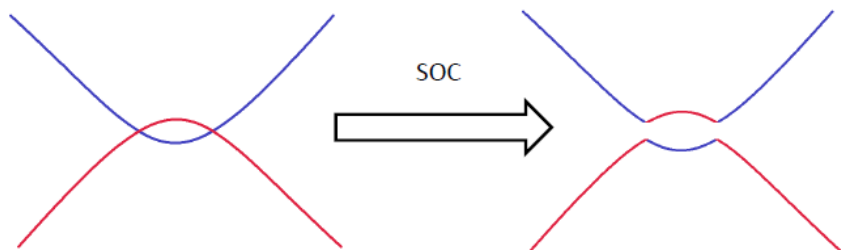
BHZ model, minimal Hamiltonian

$$H(k) = \epsilon(k)\mathbb{1}_{4 \times 4} + \begin{pmatrix} M(k) & Ak_+ & & \\ Ak_- & -M(k) & & \\ & & M(k) & -Ak_- \\ & & -Ak_+ & -M(k) \end{pmatrix} \quad M(k) = M_0 - B k_{//}^2 - G k_z^2$$



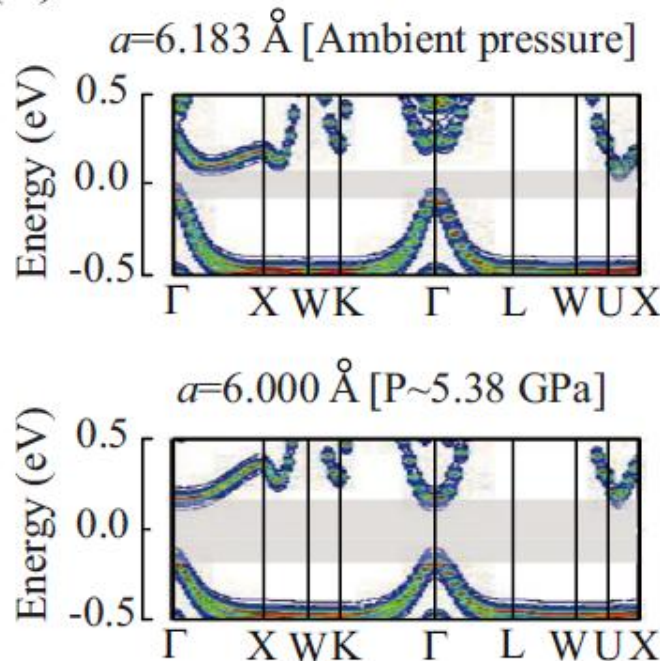
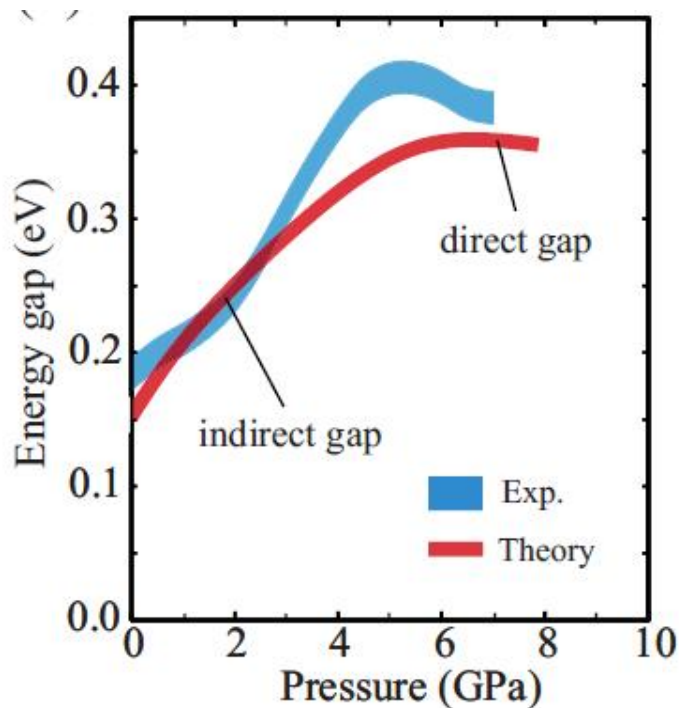


Pu with the largest SOC



XYZ Heusler compounds

H																	He
Li	Be											B	C	N	O	F	Ne
0.98	1.57											2.04	2.55	3.04	3.44	3.98	
Na	Mg											Al	Si	P	S	Cl	Ar
0.93	1.31											1.61	1.90	2.19	2.58	3.16	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.82	1.00	1.36	1.54	1.63	1.66	1.55	1.83	1.88	1.91	1.90	1.65	1.81	2.01	2.18	2.55	2.96	3.00
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.82	0.95	1.22	1.33	1.60	2.16	1.90	2.20	2.28	2.20	1.93	1.69	1.78	1.96	2.05	2.10	2.66	2.60
Cs	Ba	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
0.79	0.89	1.30	1.50	1.70	1.90	2.20	2.20	2.20	2.40	1.90	1.80	1.80	1.90	2.00	2.20		
Fr	Ra																
0.70	0.90																
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
		1.10	1.12	1.13	1.14	1.13	1.17	1.20	1.20	1.10	1.22	1.23	1.24	1.25	1.10	1.27	
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	
		1.10	1.30	1.50	1.70	1.30	1.28	1.13	1.28	1.30	1.30	1.30	1.30	1.30	1.30	1.30	



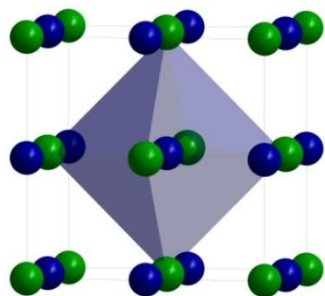
T. Gouder, P. M. Oppeneer, et al. Phys. Rev. B 72, 115122 (2005).

L. MÜchler, et al, Angewandte Chemie **124** 7333 (2012)

Xiao Zhang, Haijun Zhang, Claudia Felser, Shou-Cheng Zhang, Science **335** (2012) 1464

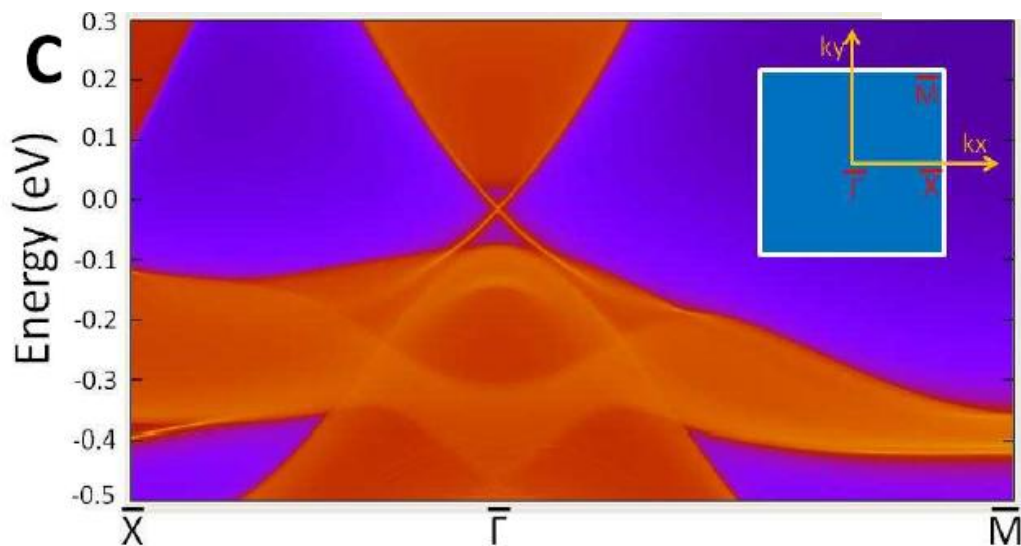


PuTe and AmN, cubic 3D correlated TI



Topological Mott Insulator,
with a Dirac cone at Γ

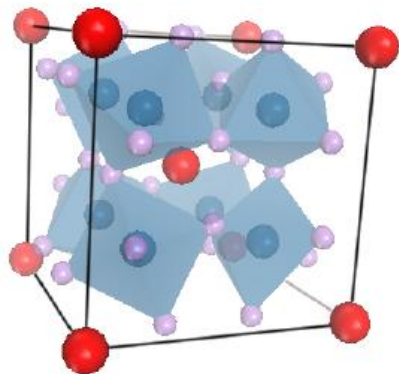
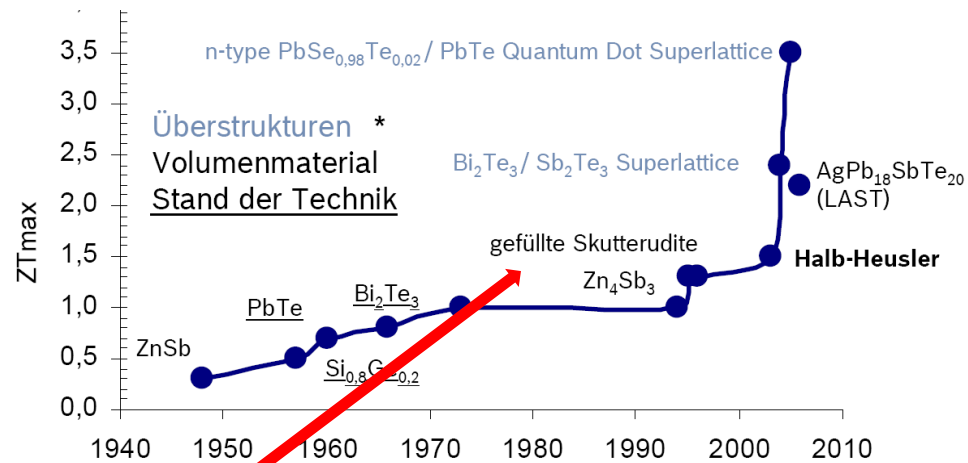
	E_g	Γ	$3X$	$4L$	Tot.
AmN	0.100eV	—	+	—	—
AmP	0.085eV	—	+	—	—
AmAs	0.080eV	—	+	—	—
AmSb	0.055eV	—	+	—	—
AmBi	0.040eV	—	+	—	—
PuSe	0.2eV	—	+	—	—
PuTe	0.178eV	—	+	—	—



Band inversion between **d** and **f**
bands of different parity
PuTe under pressure has a band
gap up to 0.4 eV



Intrinsic Nanostructures ...



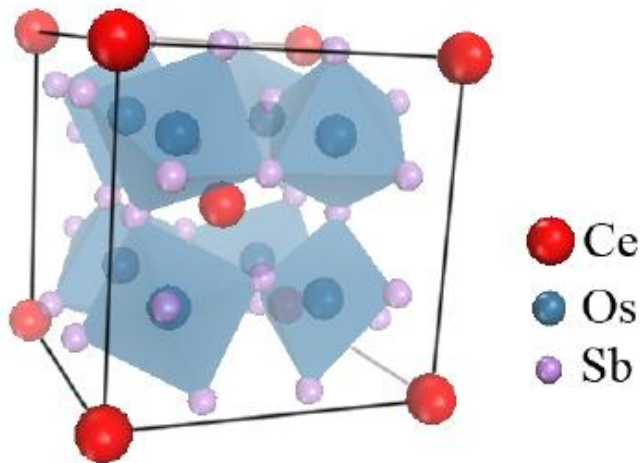
- Ce
- Os
- Sb

Kondo insulating behaviour in the filled skutterudite compound $CeOs_4Sb_{12}$

E D Bauer, A Ślebarski¹, E J Freeman, C Sirvent² and M B Maple

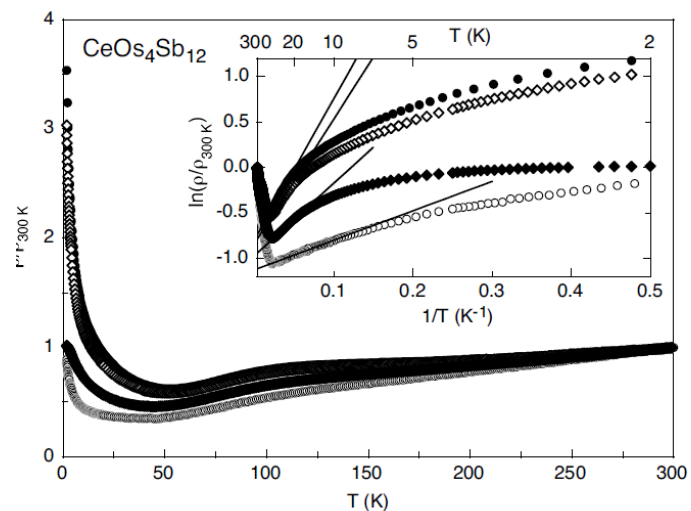
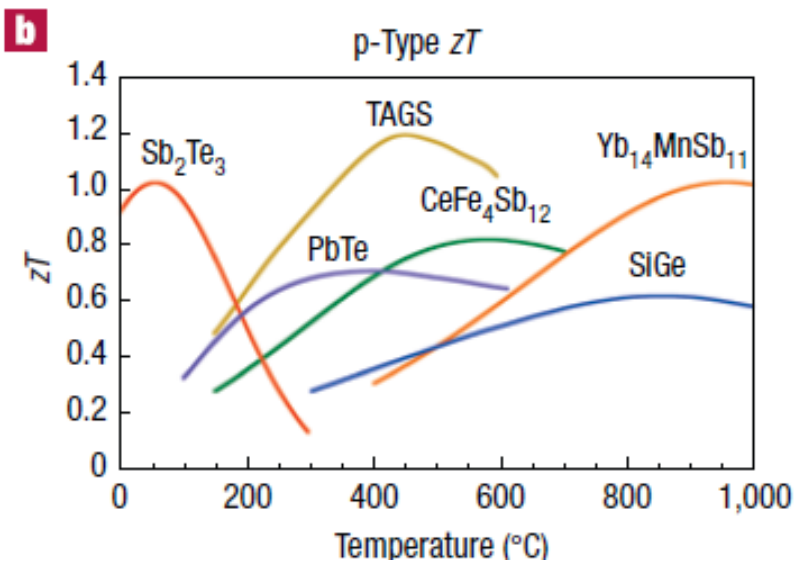


Skutterudites



Kondo insulating behaviour in the filled skutterudite compound $\text{CeOs}_4\text{Sb}_{12}$

E D Bauer, A Šlebarski¹, E J Freeman, C Sirvent² and M B Maple

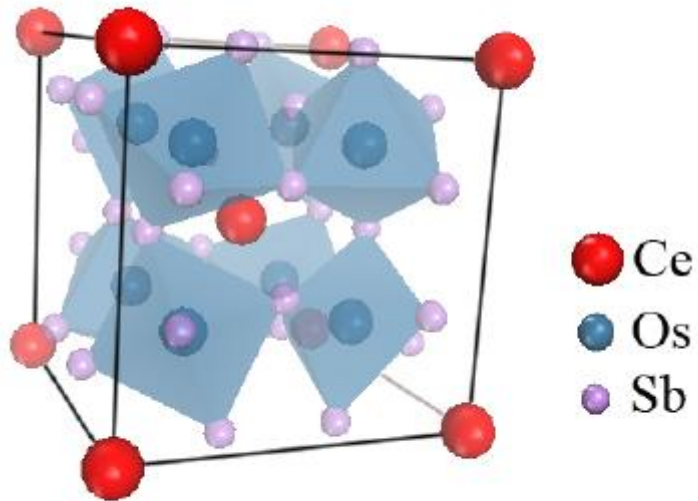


J. Phys.: Condens. Matter 13 (2001) 4495

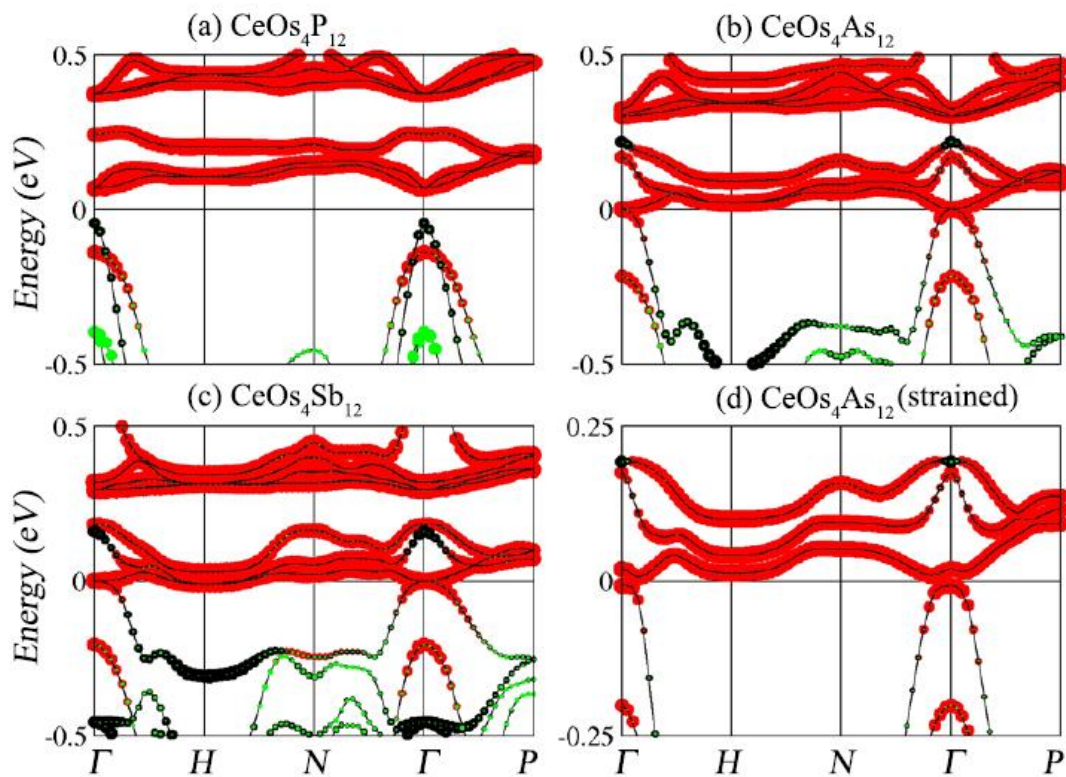
Superconductor
 $\text{PrOs}_4\text{Sb}_{12}$



Skutterudites

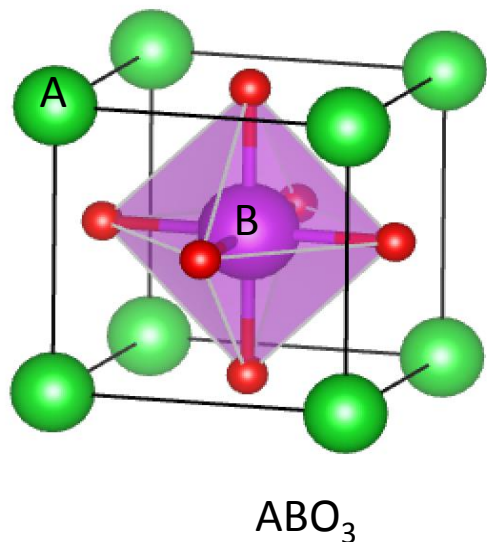


Band inversion between **d** and **f** bands of different parity





Topological Perovskite Oxides



BaBiO₃ has a formal charge of +4 for Bi 6s¹

BiO₆-octahedra are tilted 159.9° not 180°

Bi⁵⁺ and Bi³⁺ lead to BiO₆ octahedra breathing in and out

Hole doped BaBiO₃ is superconducting with a maximum

T_c is 34 K for Ba_{0.6}K_{0.4}BiO_{3.8}

Ba_{1-x}K_xBiO₃ (BKBO) crystallizes in the cubic structure

0.375 < x < 0.5 no breathing mode, but superconducting

Can perovskites exhibit topological quantum states?

- Stable against against surface oxidization and degrading
- Multi-functionality, superconductivity, magnetic, ferroelectric
- Experiment fabrication

First example: BaBiO₃

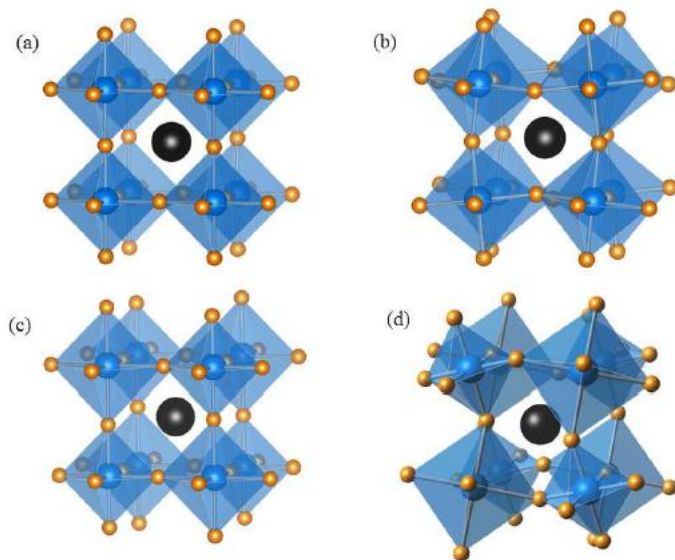


The lone pair - RbTiCl_3

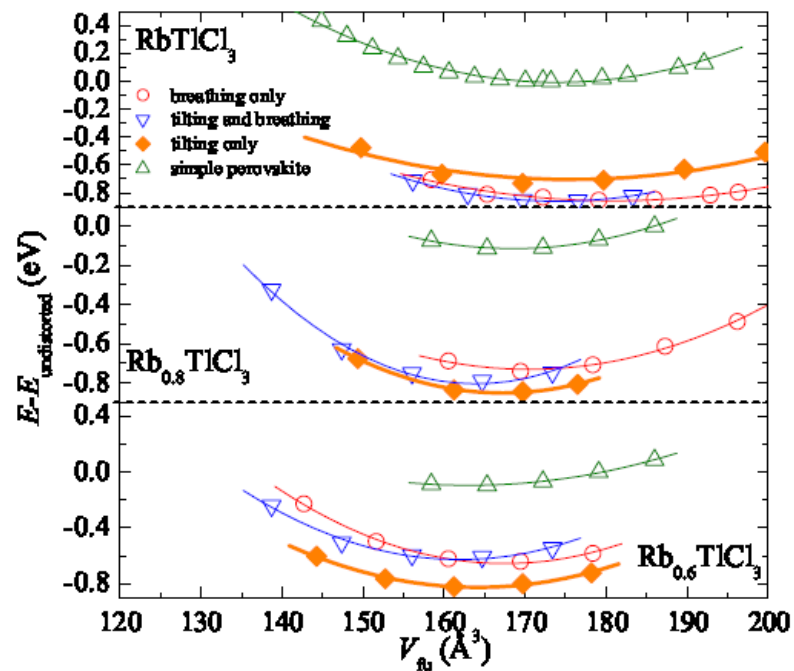
Lone Pair Effect, Structural Distortions, and Potential for Superconductivity in TI Perovskites

Leslie M. Schoop,^{*,†,‡} Lukas Muechler,[§] Claudia Felser,^{§,||} and R. J. Cava[†]

RbTiCl_3 has a formal charge of +2 for TI $6s^1$



- (a) Undistorted ideal
- (b) Tilted octahedra
- (c) Breathing no tilting
- (d) Breathing and tilting

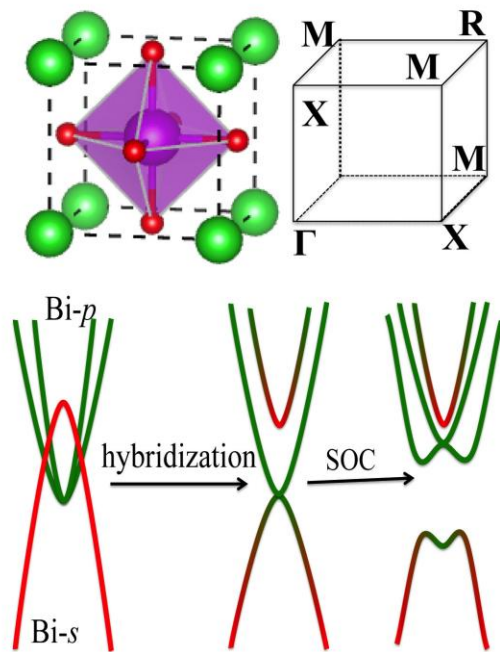




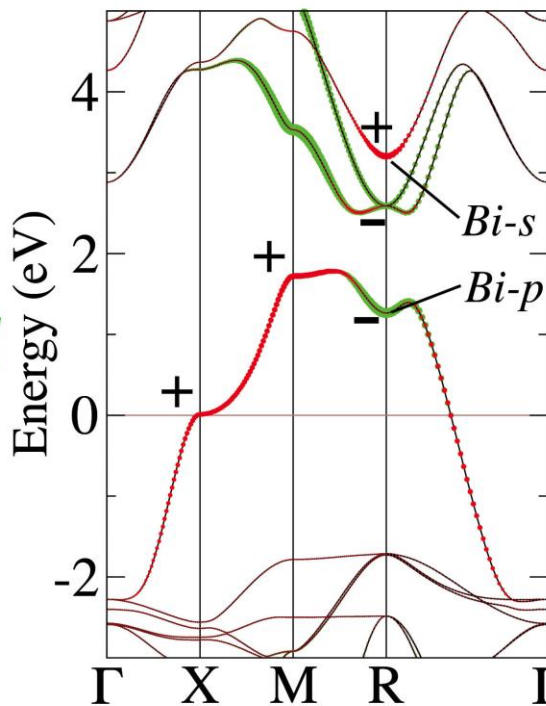
Oxide Topologic Insulator

BaBiO₃ has a formal charge of +4 for Bi 6s¹

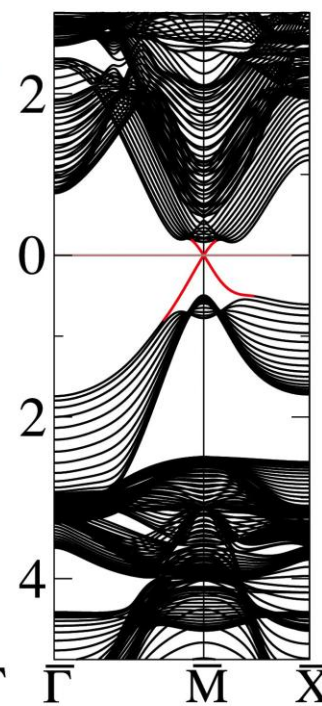
6s²



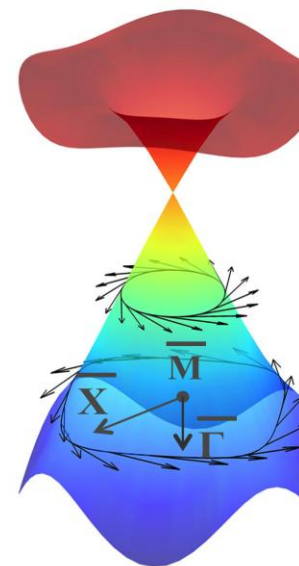
(A)



(B) cubic bulk



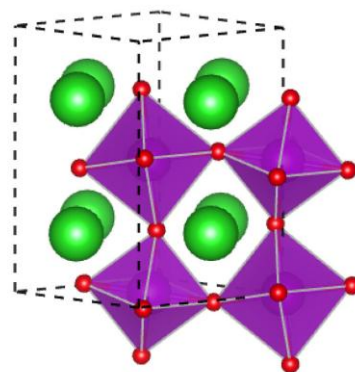
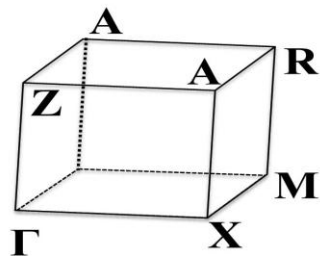
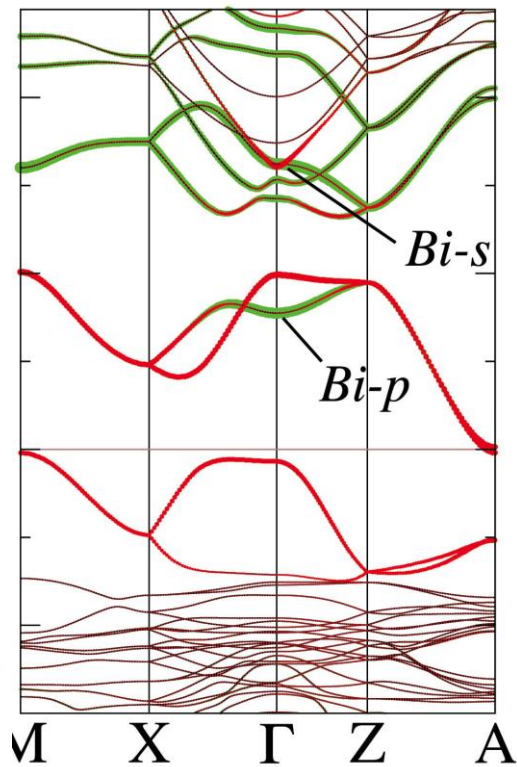
(C) surface (electron-doped)



- 3D strong TI with Z_2 (1;111)
- Largest E_g of 0.7 eV among all known TIs



Robust against lattice distortion



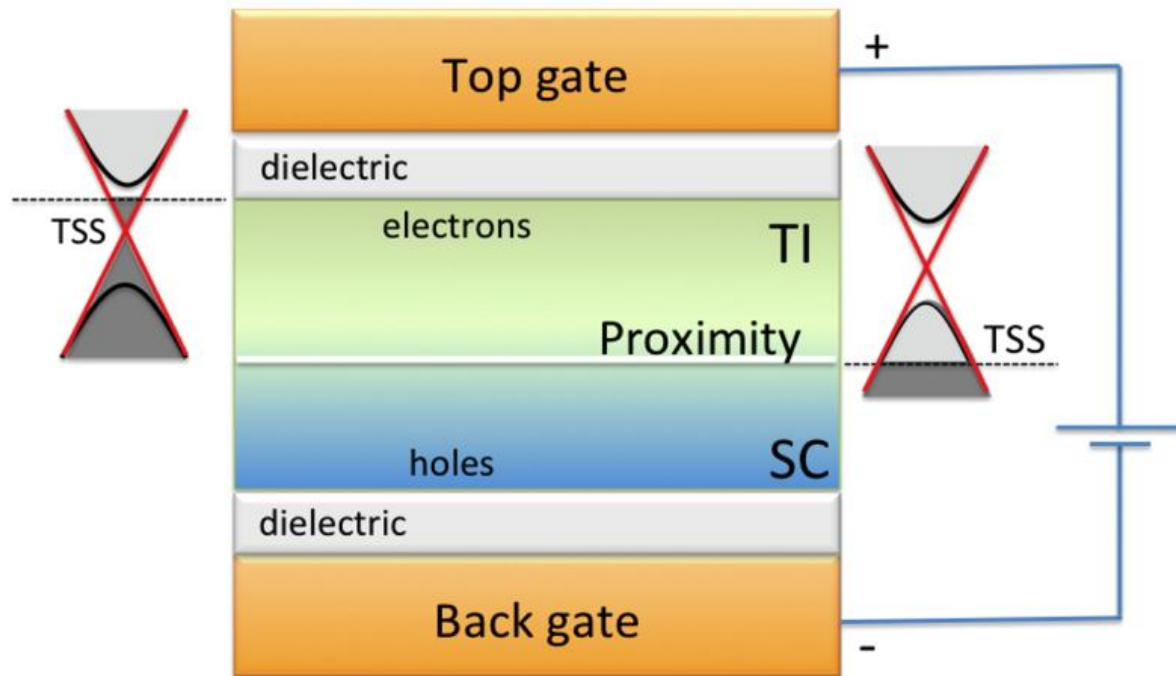
O-breathing
Octahedral distortion

(D) monoclinic bulk



TI + SC interface

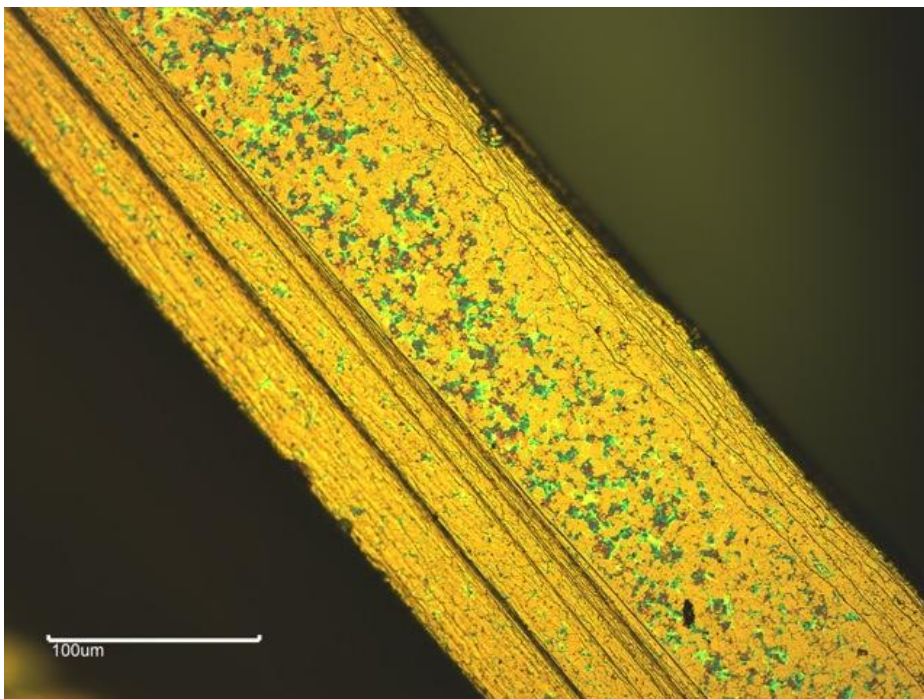
A platform for Majorana fermions



SC: p-type
TI: n-type



Mixed valent BaBiO_3



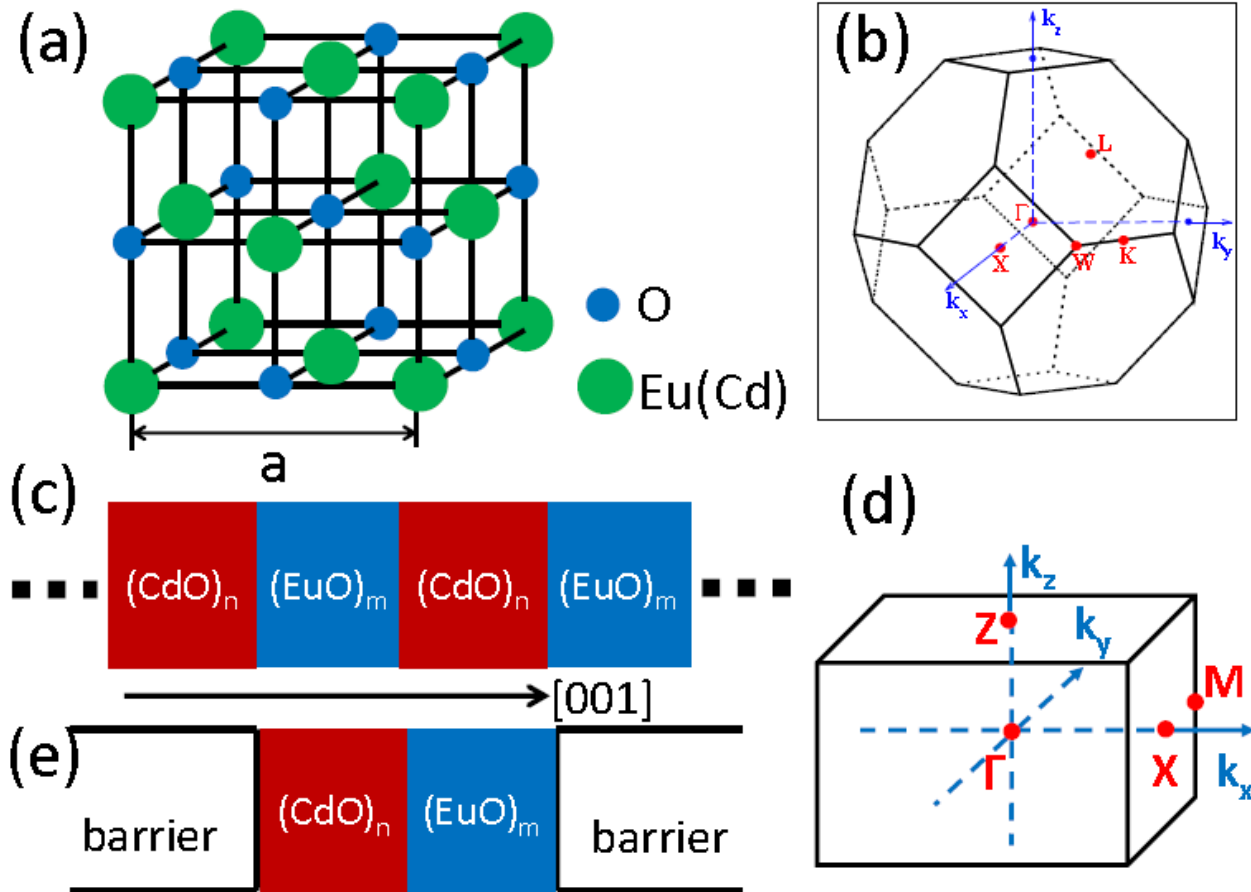
Single Crystals



Prediction in multilayer

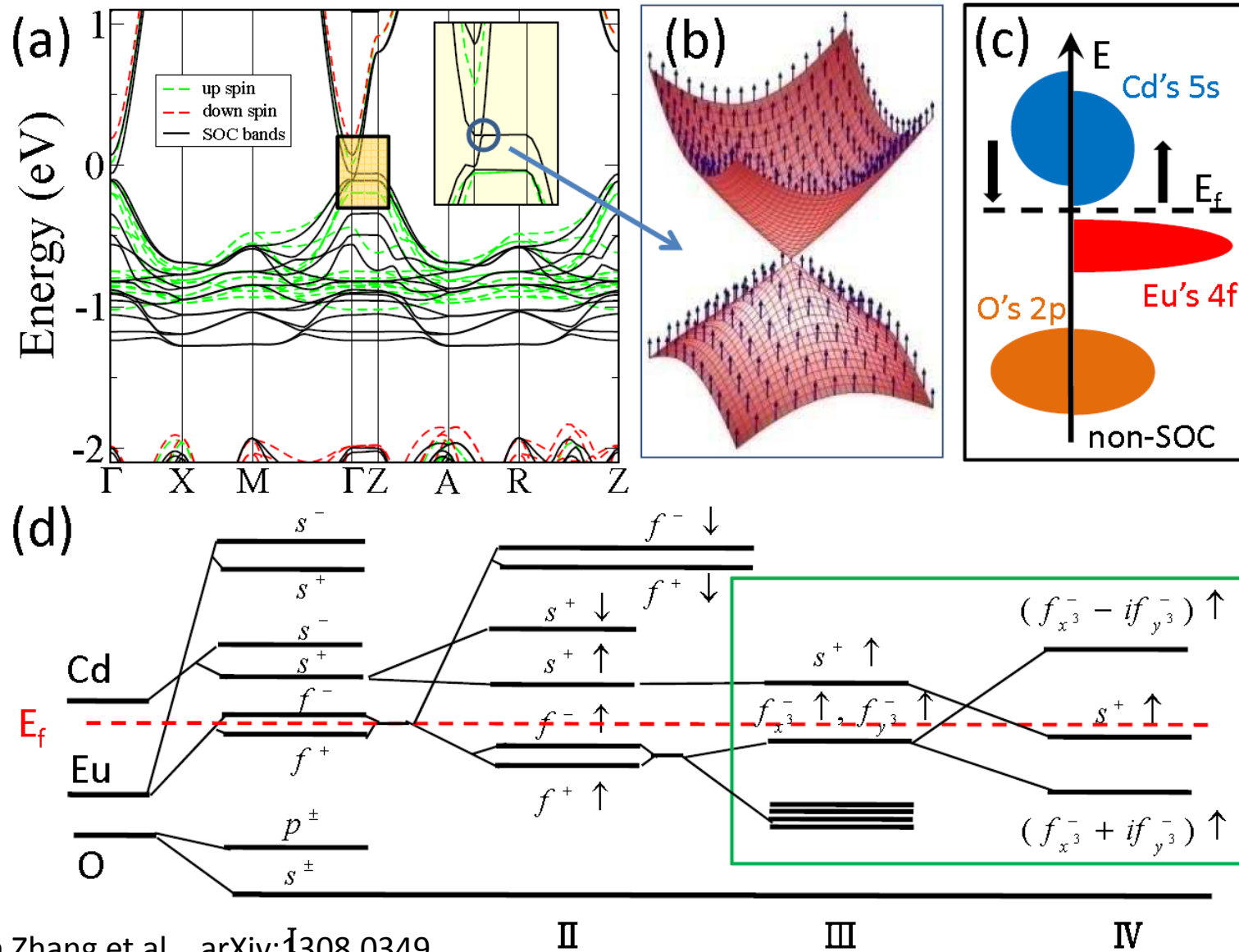
Topological States in Ferromagnetic CdO/EuO Quantum Well

Haijun Zhang, Jing Wang, Gang Xu, Yong Xu and Shou-Cheng Zhang
Department of Physics, McCullough Building, Stanford University, Stanford, CA 94305-4045, USA
(Dated: August 5, 2013)





Prediction in multilayer





Summary

Half Heusler as multifunctional TI

- Linear dispersion via ARPES
- TI plus superconductivity, Kondo, Magnetism

Correlated TIs with d – f inversion

- Skutterudites
- PuTe
- SmB_6 (Fisk) ...

New oxide TI: BaBiO_3

- Large gap 0.7 eV
- Possible TI + SC interface
- Other s^2 systems such $\text{Tl}^+ \text{Pb}^{2+} \text{Bi}^{3+}$ for TI
- Other s^1 system stable against breathing for superconductivity such as CsPbCl_2O or BaPbO_2F

What is next? Correlated oxides