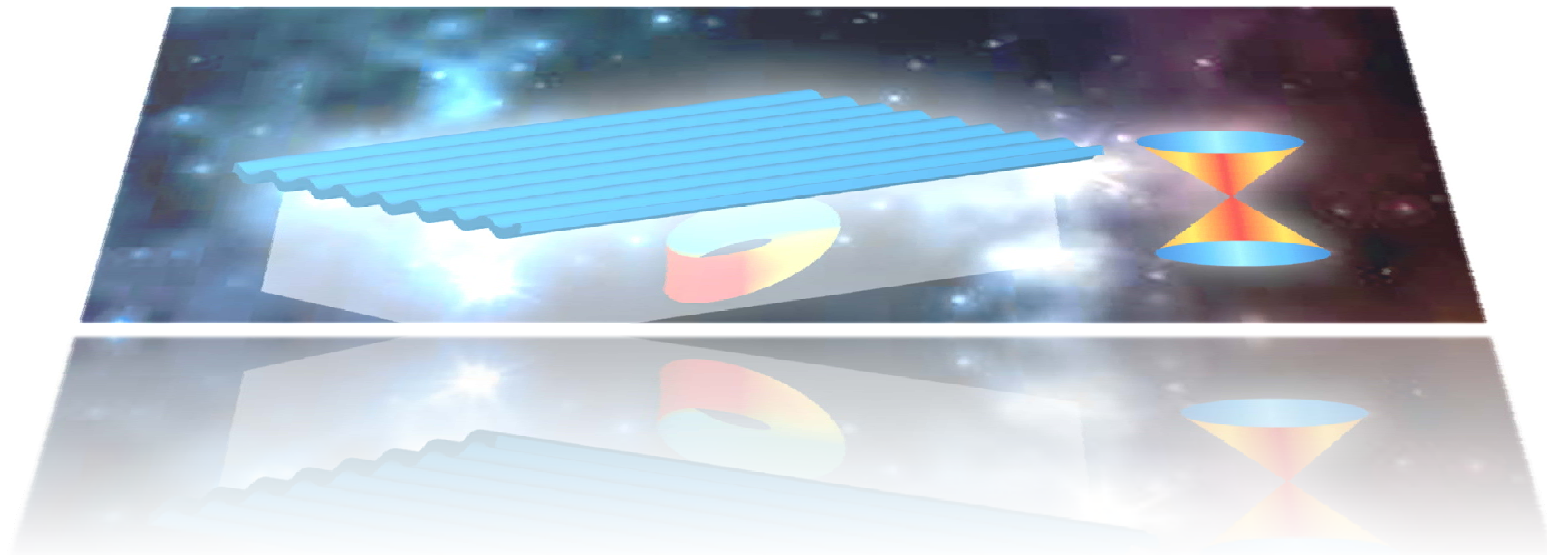




Topology – from the materials perspective



Special thanks to Binghai Yan, Shekhar Chandra, Lukas MÜchler, Leslie Schoop, Stas Chadov, Sun Yan, Yulin Chen, Shoucheng Zhang, Stuart Parkin

Claudia FELSER



Co-workers in Dresden and elsewhere



Andrei Bernevig, Princeton, CNR Rao, Bangalore, India
Uli Zeitler, et al. HFML - EMFL, Nijmegen; J. Wosnitza et al., HFML Rossendorf
Yulin Chen et al., Oxford; Günter Reiss, Bielfeld
S.C.Zhang et al. and A. Kapitulnik, Stanford
S. S. P. Parkin et al., IBM Almaden, MPI Halle



Topological Insulators



Topology



\mathbb{S}^2



\mathbb{R}^2



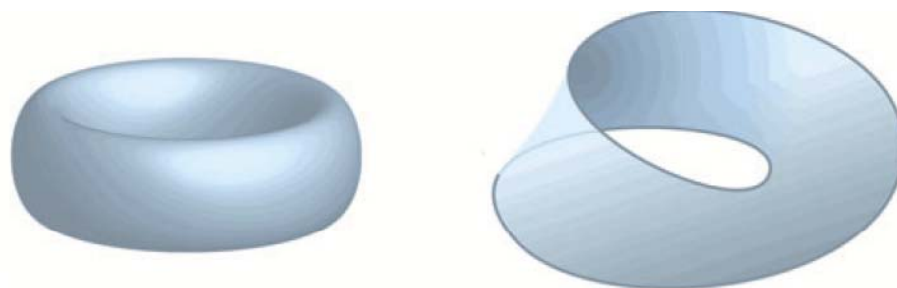
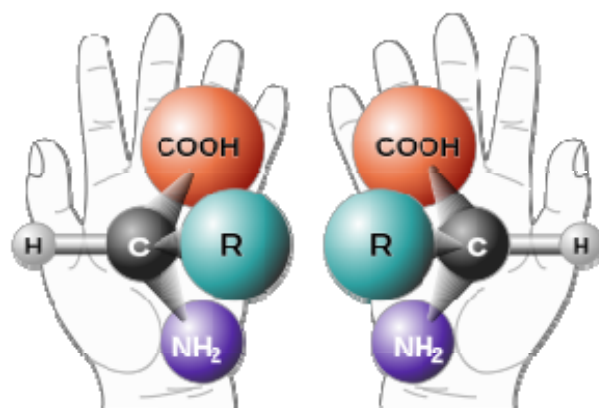
\mathbb{S}^1





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



Universe – particles – condensed matter

Theoretician – from model to materials predictions



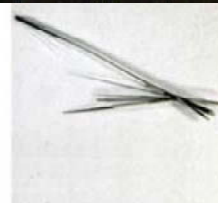
Ag₂Se 1000 μm



BiTeBr 3000 μm



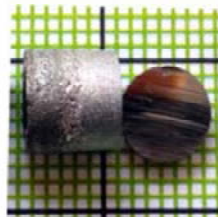
CaPd₃O₄ 100 μm



HfTe₅ 1000 μm



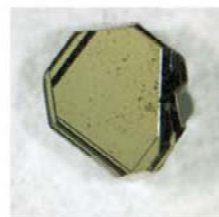
Mn₃Ge 1 cm



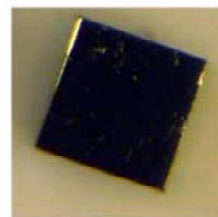
Mn₃Ir 3000 μm



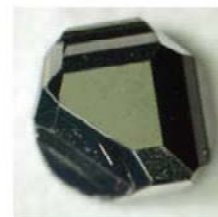
NbAs 2000 μm



NbP 8000 μm



SrPd₃O₄ 100 μm

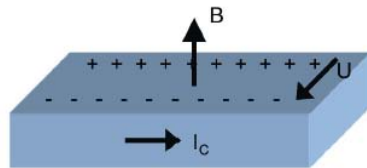


TaAs 2000 μm

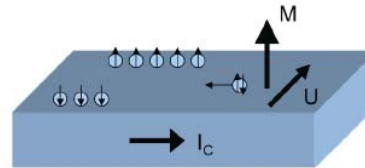


Family of quantum Hall effects

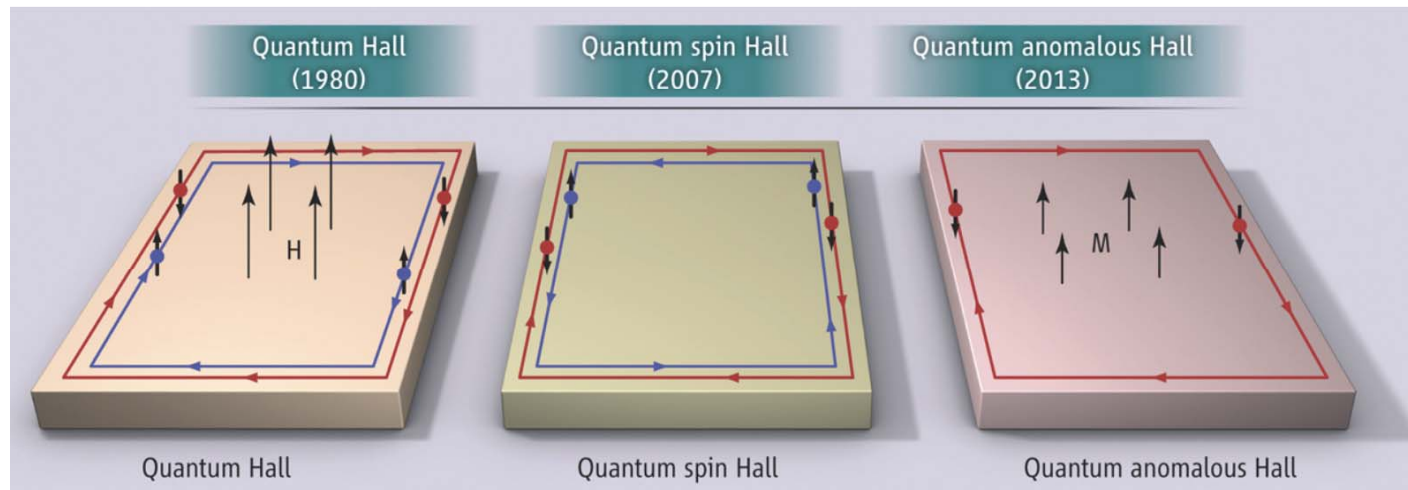
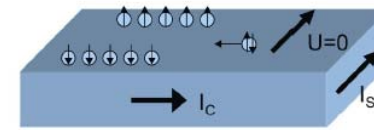
Hall effect
1879



Anomalous Hall effect
1881



Spin Hall effect
2004



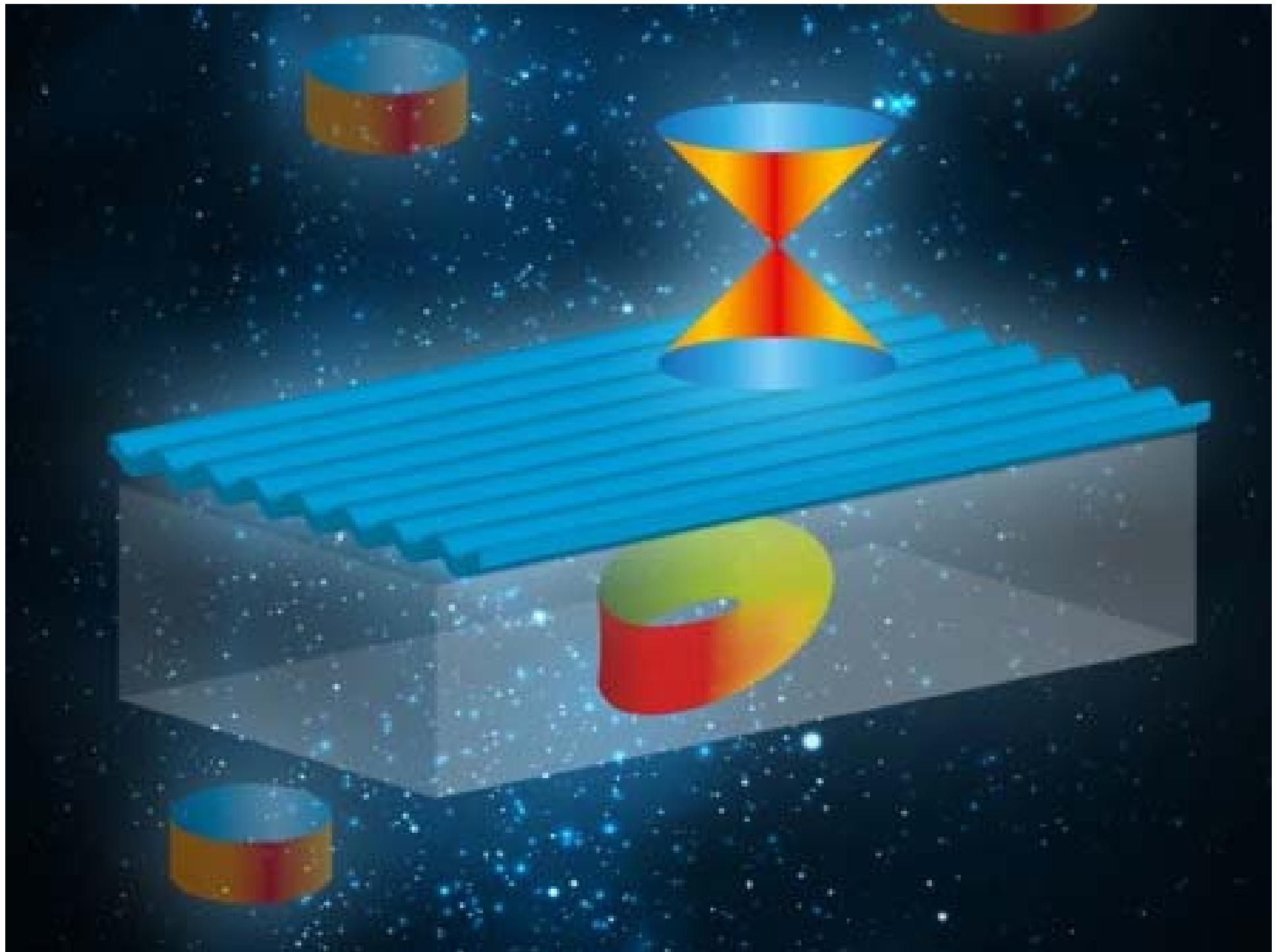
1985
Klaus von Klitzing

1998
Horst Ludwig Störmer and Daniel Tsui

2010
Andre Geim and Konstantin Novoselov

2016
David Thouless, Duncan Haldane und Michael Kosterlitz

S Oh Science 340 (2013) 153



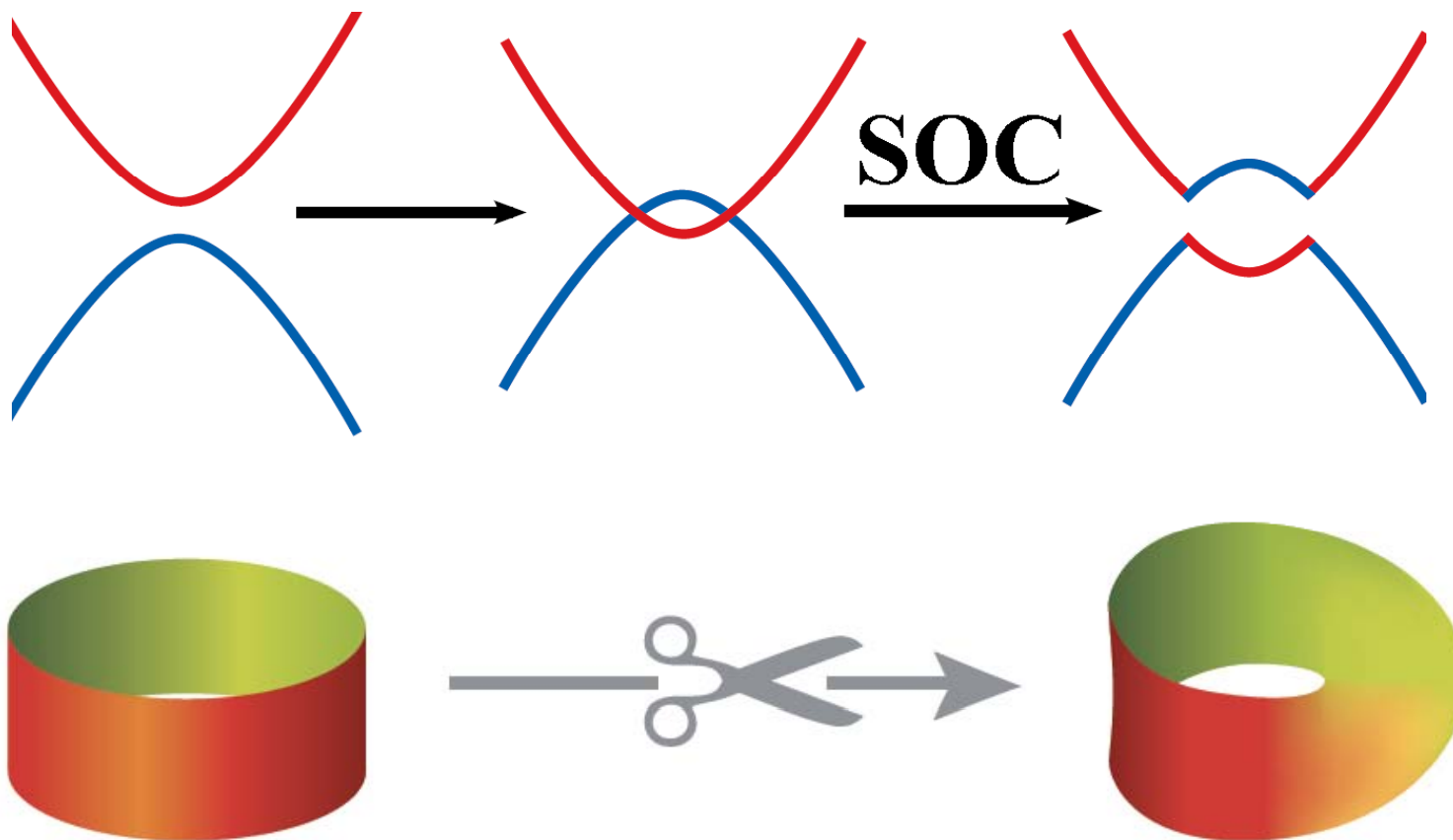


Trivial and topological insulators

Trivial semiconductor
CdS

Topological Insulator
Without spin orbit coupling

Topological Insulator
With spin orbit coupling





Topological insulator

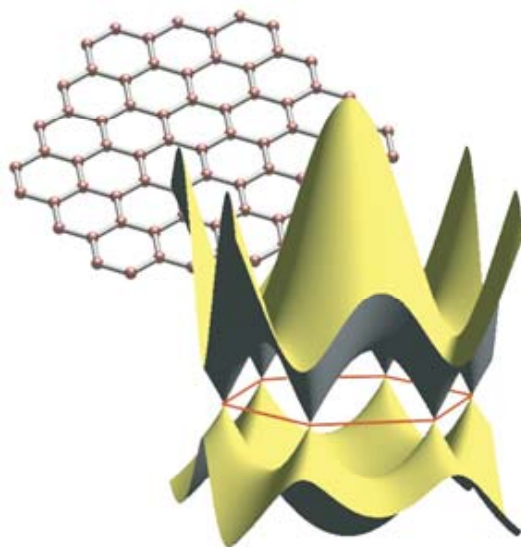
Z₂ Topological Order and the Quantum Spin Hall Effect

C.L. Kane and E. J. Mele

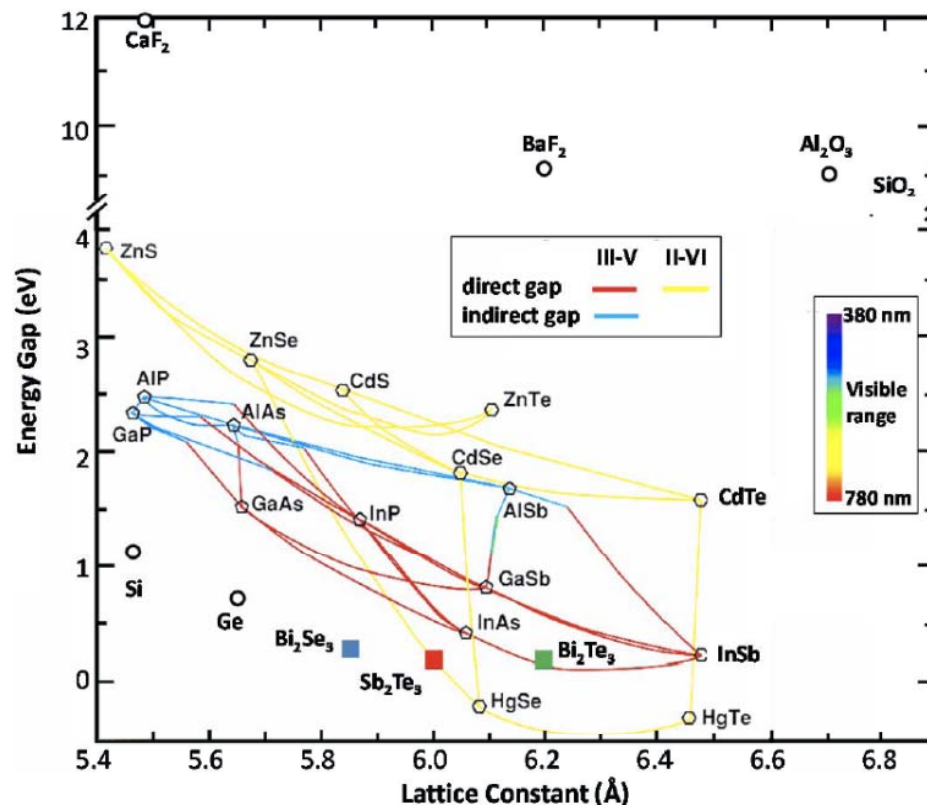
Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA

(Received 22 June 2005; published 28 September 2005)

The quantum spin Hall (QSH) phase is a time reversal invariant electronic sta band gap that supports the transport of charge and spin in gapless edge states. W associated with a novel Z₂ topological invariant, which distinguishes it from an o classification, which is defined for time reversal invariant Hamiltonians, is analog classification of the quantum Hall effect. We establish the Z₂ order of the QSI model of graphene and propose a generalization of the formalism applicable to n systems.



First prediction in graphene by Kane



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)



First success

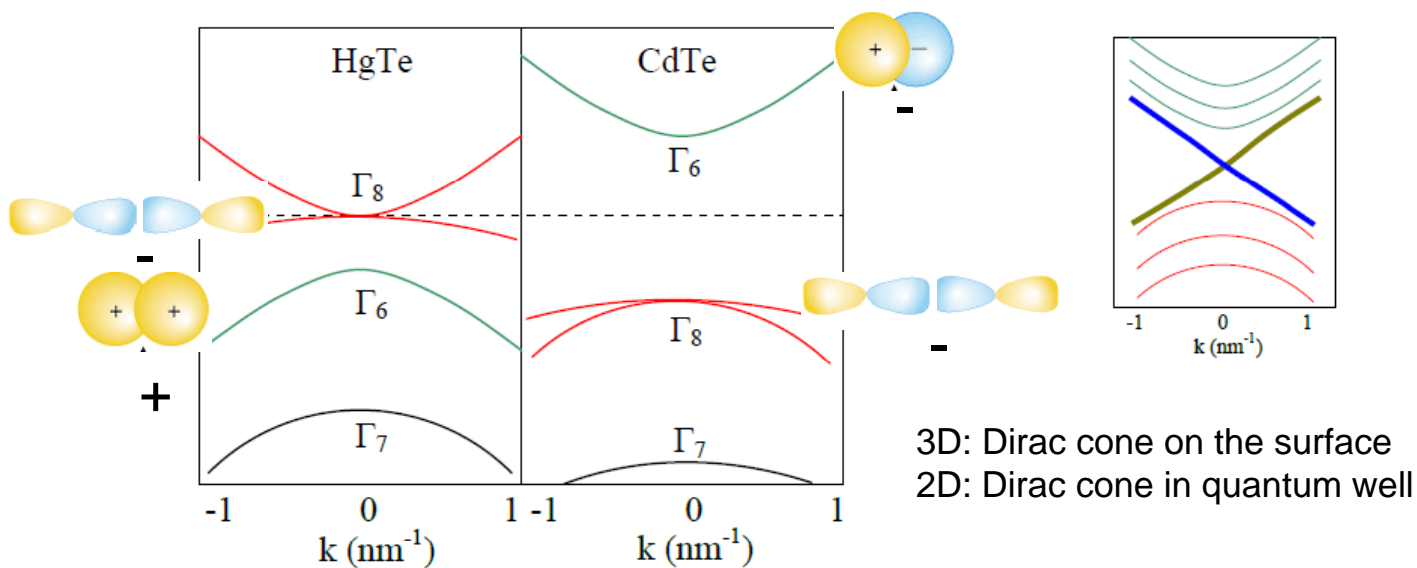


Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells

B. Andrei Bernevig, *et al.*

Science **314**, 1757 (2006);

DOI: 10.1126/science.1133734



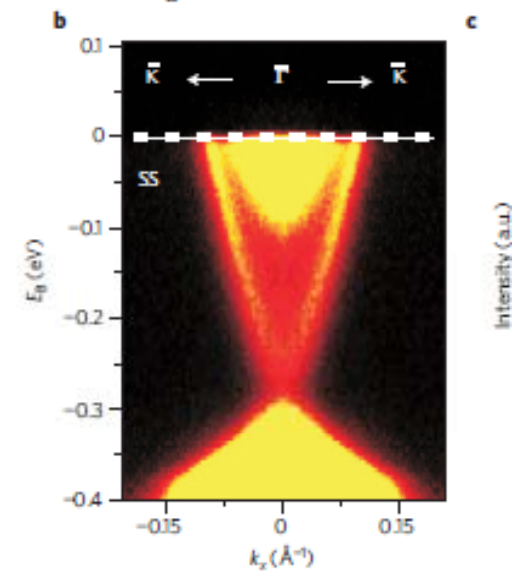
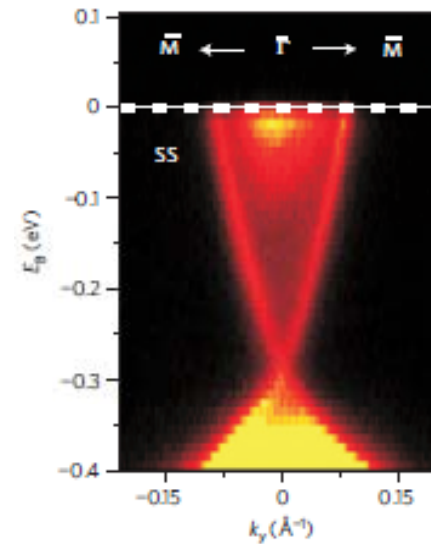
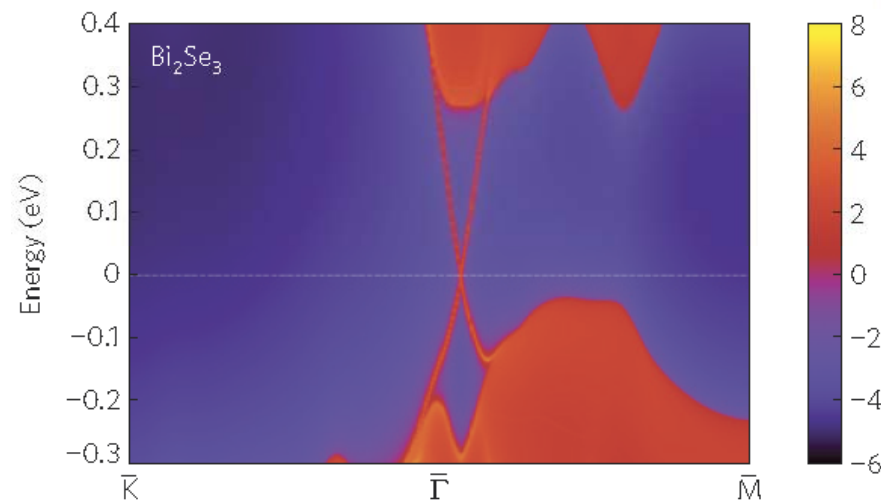
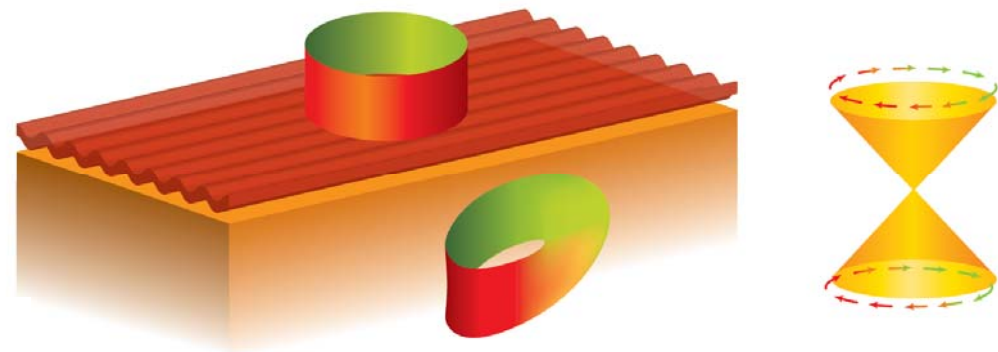


Theory and experiment

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)

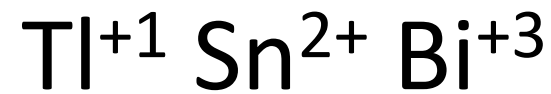
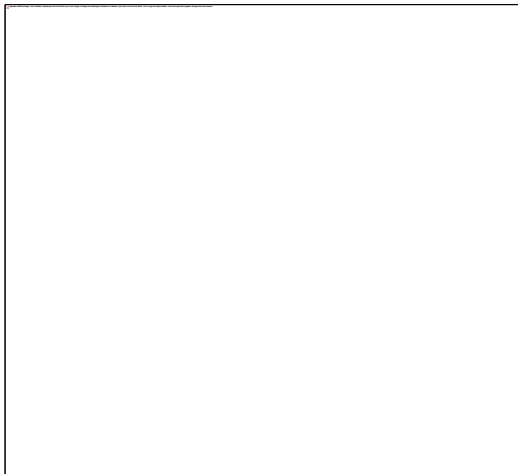


Materials

Table I. Proposed topological insulator materials grouped into several different material classes.^{4,12,13,19,23-29}

HgTe-type	Bi ₂ Se ₃ -type	Honey Comb Lattice	Bismuth-Alloys	NaCl Structure	Oxides	Correlated Materials	Super-conductors
HgTe	Bi ₂ Se ₃ , Bi ₂ Te ₃ , and Sb ₂ Te ₃	Graphene	Bi-Sb	SnTe PbTe	Doped BaBiO ₃	Iridates	Cu _x Bi ₂ Se ₃
Half-Heuslers such as LaPtBi	Bi ₂ Te ₂ Se	LiAuTe		PuTe AmN	Iridates	SmB ₆	LaPtBi YPtBi LuPtBi
α -Sn, HgSe β -HgS	(Bi _x Sb _{1-x}) ₂ Te ₃					YbPtBi	TiBiSe ₂ TiBiTe ₂
Chalco-pyrites	TiBiSe ₂ and TiBiTe ₂					Skutterudites	
AlSb/InAs/GaSb	Bi ₁₄ Rh ₃ I ₉					PuTe, AmN	

Claudia Felser and Xiao-Liang Qi , Guest Editors, MRS Bull. 39 (2014) 843.



Inert pair effect



Rewriting the text book: Au



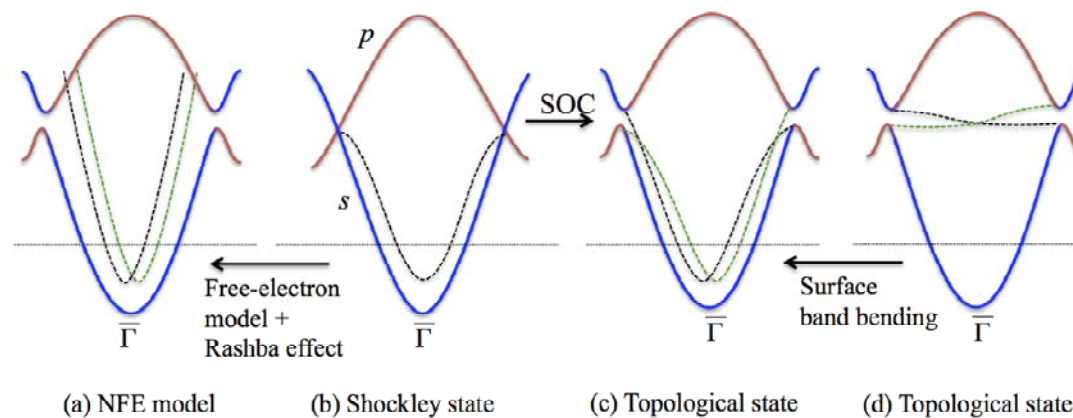
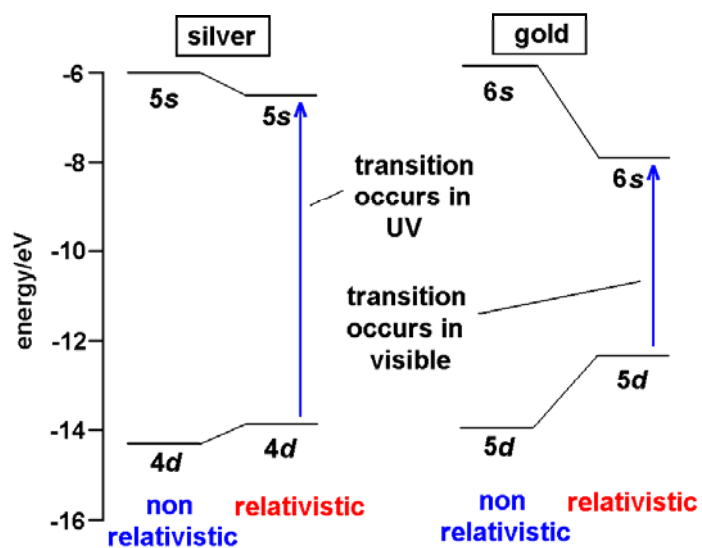
AUGUST 15, 1939

PHYSICAL REVIEW

VOLUME 56

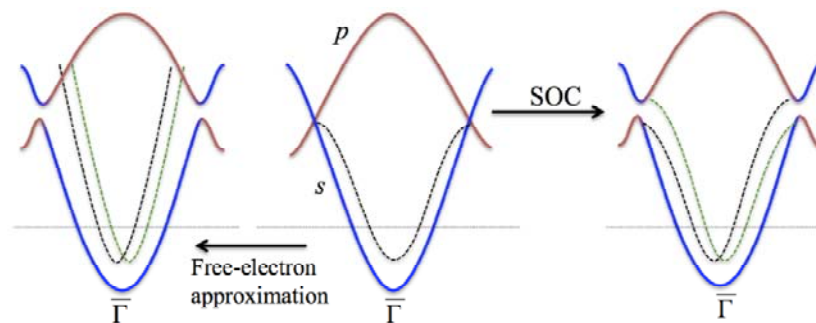
On the Surface States Associated with a Periodic Potential

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





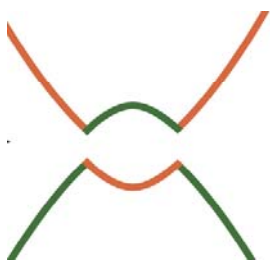
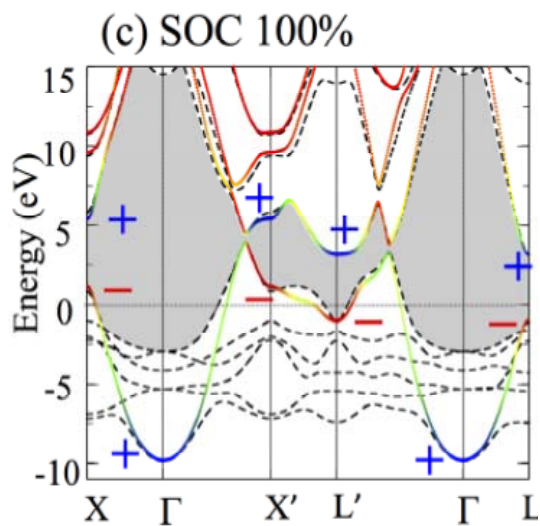
Rewriting the text book: Au



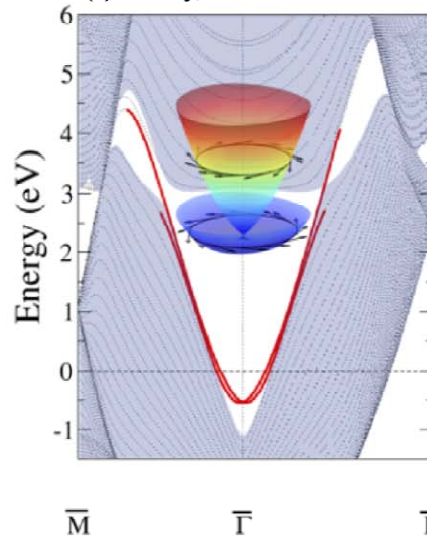
(a) NFE model

(b) Shockley state

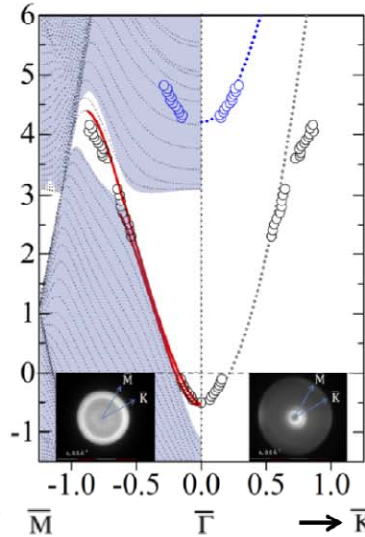
(c) Topological surface states



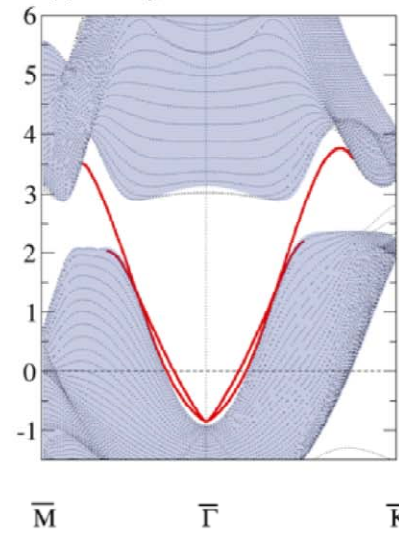
(a) Theory, SOC 100%



(b) Experiment vs. theory



(c) Theory, SOC 350%

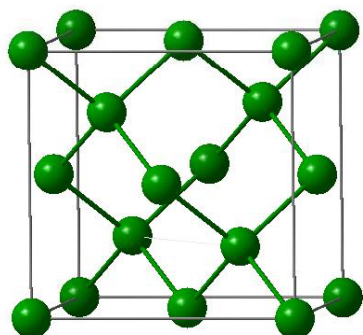


Cs⁺Au⁻

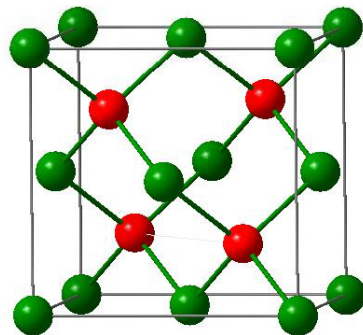


Heusler compounds

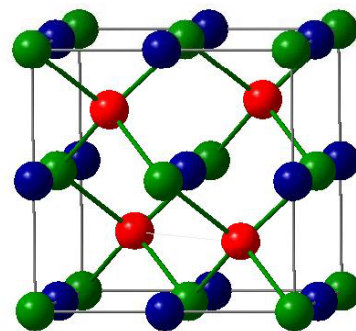
Diamond



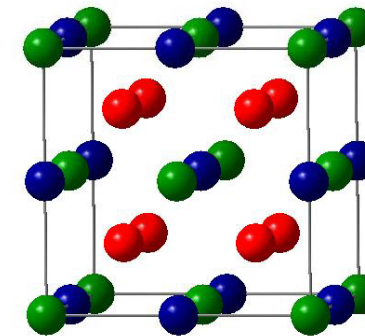
ZnS



Heusler XYZ C1_b



X₂YZ L2₁

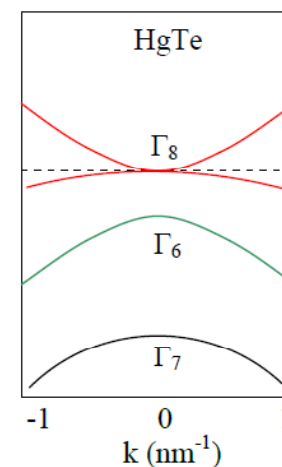
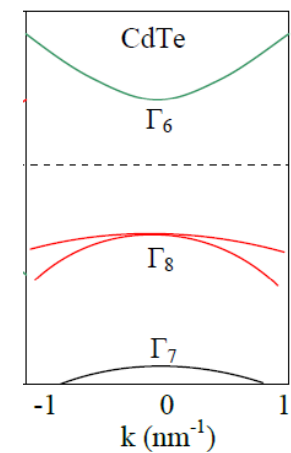
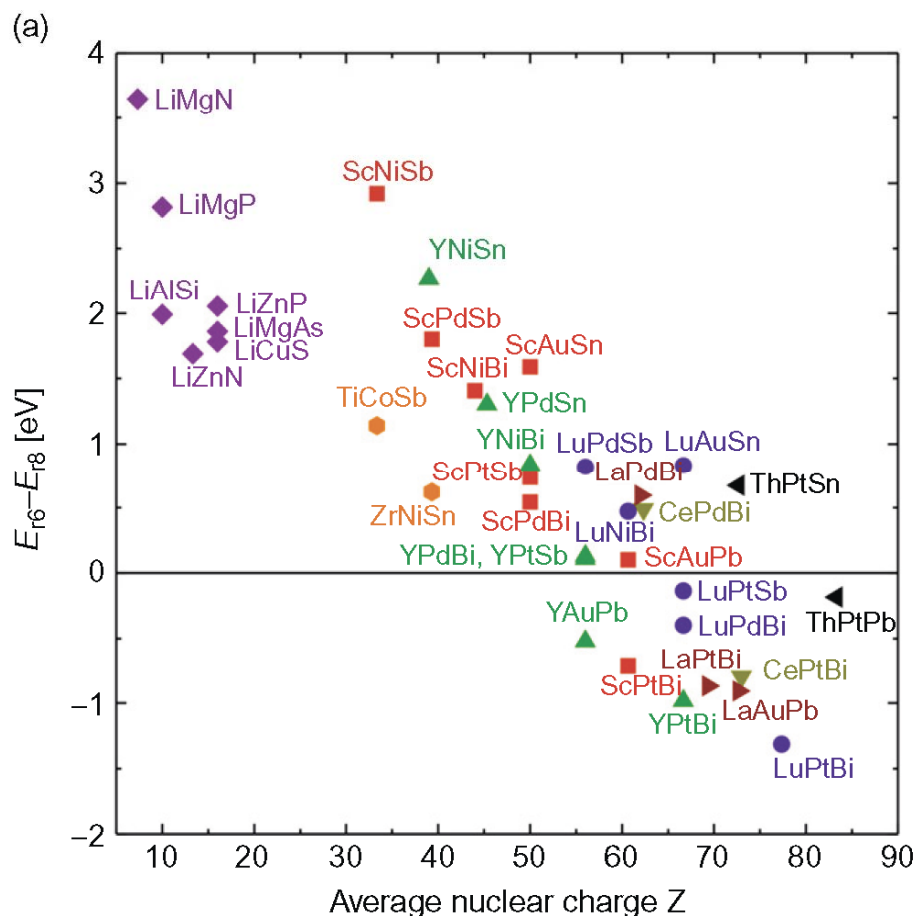
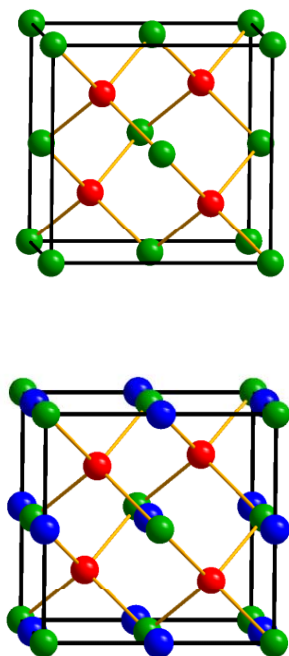


H 2.20																	He	
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne	
Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar	
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00	
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 2.40	Au 1.90	Hg 1.80	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 T, Felser C, Parkin SSP, IEEE TRANSACTIONS ON MAGNETICS 47 (2011) 367
 Graf T, Felser C, Parkin SSP, Progress in Solid State Chemistry Chemistry 39 (2011) 1



Predicting new compounds

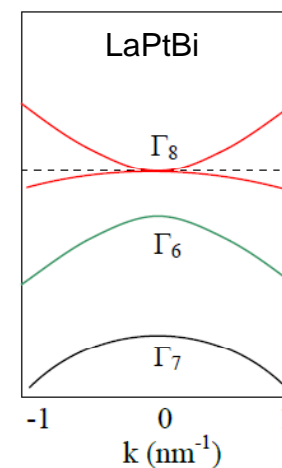
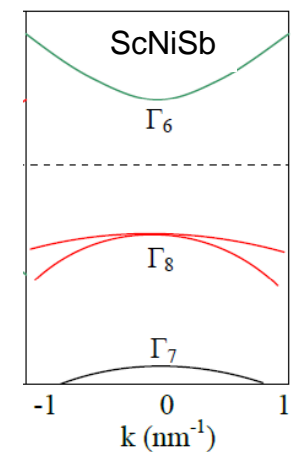
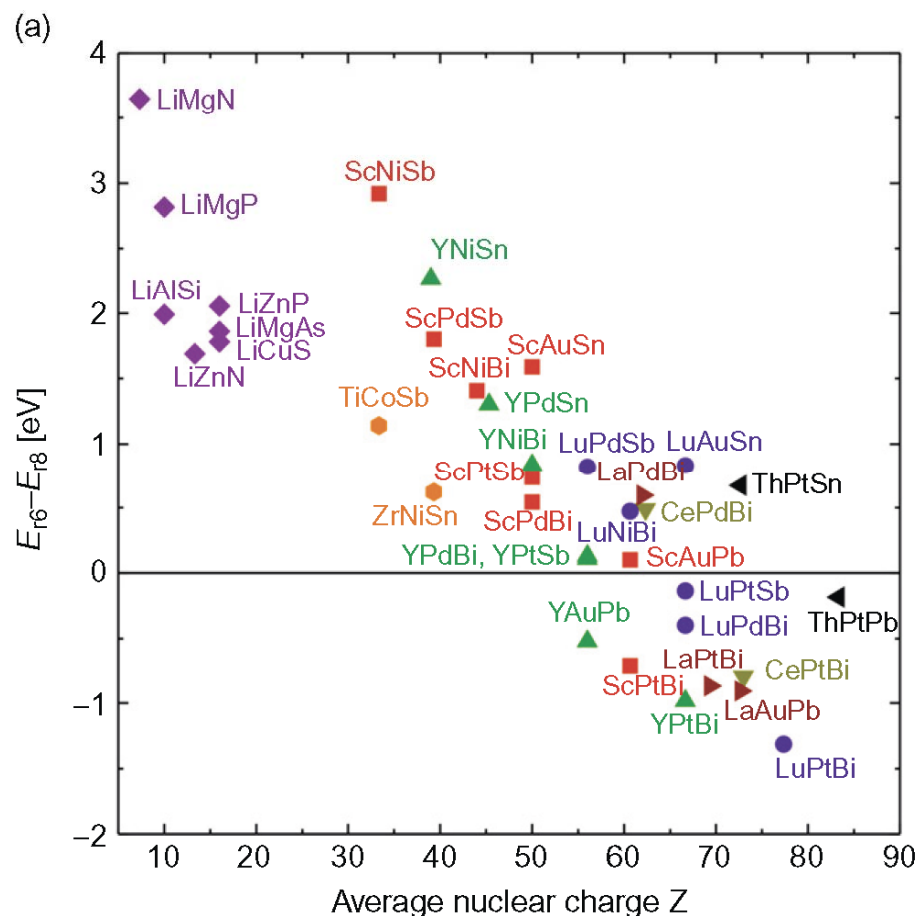
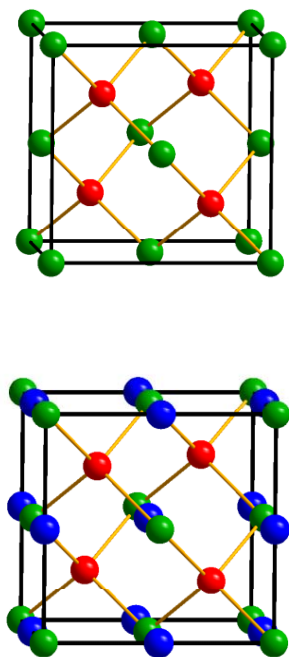


S. Chadov et al., Nat. Mater. 9, 541 (2010).

H. Lin et al., Nat. Mater. 9, 546 (2010).



Predicting new compounds

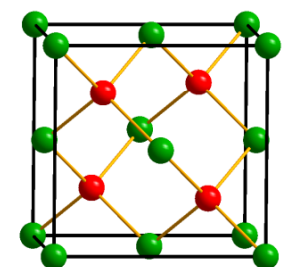


S. Chadov et al., Nat. Mater. 9, 541 (2010).

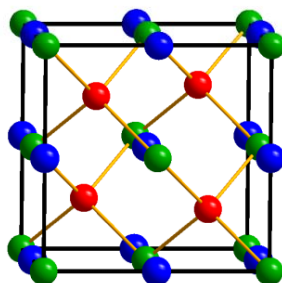
H. Lin et al., Nat. Mater. 9, 546 (2010).



Electronic structure

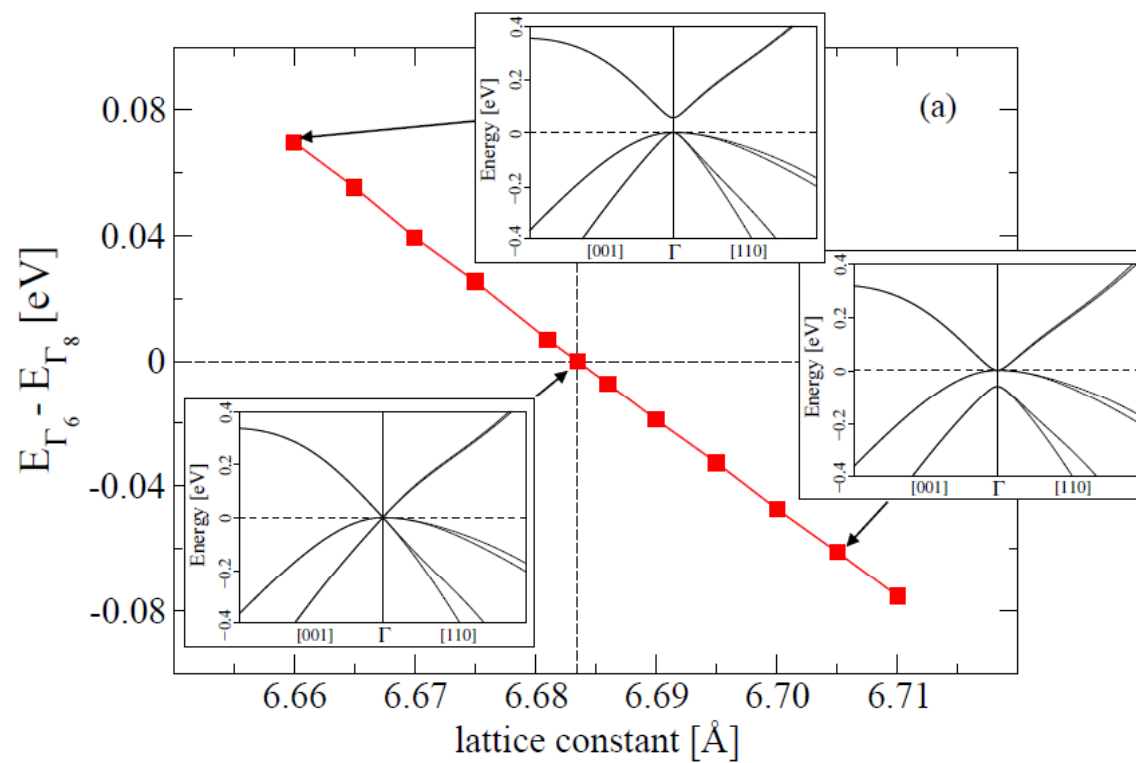


CdTe



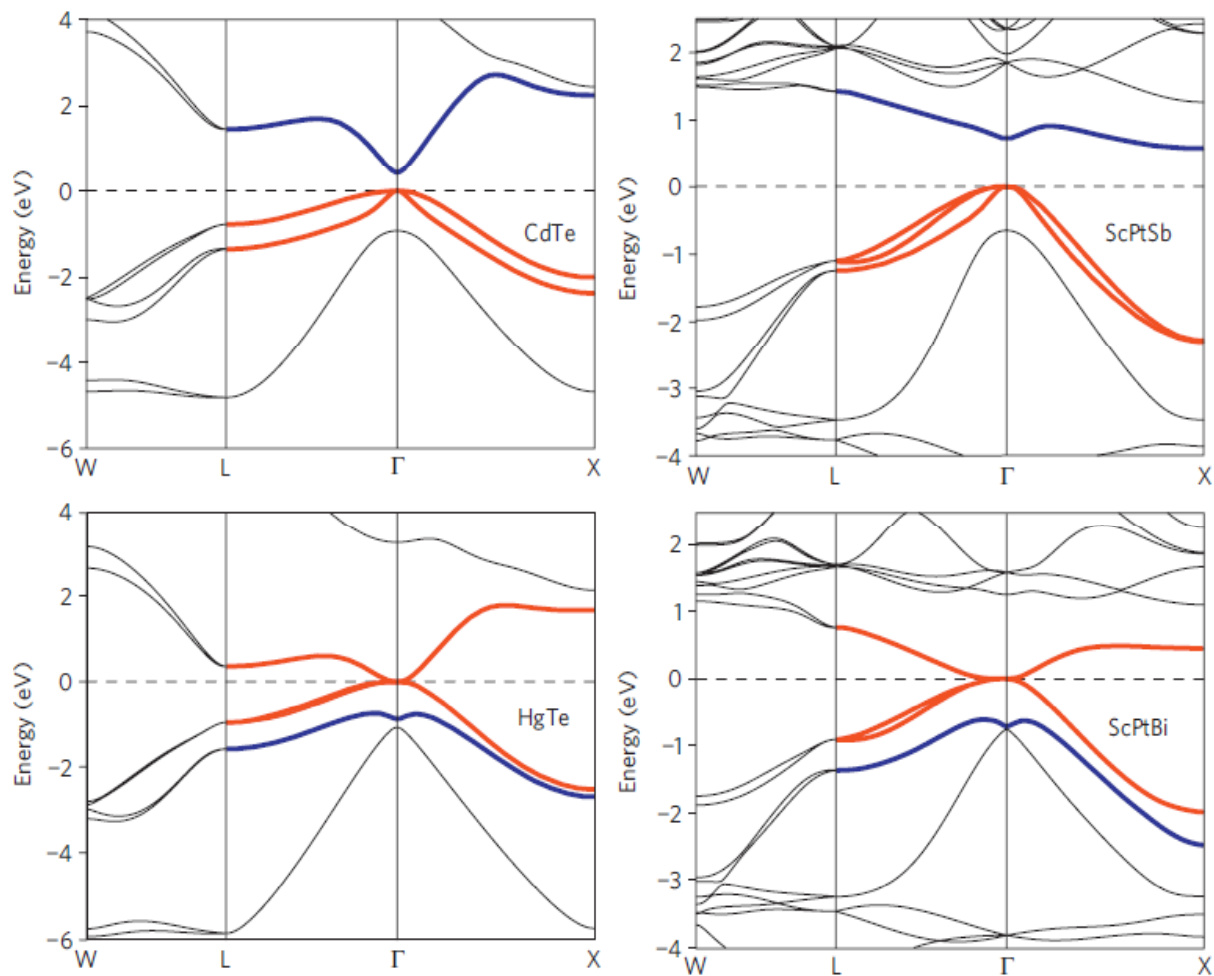
ScPtSb

ScPtBi





Electronic structure

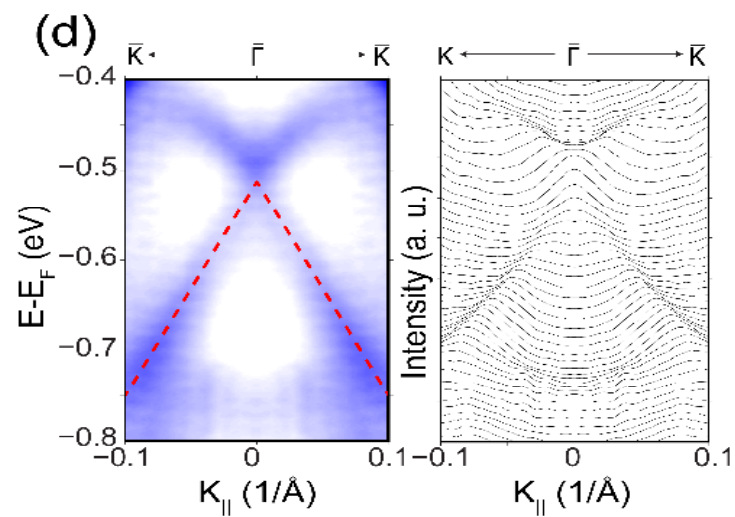
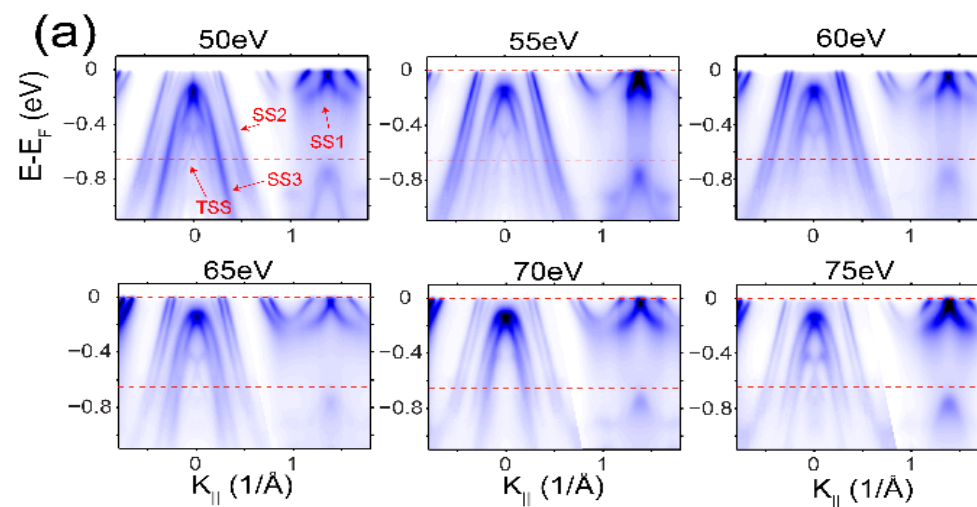
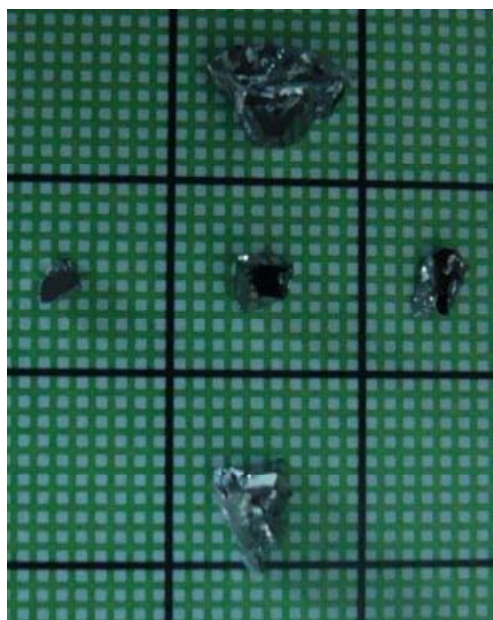


S. Chadov et al., *Nat. Mater.* 9, 541 (2010).

H. Lin et al., *Nat. Mater.* 9, 546 (2010).

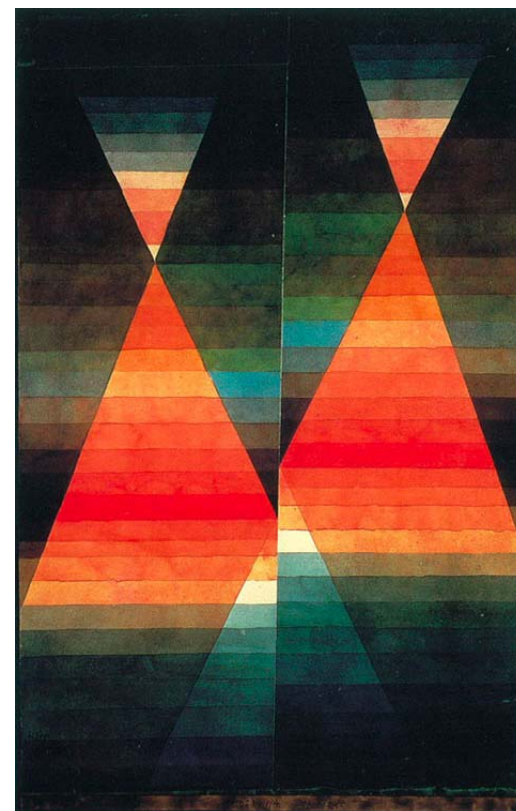
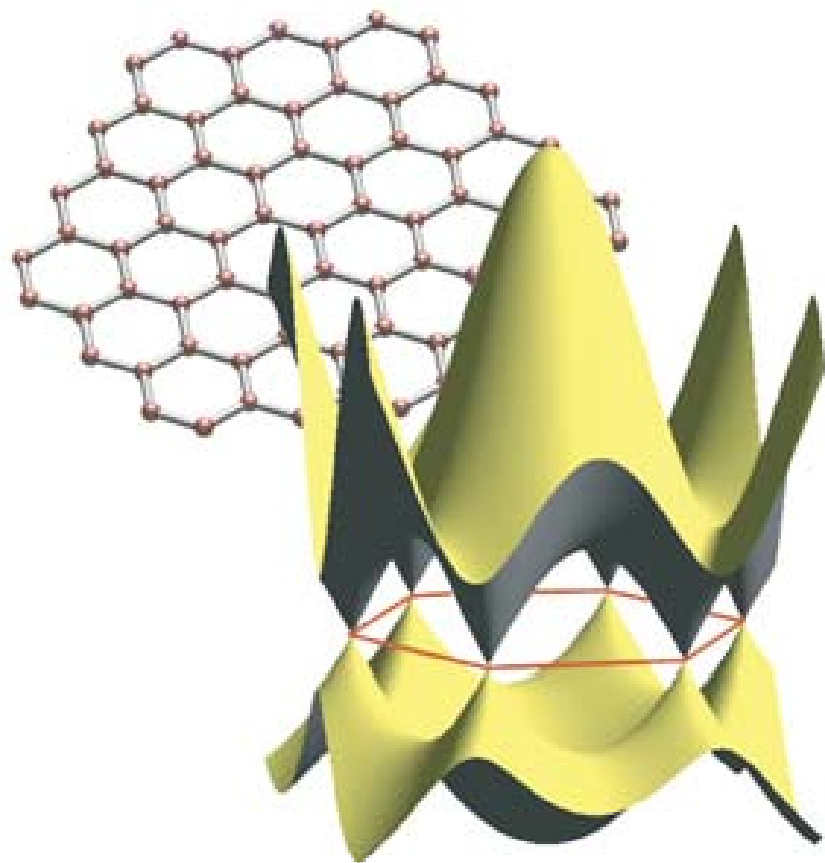


ARPES of LnPtBi





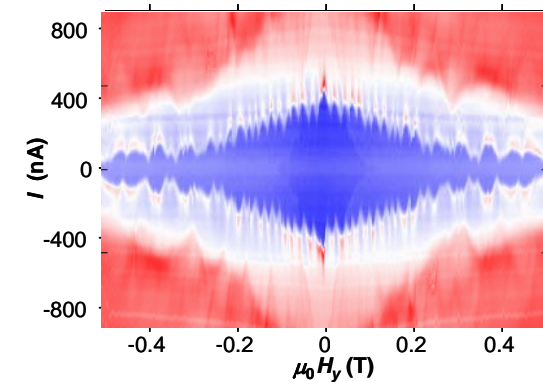
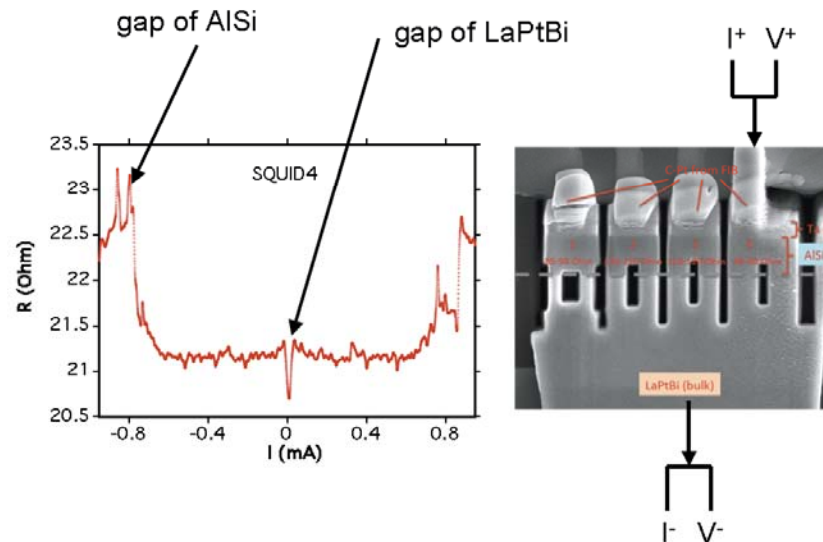
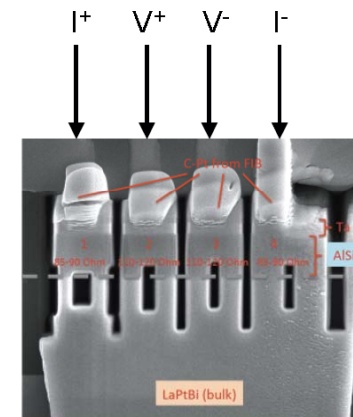
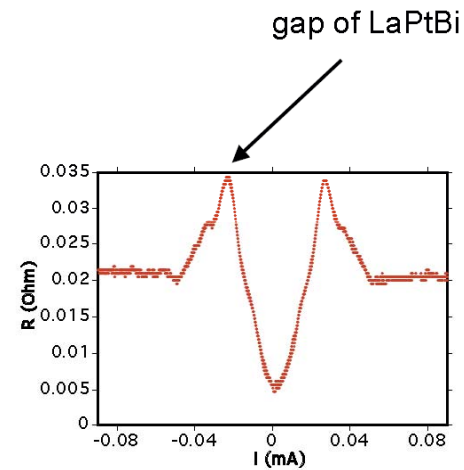
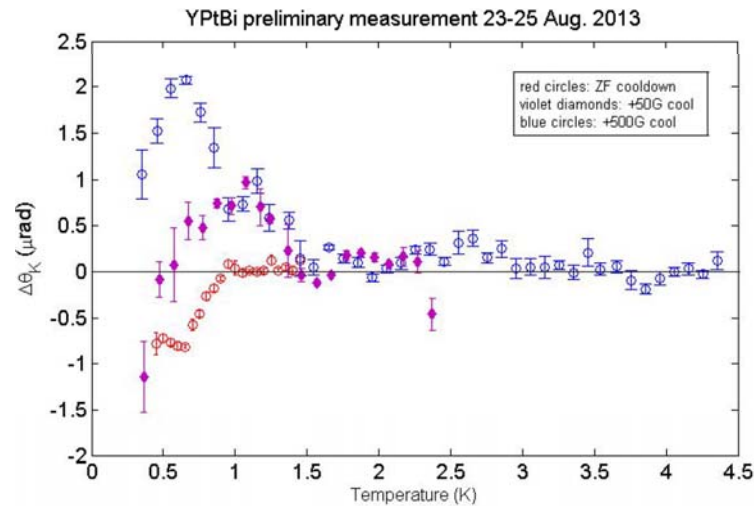
Dirac and Weyl semimetals



Paul Klee



Hunting Majorana



The nontrivial Josephson coupling leads to a current-flux relation with a **half period** in a superconducting quantum interference device geometry



Topological RPdBi half-Heusler semimetals A new family of noncentrosymmetric magnetic superconductors

Yasuyuki Nakajima,¹ Rongwei Hu,¹ Kevin Kirshenbaum,¹ Alex Hughes,¹ Paul Syers,¹ Xiangfeng Wang,¹ Kefeng Wang,¹ Renxiong Wang,¹ Shanta R. Saha,¹ Daniel Pratt,² Jeffrey W. Lynn,² Johnpierre Paglione^{1*}

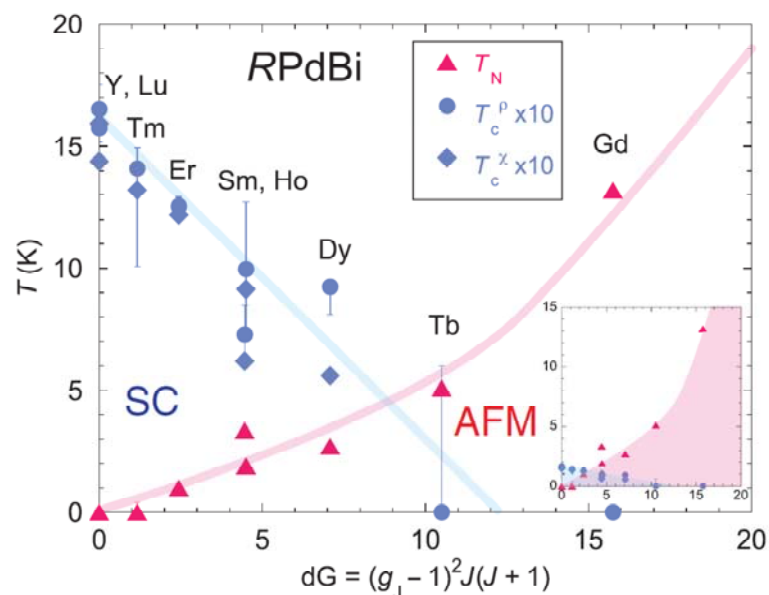


Fig. 5. Phase diagram of RPdBi series, indicating evolution of superconducting and antiferromagnetic ground states as a function of de Gennes factor $dG = (g_j - 1)^2 J(J + 1)$. The superconducting transition T_c

Pairing of $j = 3/2$ Fermions in Half-Heusler Superconductors

P. M. R. Brydon,^{1,2,*} Limin Wang,³ M. Weinert,⁴ and D. F. Agterberg⁴

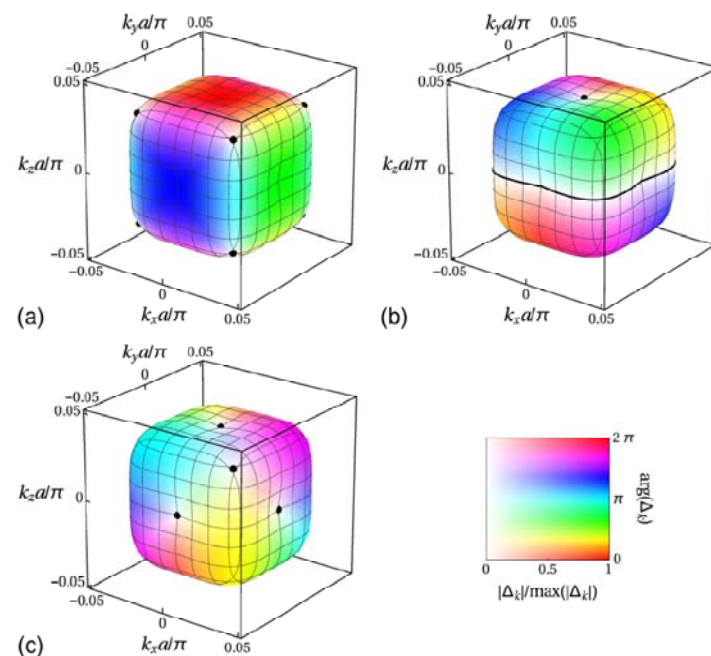
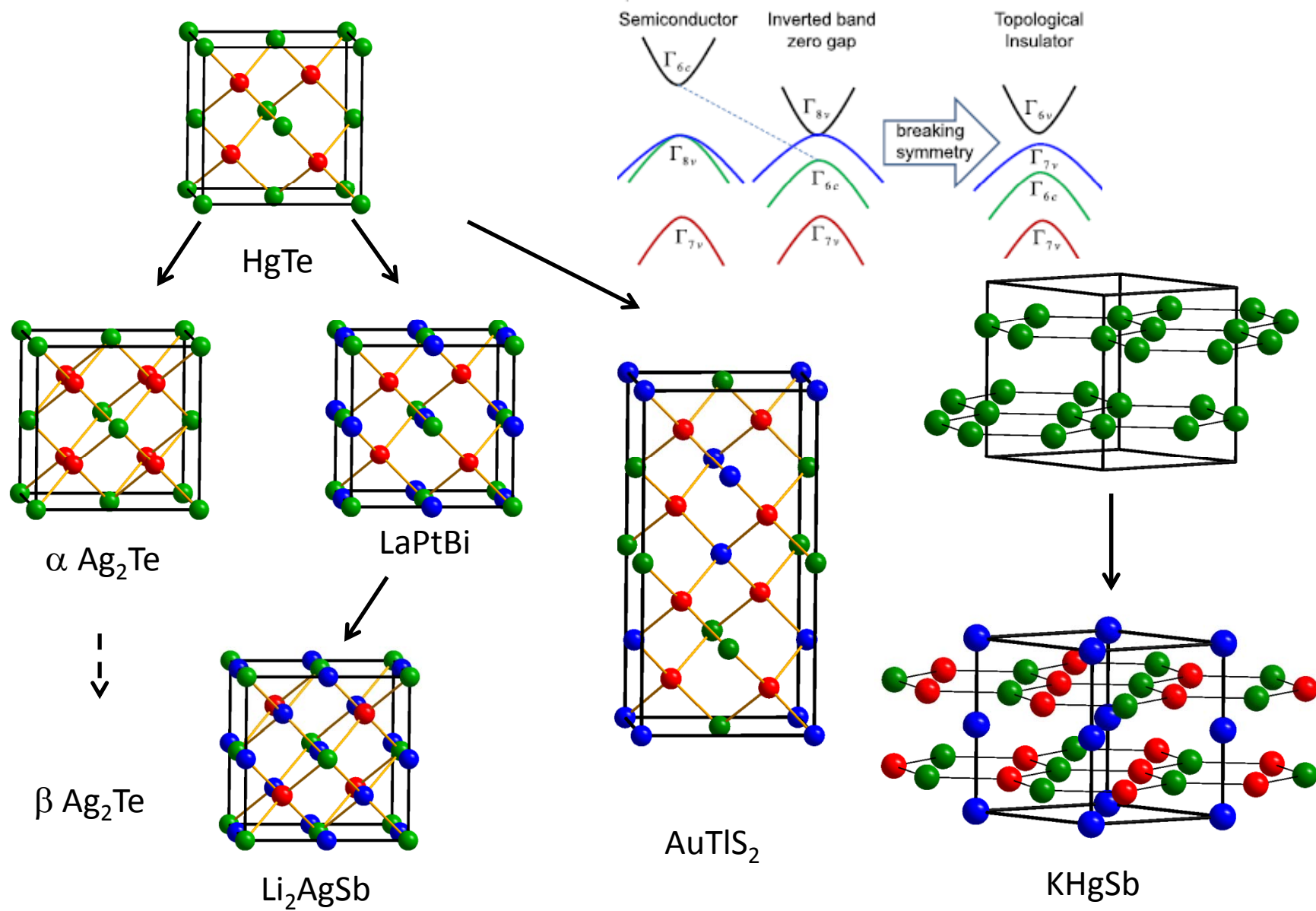


FIG. 4. Time-reversal symmetry-breaking quintet pairing states: (a) the E pairing state; (b) the T_2 pairing state with $\mathbf{l} = (1, i, 0)$; (c) the T_2 pairing state with $\mathbf{l} = (1, -e^{2\pi i/3}, e^{4\pi i/3})$. The color indicates the phase while the saturation gives the gap magnitude. Black points or lines indicate nodes of the gap.

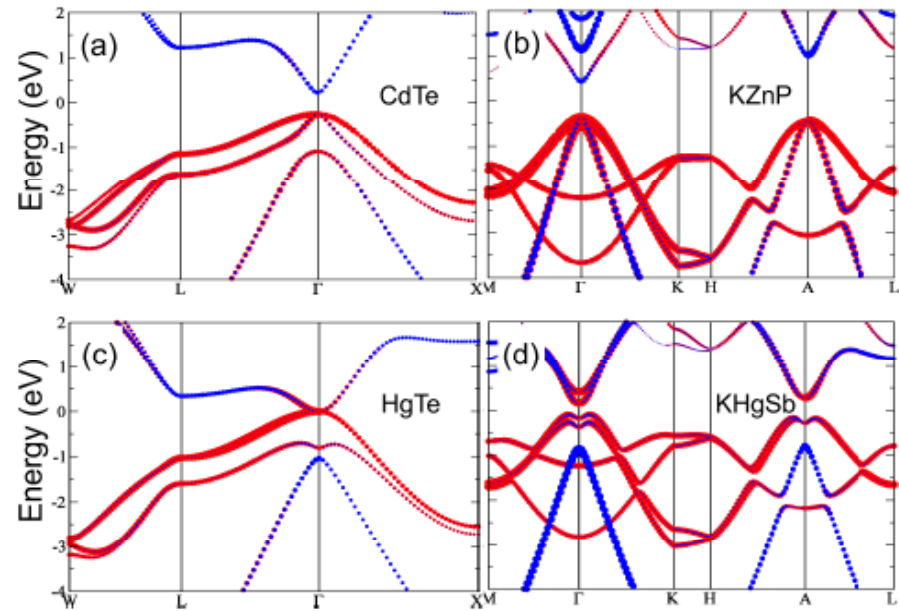
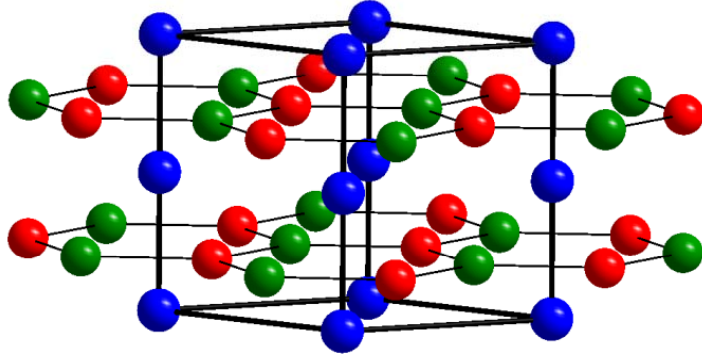


Structure to Property





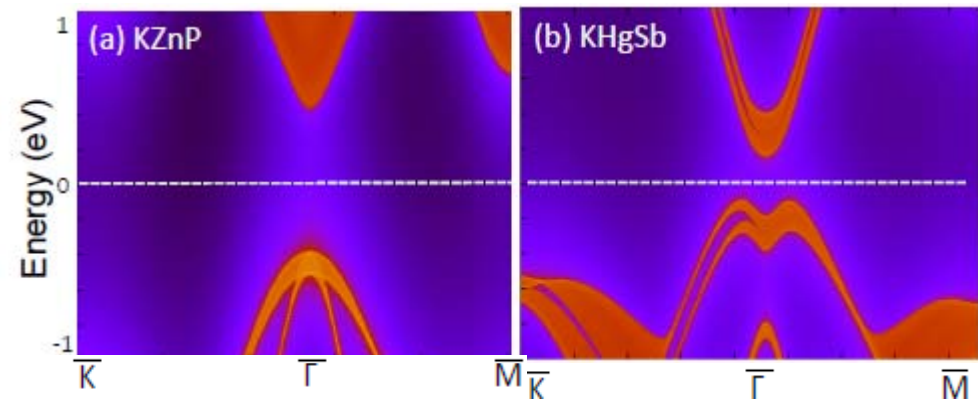
Honeycomb from sp^3 to sp^2



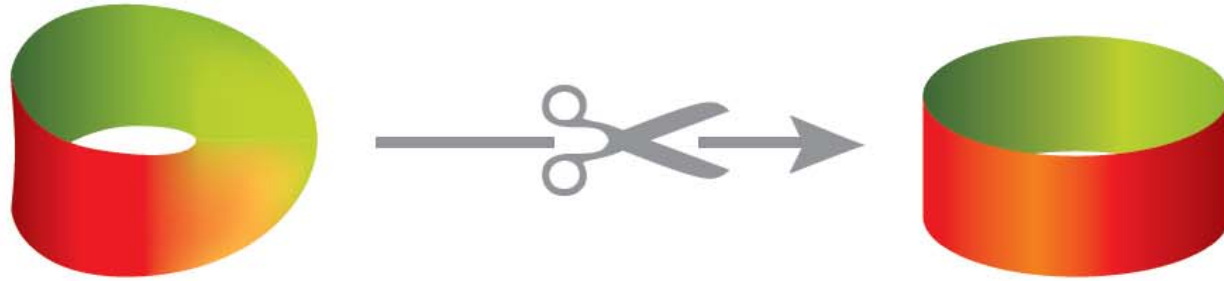
Band inversion is found in the heavier compounds

No surface state? Why ?

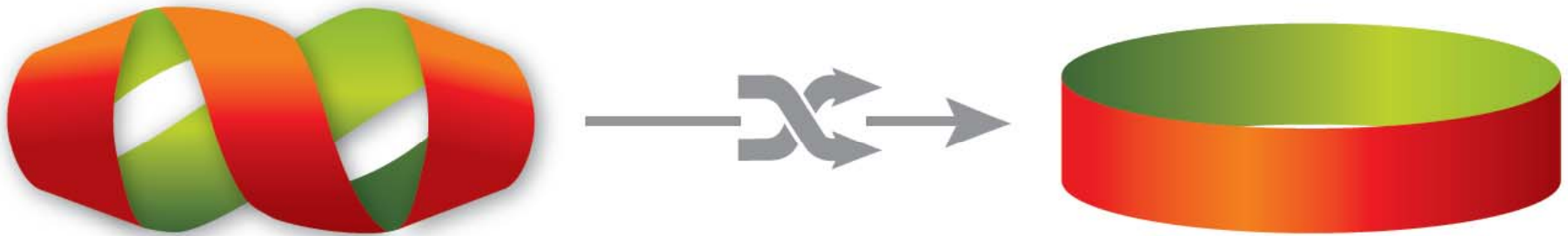
→ Interaction between the two layers in the unit cell and two Dirac Cones



a)

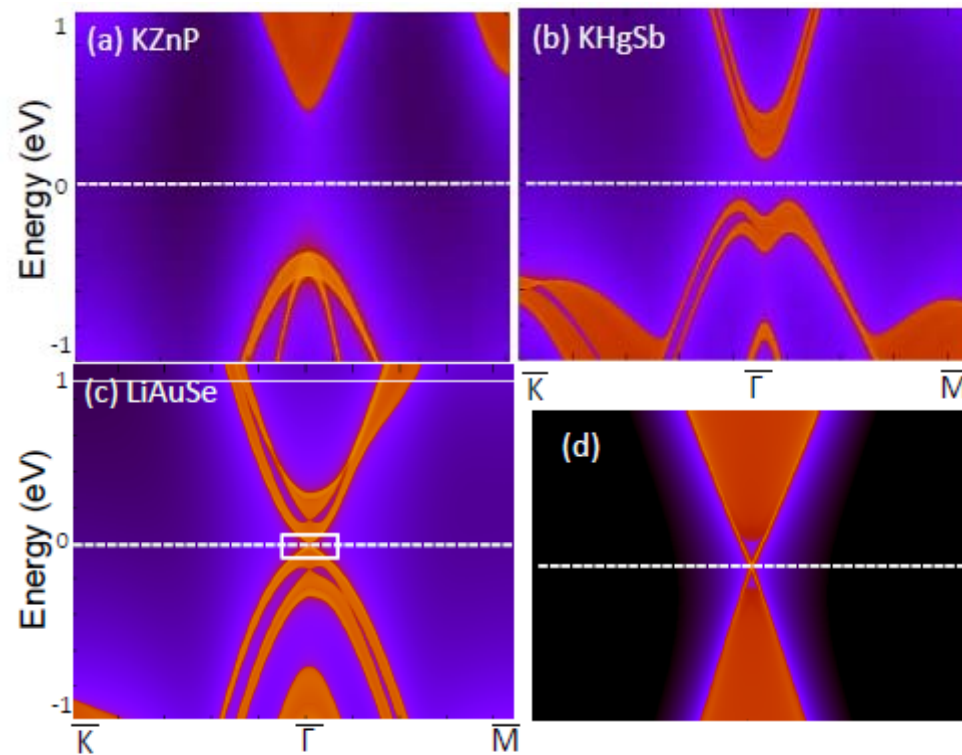
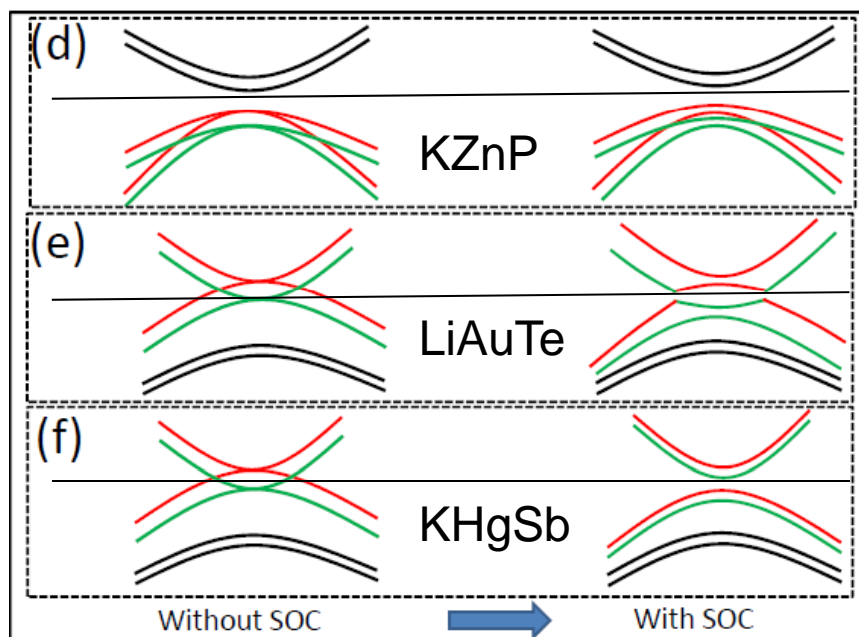
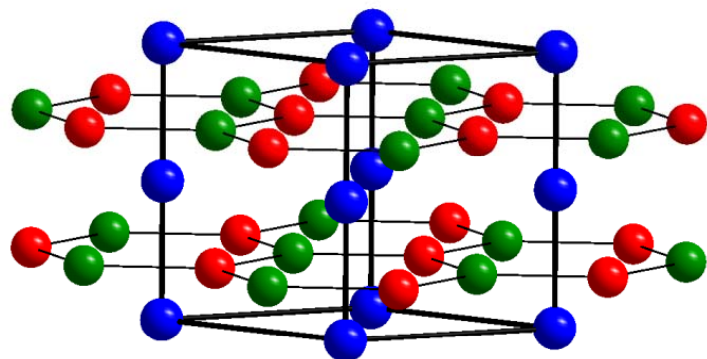


b)





Honeycomb from sp^3 to sp^2





Honeycomb: Weak TI



Sb-s Sb-s
Crystal field SOC

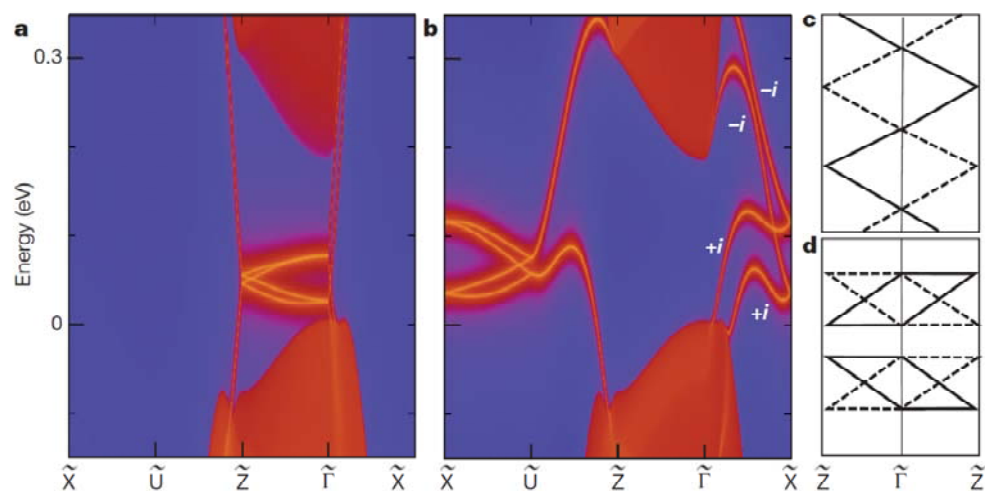




ARTICLE

Hourglass fermions

Zhijun Wang^{1*}, A. Alexandradinata^{1,2*}, R. J. Cava³ & B. Andrei Bernevig¹



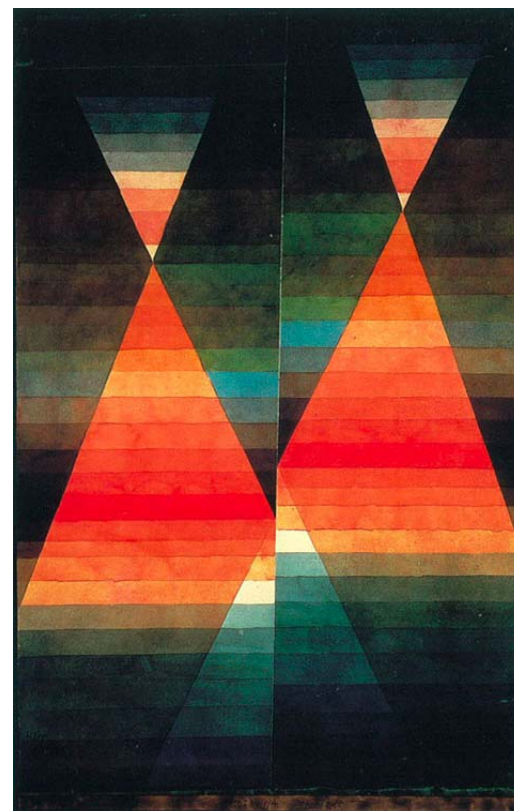
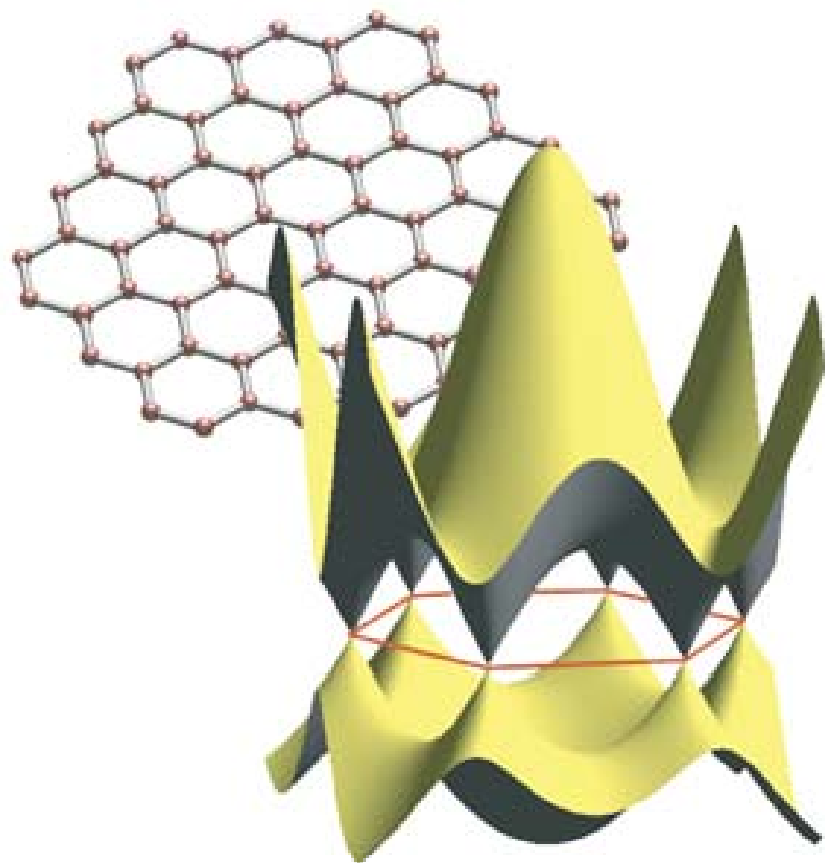


Weyl Semimetals

Breaking symmetry - TaAs



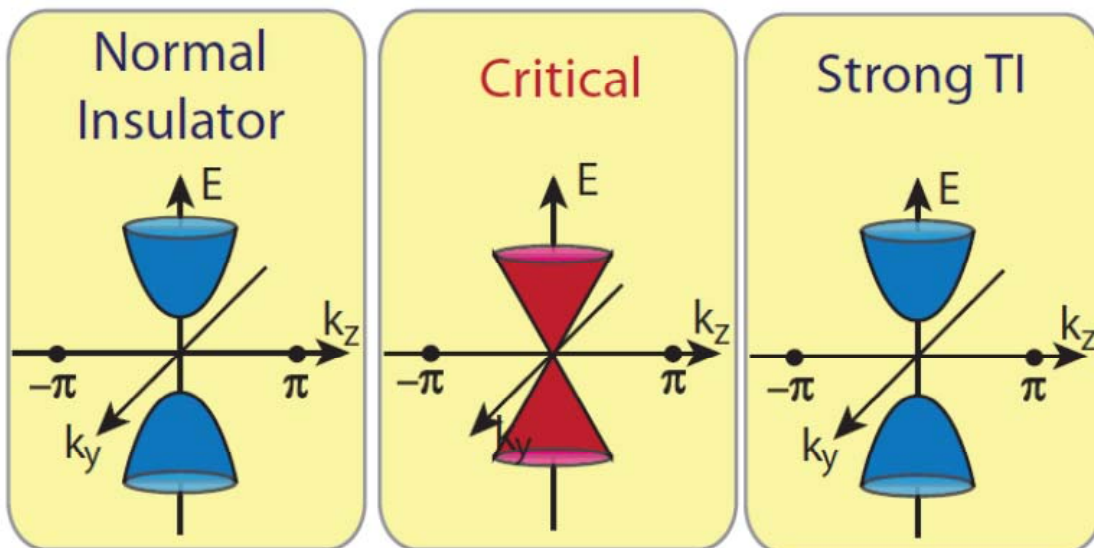
Dirac and Weyl semimetals



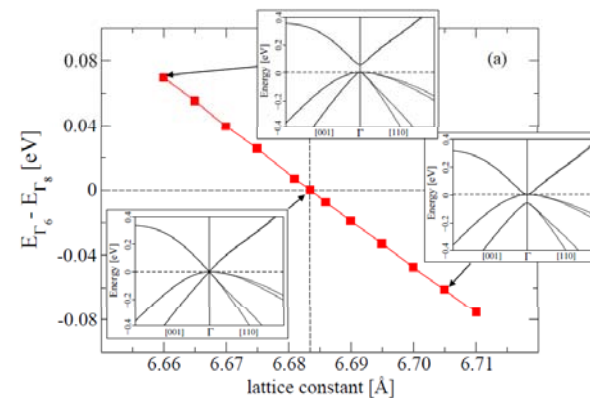
Paul Klee



Dirac semimetals



Bohm-Jung Yang and Naoto Nagaosa, arXiv:1404.0754



ARTICLE

Received 2 Dec 2013 | Accepted 2 Apr 2014 | Published 7 May 2014

DOI: 10.1038/ncomms4786

Observation of a three-dimensional topological Dirac semimetal phase in high-mobility Cd₃As₂

Madhab Neupane^{1,*}, Su-Yang Xu^{1,*}, Raman Sankar^{2,*}, Nasser Alidoust¹, Guang Bian¹, Chang Liu¹, Ilya Belopolski¹, Tay-Rong Chang³, Horng-Tay Jeng^{3,4}, Hsin Lin⁵, Arun Bansil⁶, Fangcheng Chou² & M. Zahid Hasan^{1,7}



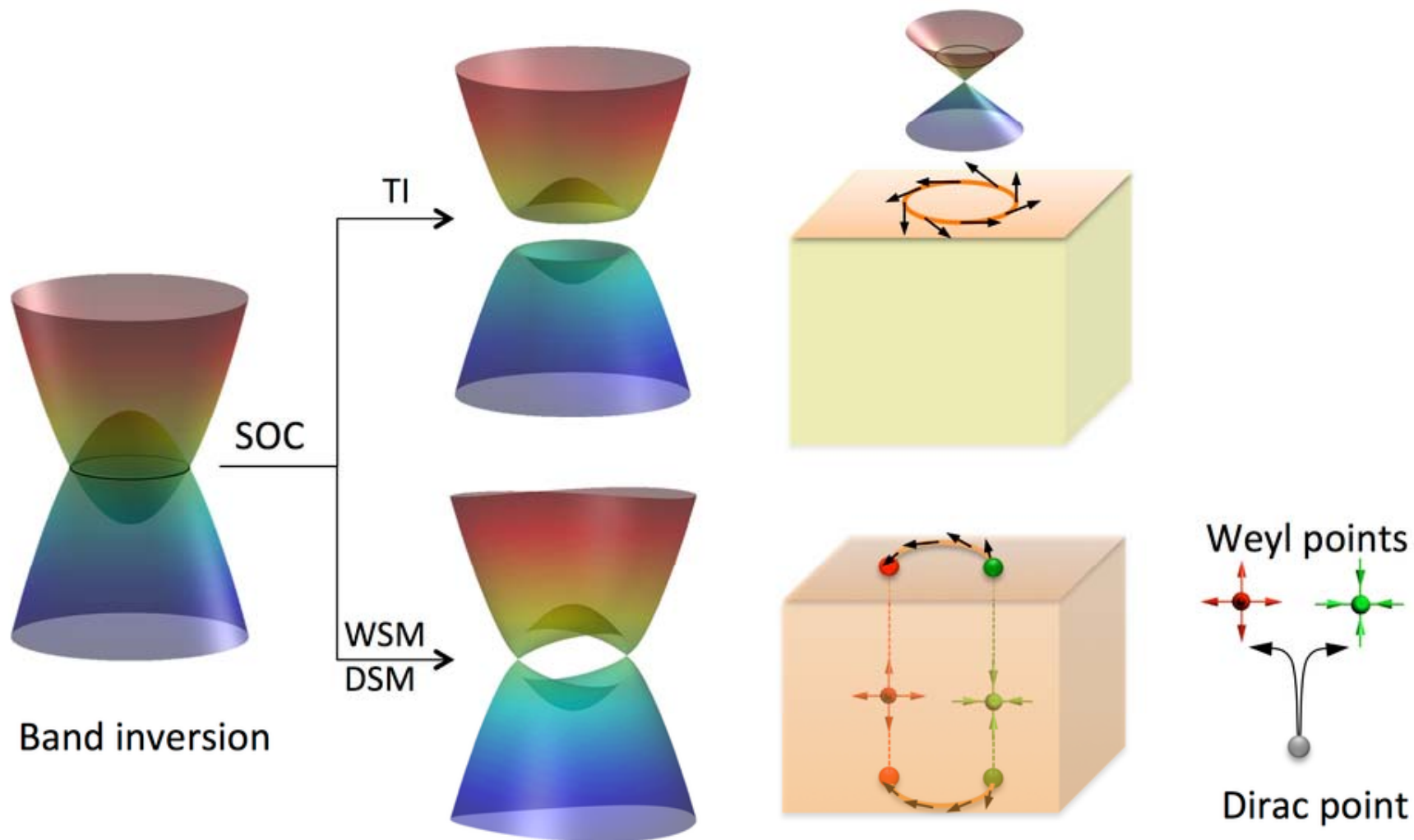
Observation of Fermi arc surface states in a topological metal

Su-Yang Xu *et al.*
Science **347**, 294 (2015);
DOI: 10.1126/science.1256742





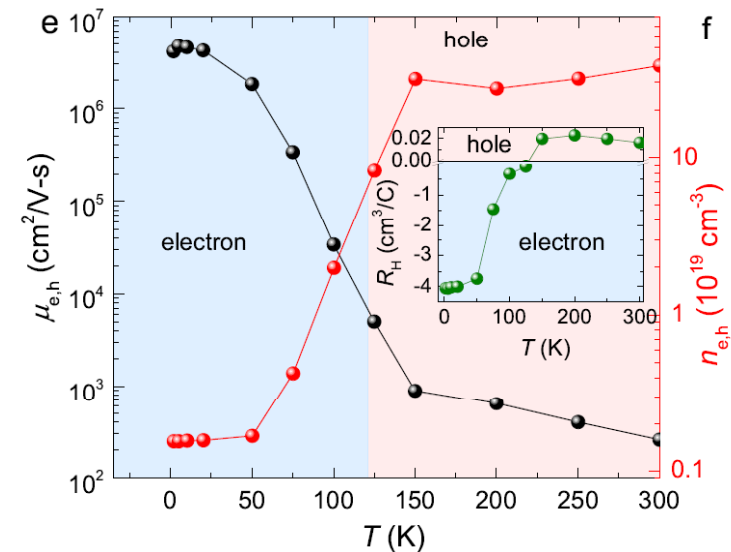
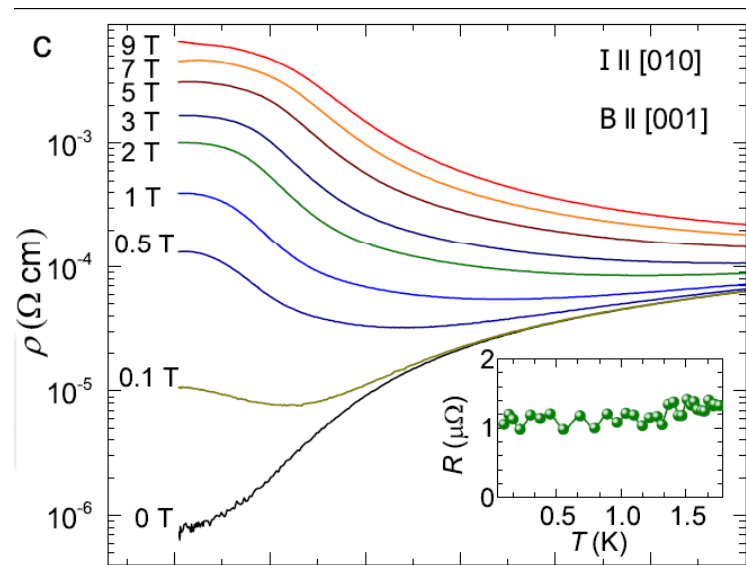
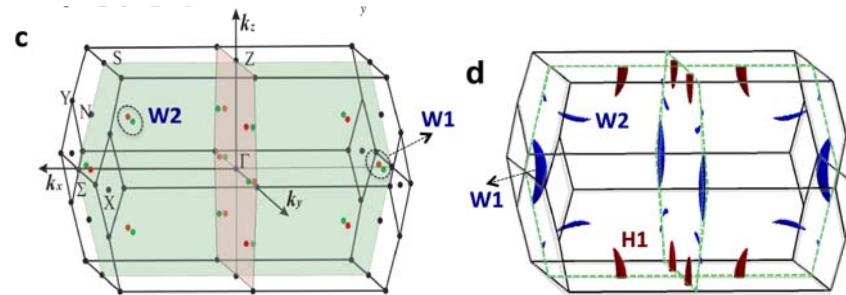
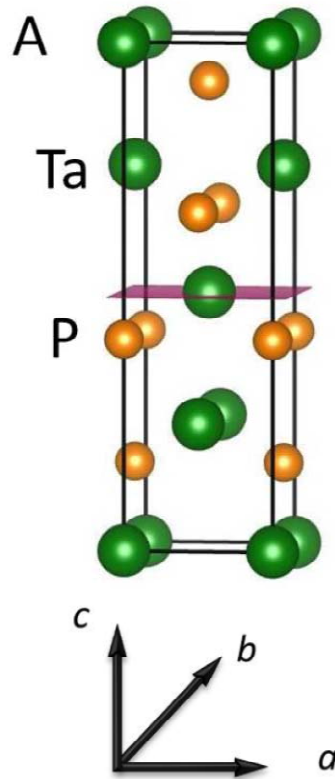
Weyl semimetals





Weyl semimetals in non centro NbP

NbP, NbAs, TaP, TaAs



NbP is a topological Weyl semimetal

- with massless relativistic electrons
- extremely large magnetoresistance of **850,000%** at 1.85 K, 9T (250% at room temperature)
- an ultrahigh carrier mobility of **$5 \cdot 10^6 \text{ cm}^2 / \text{V s}$**

Shekhar, et al. , Nature Physics 11 (2015) 645,
Frank Arnold, et al. Nature Communication 7 (2016) 11615

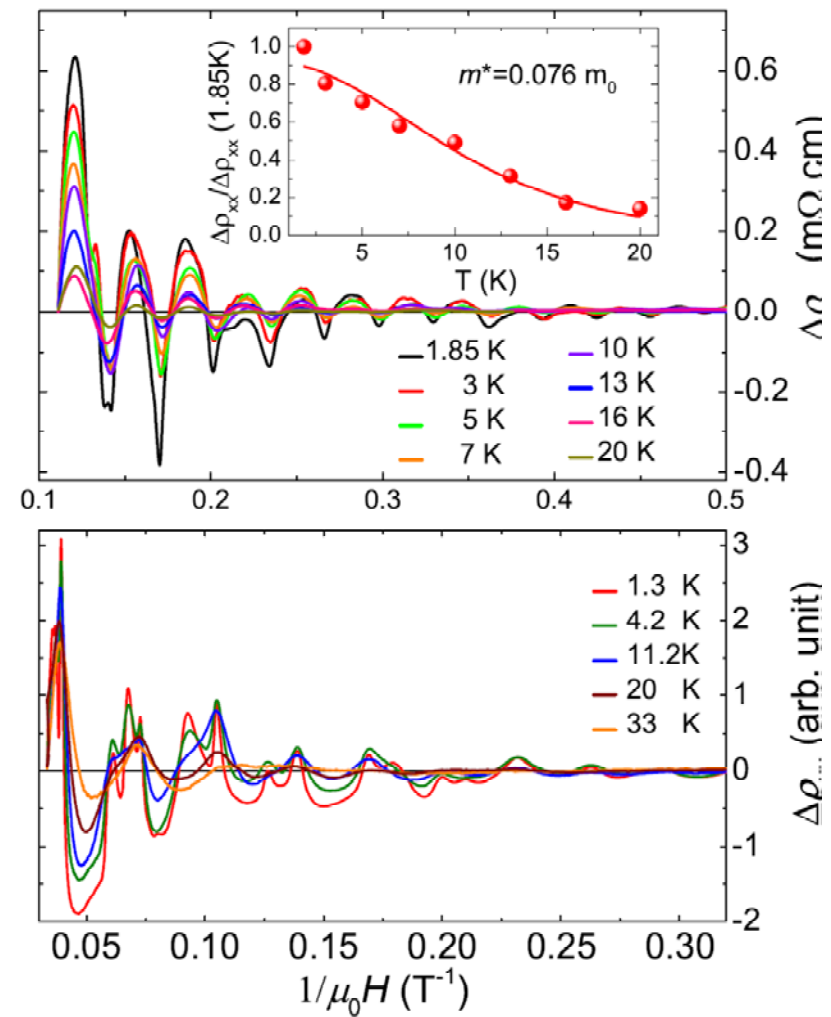
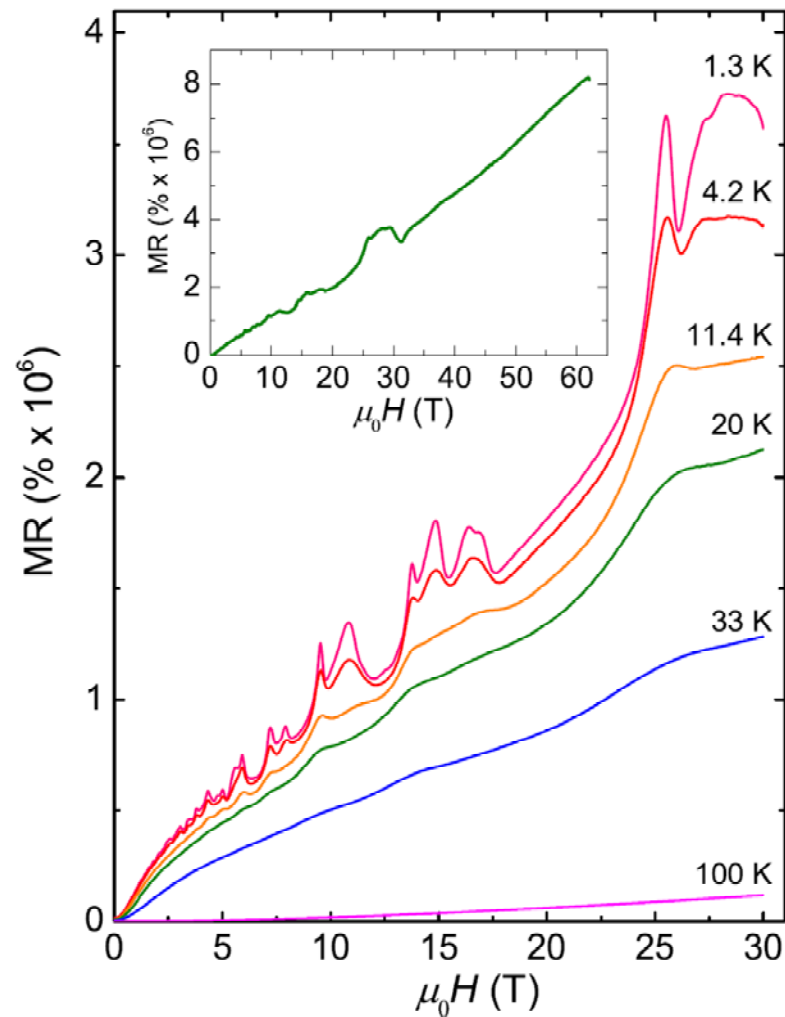
Weng, et al. Phys. Rev. X 5, 11029 (2015)

Huang . et al. preprint arXiv:1501.00755

Yang, et al. Nature Phys. 11 (2015) 728, preprint arXiv:1507.00521v1

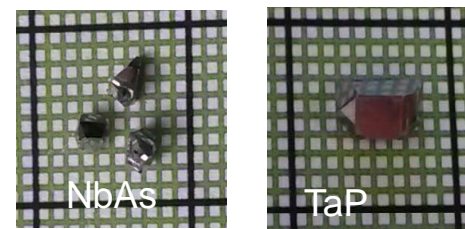
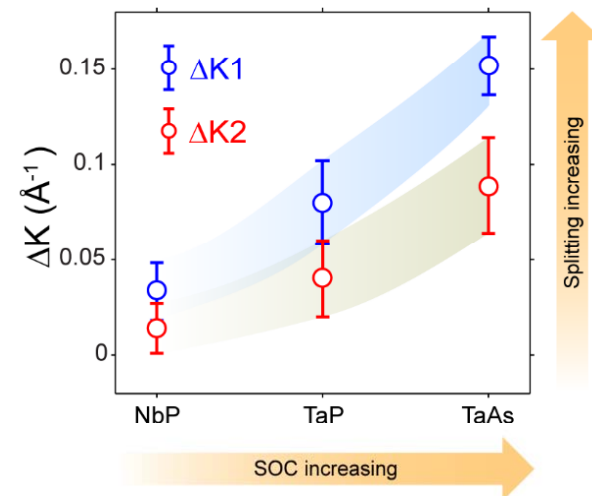
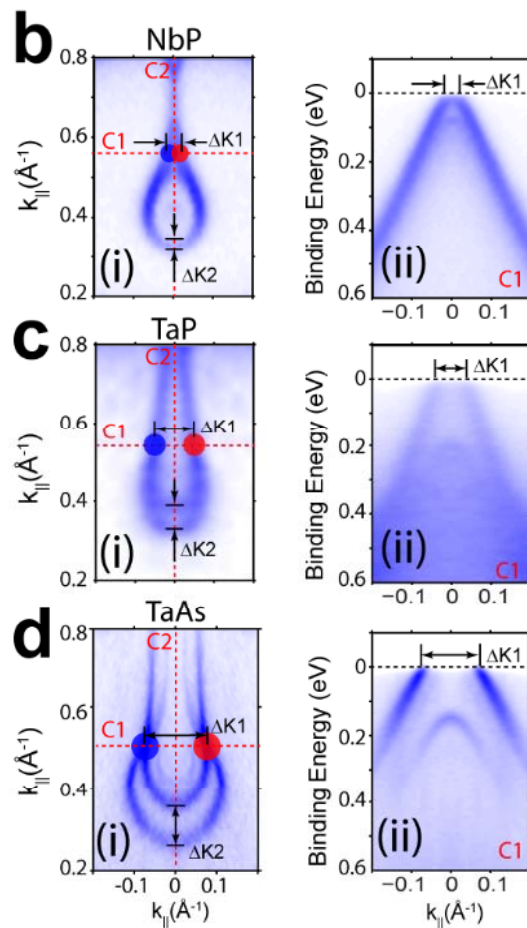
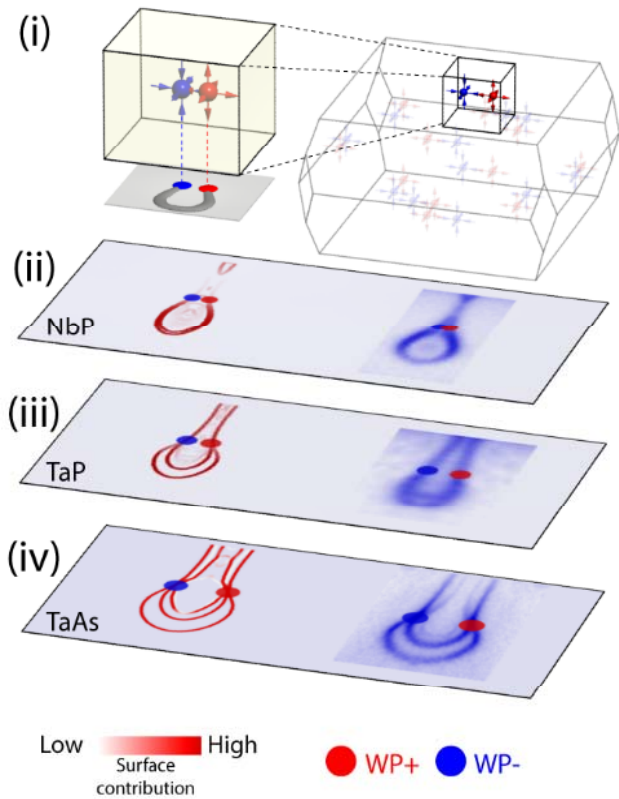


NbP quantum oscillations





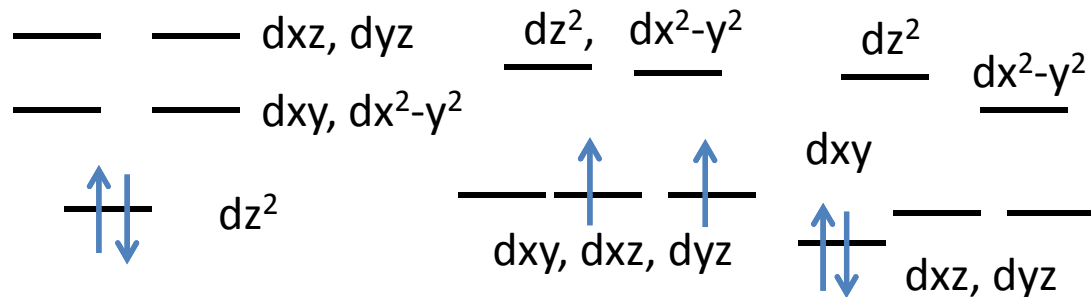
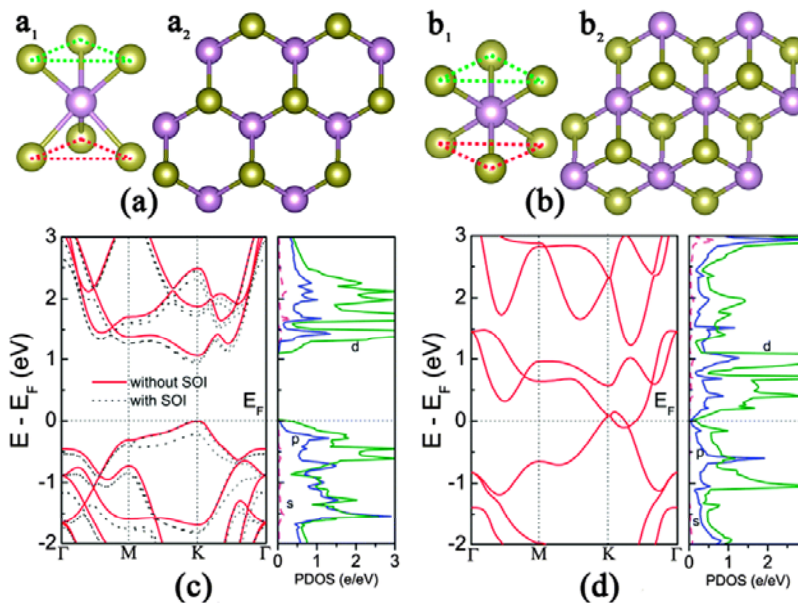
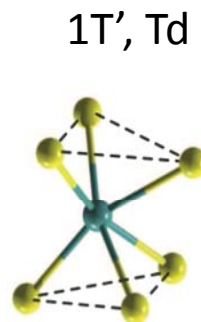
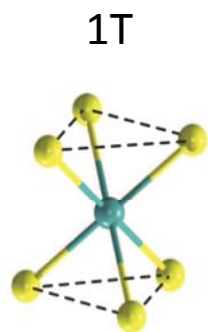
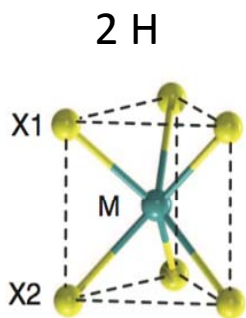
NbP, TaP, TaAs





MoS₂ : crystal field

Mo⁴⁺ (d²)
S²⁻ (s²p⁶)



Semiconductor

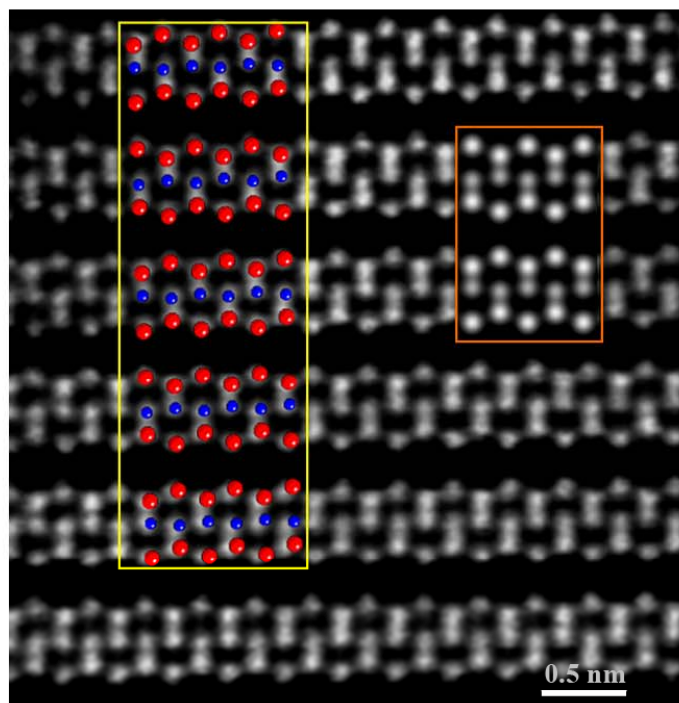
Metal

Semimetal

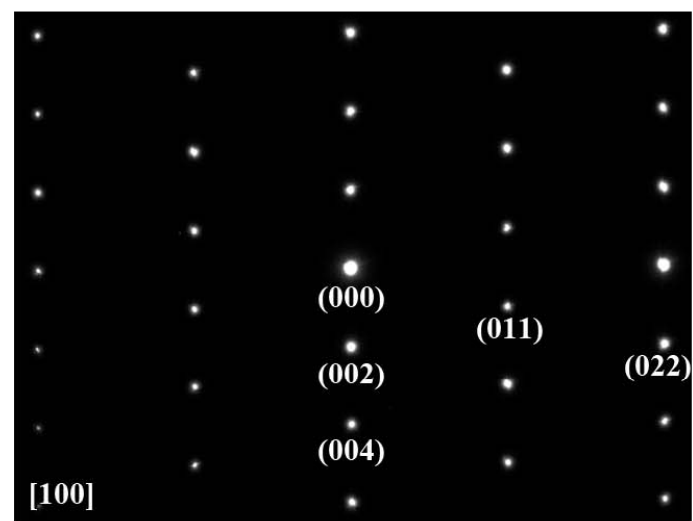


T_d-MoTe₂

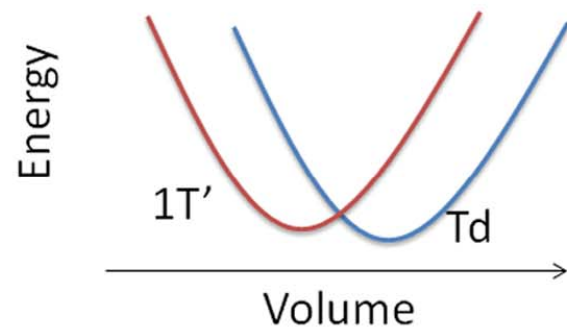
a



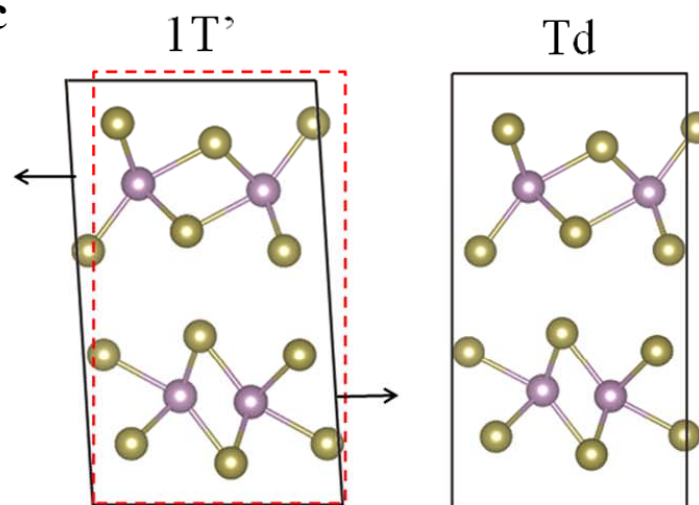
b



d

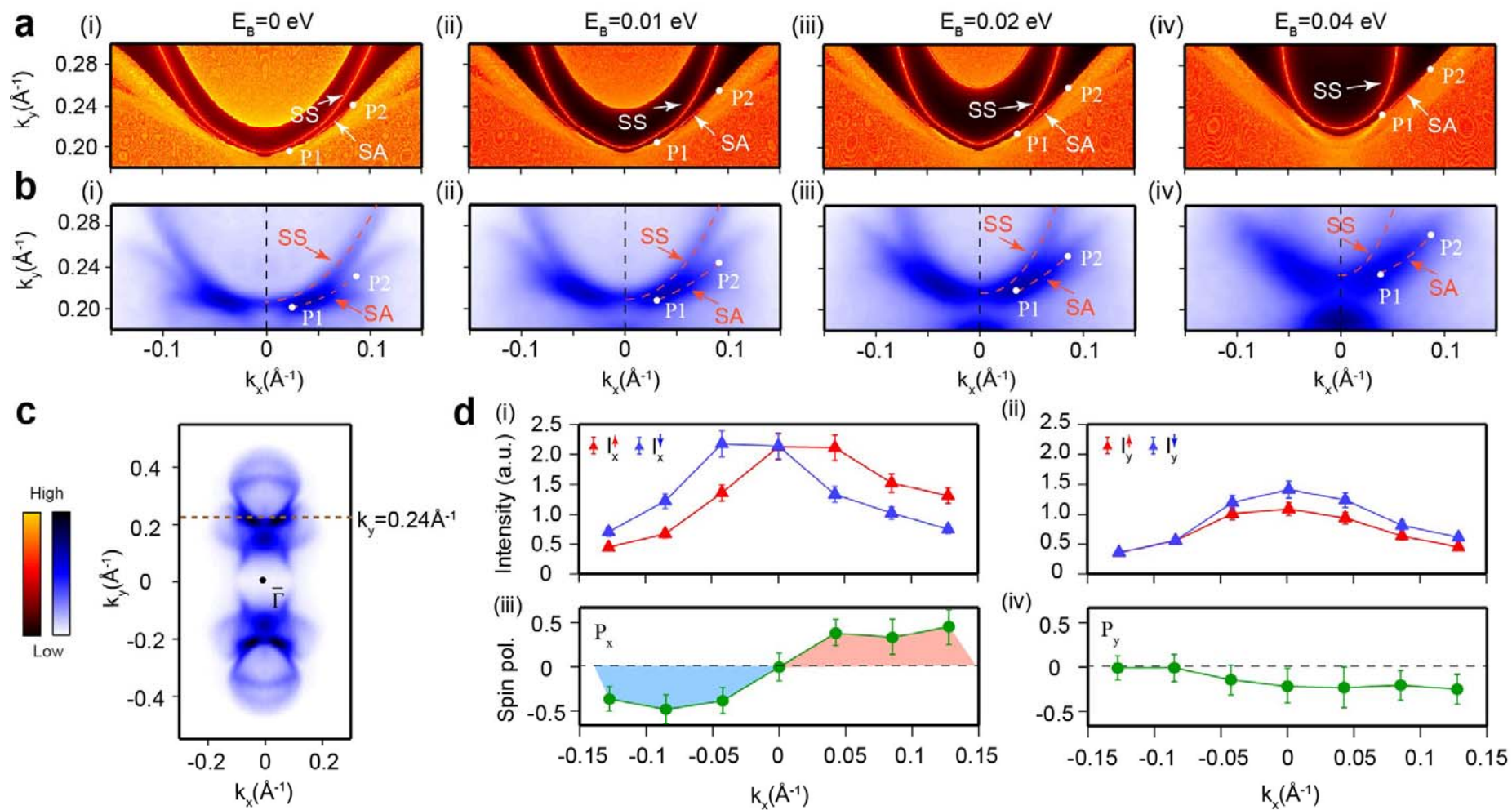


c





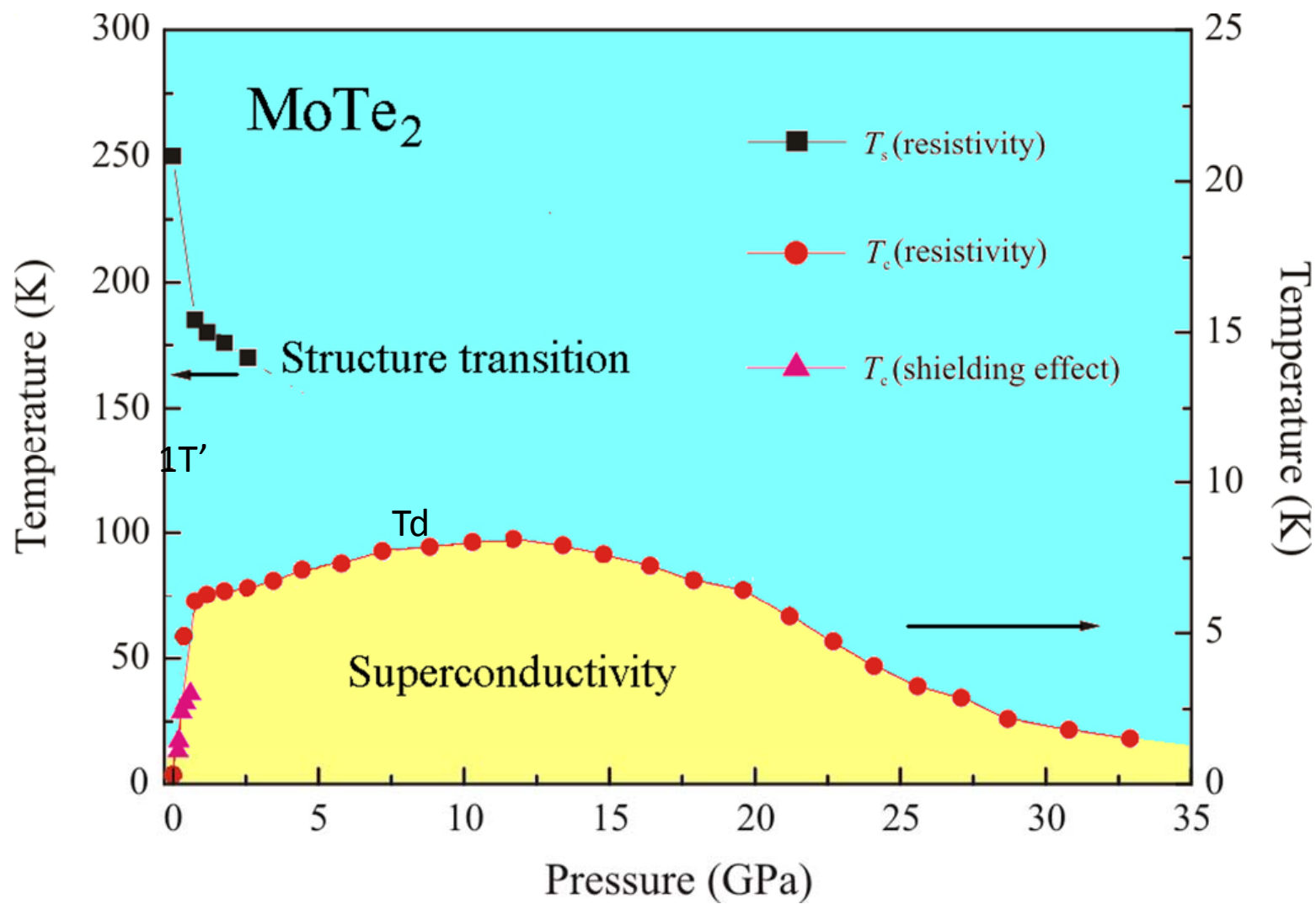
MoTe₂: Weyl Semimetal?



J. Jiang, Z. K. Liu, Y. Sun, H. F. Yang, R. Rajamathi, Y. P. Qi, L. X. Yang, C. Chen, H. Peng, C.-C. Hwang, S. Z. Sun, S.-K. Mo, I. Vobornik, J. Fujii, S. S. P. Parkin, C. Felser, B. H. Yan, Y. L. Chen, preprint: arXiv: 1604.00139



MoTe₂





Magnetic Weyl Semimetals

Induced

Intrinsic



REPtBi... 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

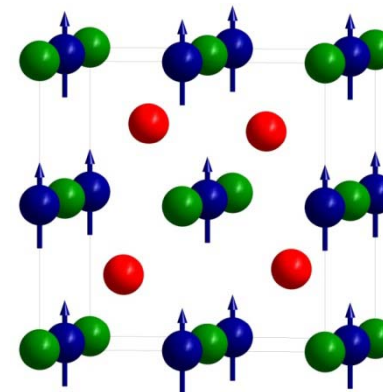
J. Appl. Phys. **70** (10), 15 November 1991

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



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

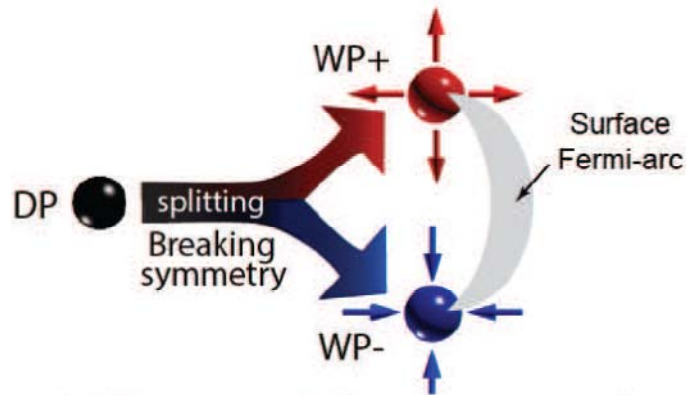


S. Chadov et al., Nat. Mater. 9, 541 (2010).

H. Lin et al., Nat. Mater. 9, 546 (2010).



Weyl semimetals



We need time reversal symmetry breaking
(Dirac points are at high symmetry points
Weyl points are not at high symmetry points)

- Structural distortion
- Application of magnetic field or magnetism

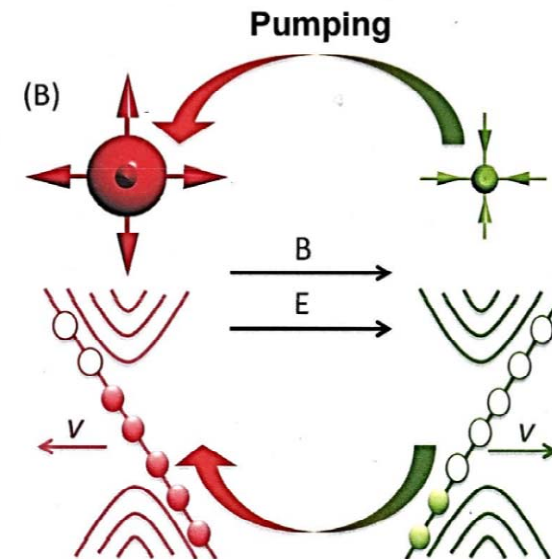
3D topological Weyl semimetals - breaking Time reversal symmetry – by transport

1. Intrinsic anomalous Hall effect

2. Chiral anomaly

$$\partial_\mu j_\chi^\mu = \chi \frac{e^3}{4\pi^2 \hbar^2} \mathbf{E} \cdot \mathbf{B}$$

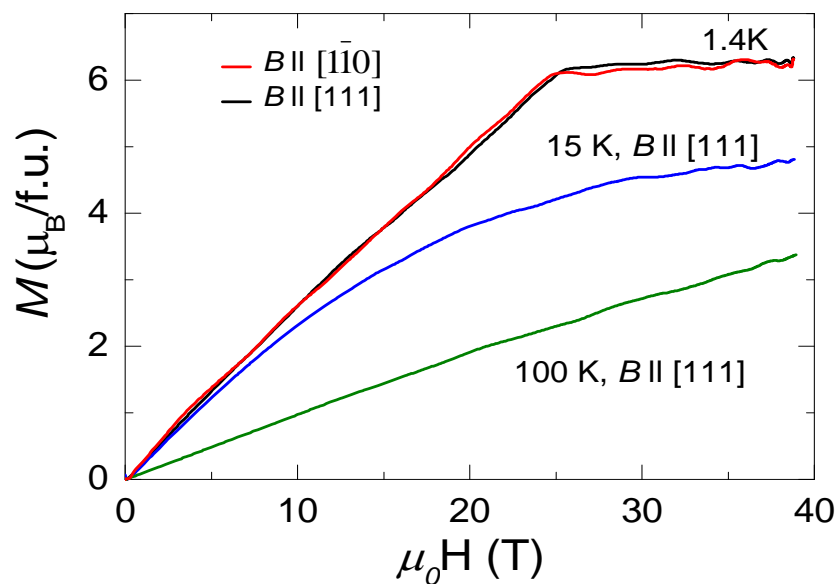
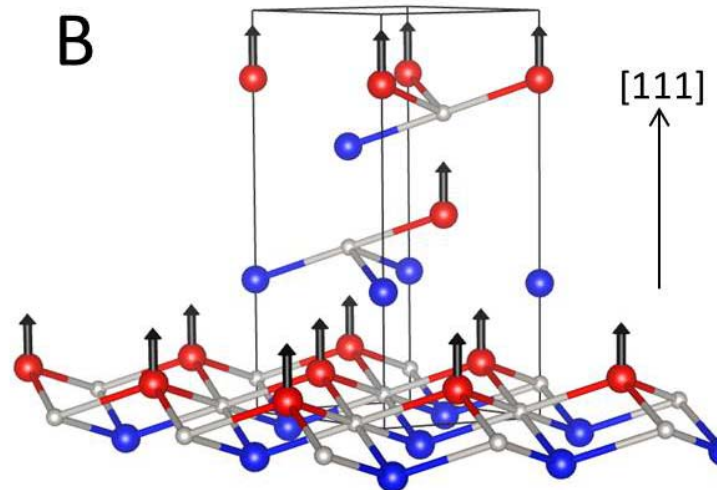
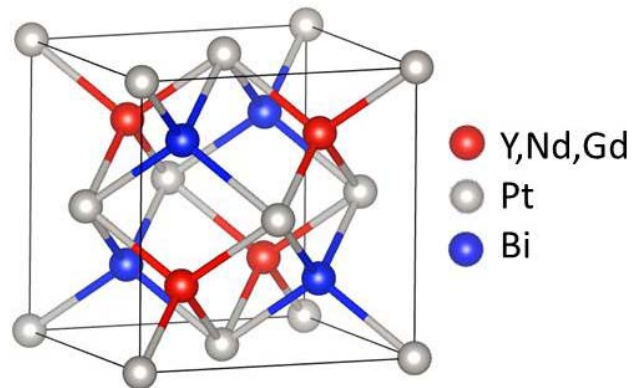
$$\sigma_a = \frac{e^3 v_f^3}{4\pi^2 \hbar \mu^2 c} B^2$$



- S. L. Adler, Phys. Rev. 177, 2426 (1969)
 J. S. Bell and R. Jackiw, Nuovo Cim. A60, 47 (1969)
 AA Zyuzin, AA Burkov - Physical Review B (2012)
 AA Burkov, L Balents, PRL 107 12720 (2012)



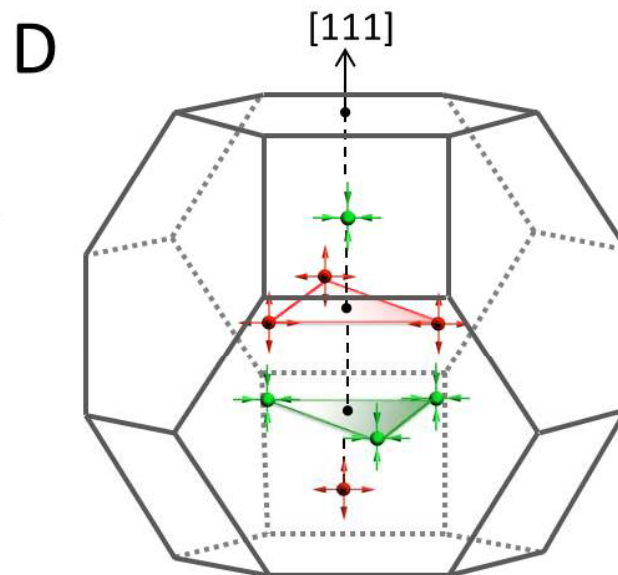
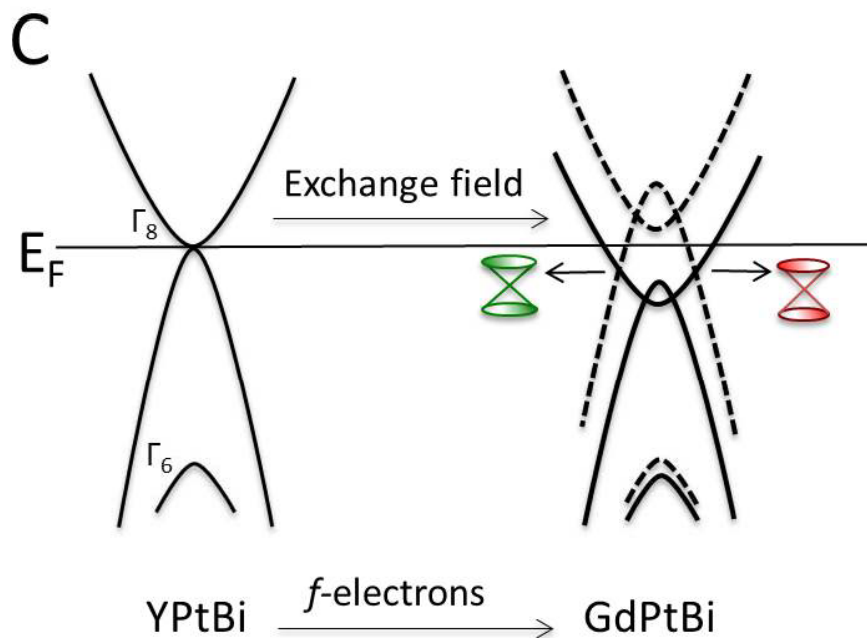
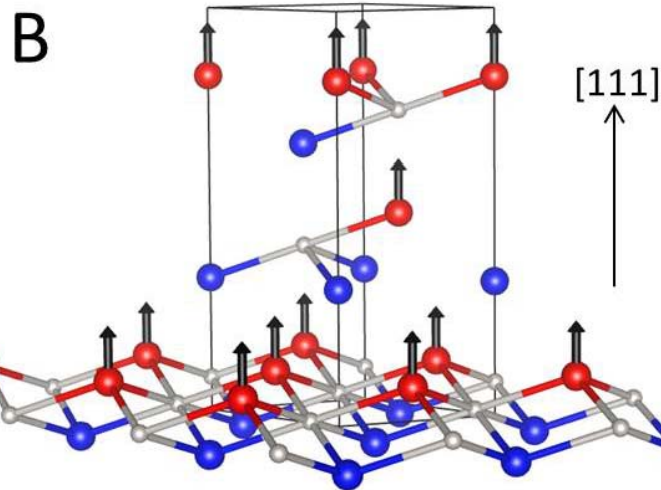
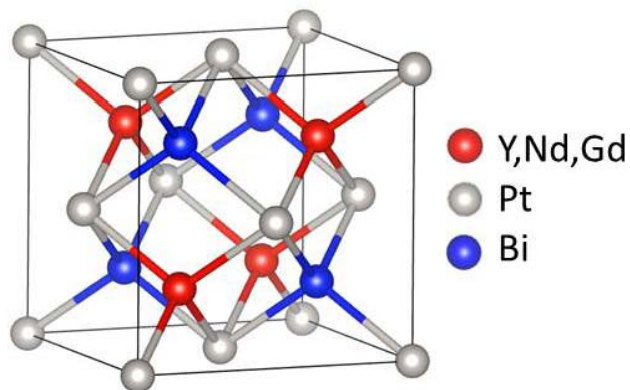
GdPtBi is magnetic



GdPtBi is an Antiferromagnet below 10 K
However it is very soft and the spins can be tuned in a magnetic field



Weyl GdPtBi in a magnetic field

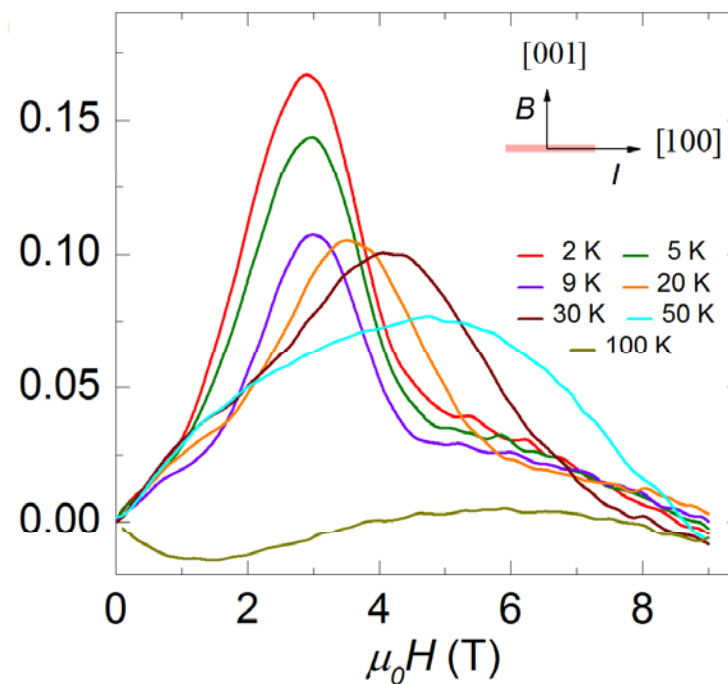
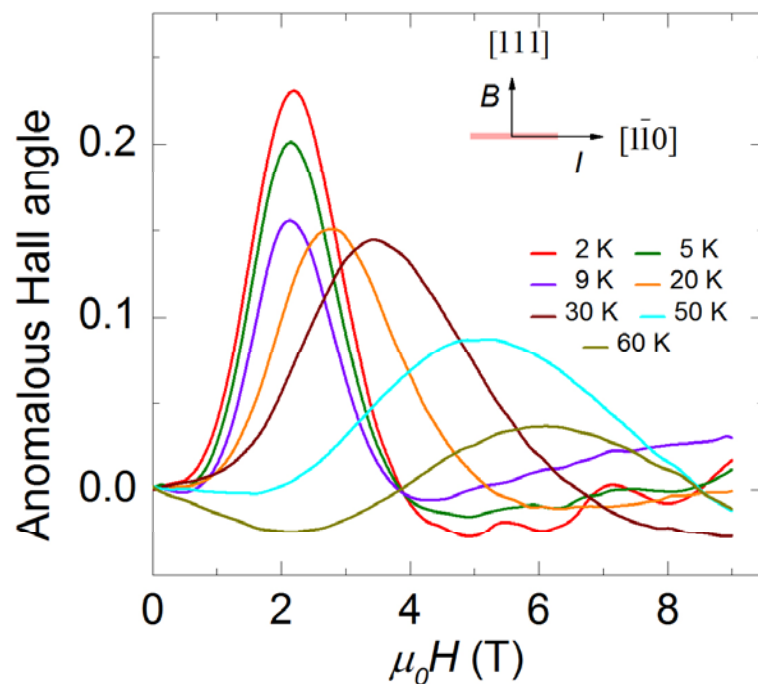


C. Shekhar et al., arXiv:1604.01641, (2016).

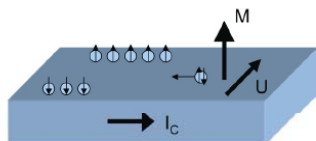
M. Hirschberger et al., Nature Mat. Online arXiv:1602.07219, (2016).



GdPtBi – Anomalous Hall Effect



Anomalous Hall effect
1881



In ferromagnets an AHE scales with the magnetic moment

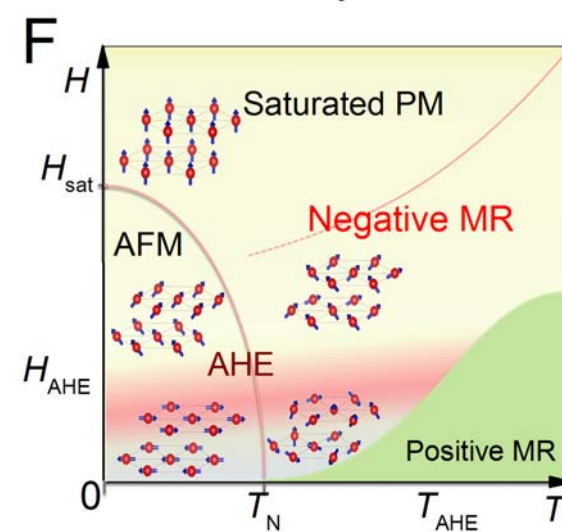
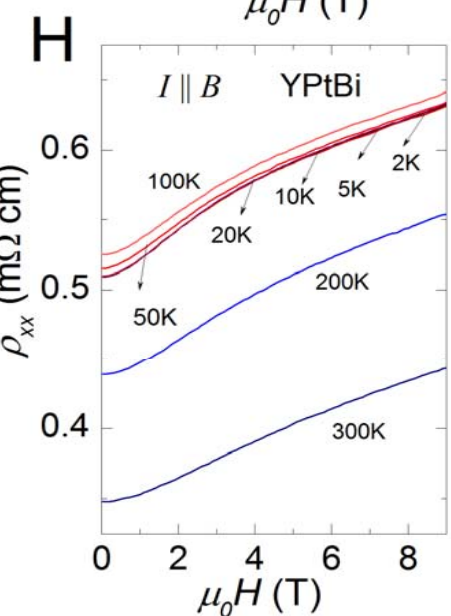
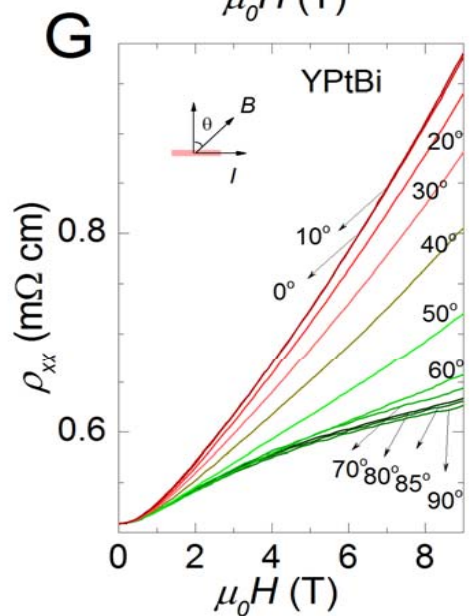
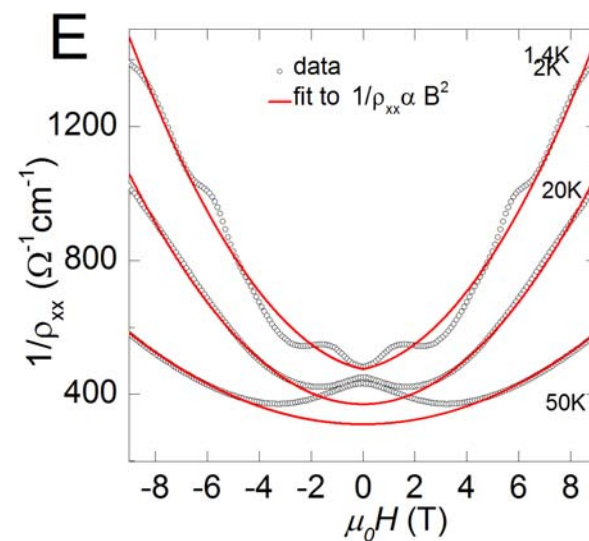
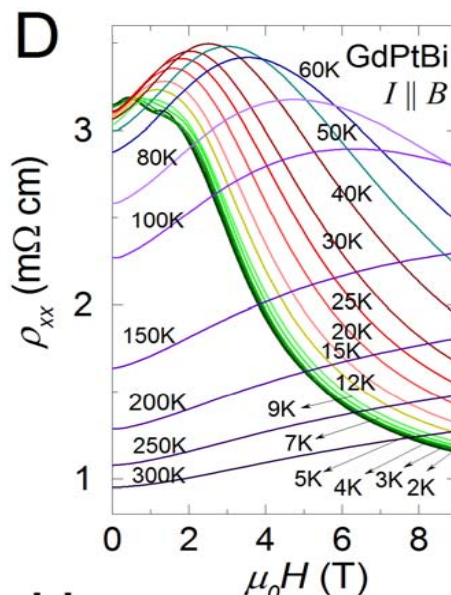
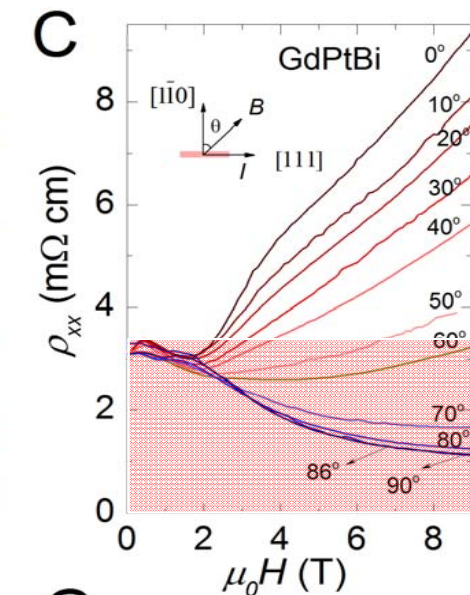
Antiferromagnet show no AHE

A Hall angle of 0.2 is exceptional – 1 would be the **Q**uantum AHE

T. Suzuki,... & J. G. Checkelsky, Nature Physics (2016) doi:10.1038/nphys3831
Shekhar et al., arXiv:1604.01641, (2016)



Chiral Anomaly – neg. quadratic MR

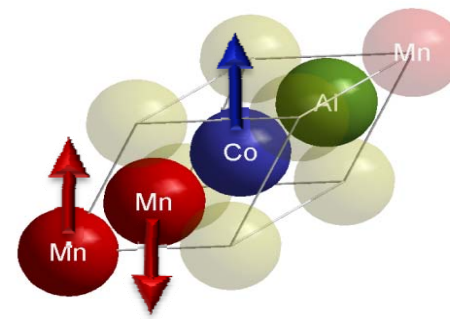
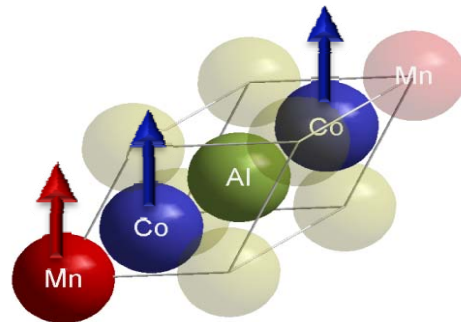
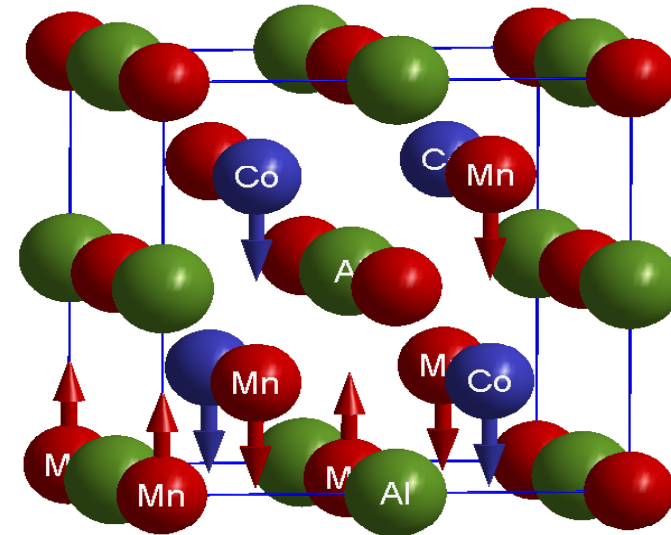
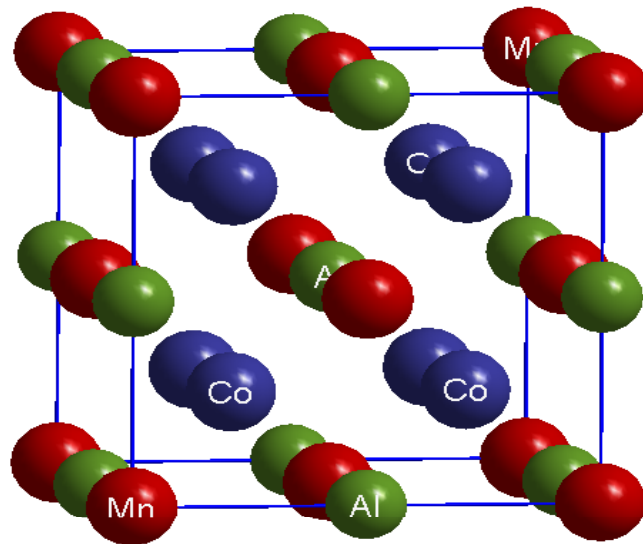


C. Shekhar et al., arXiv:1604.01641, (2016).

M. Hirschberger et al. Nature Mat. online, arXiv:1602.07219, (2016).



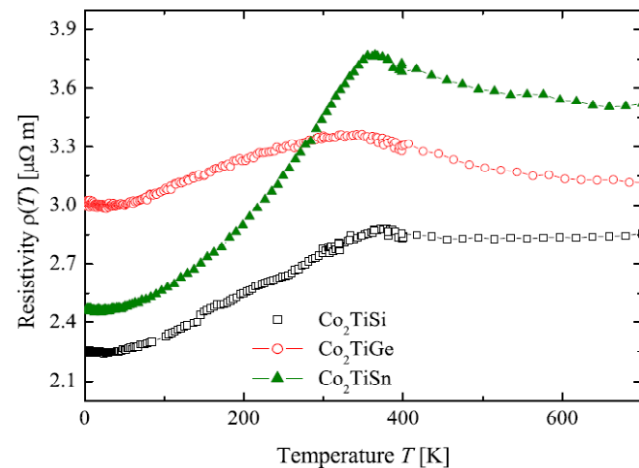
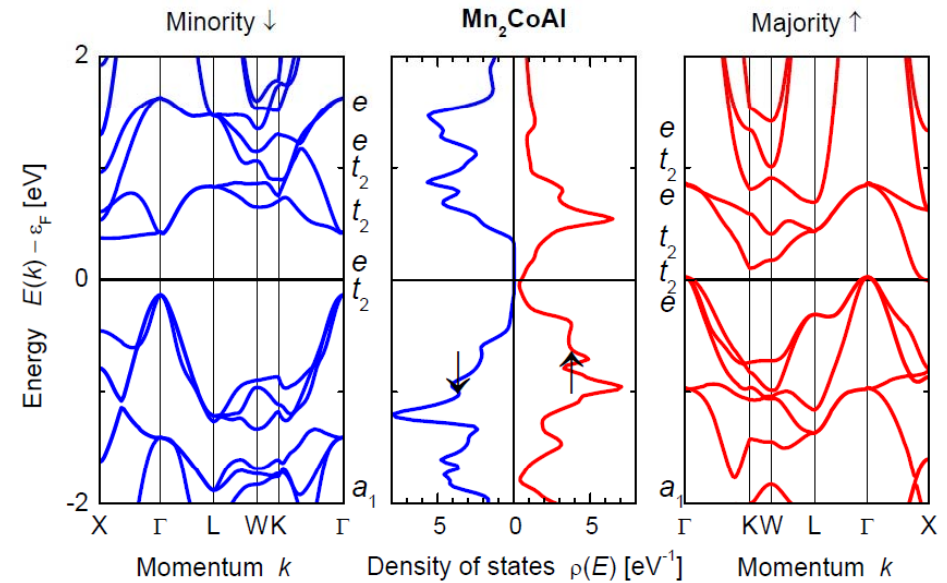
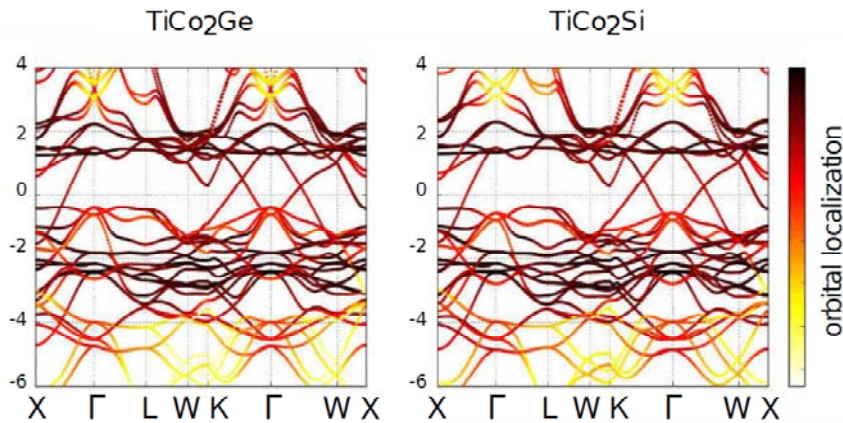
Magnetic Heusler compounds with and without inversion



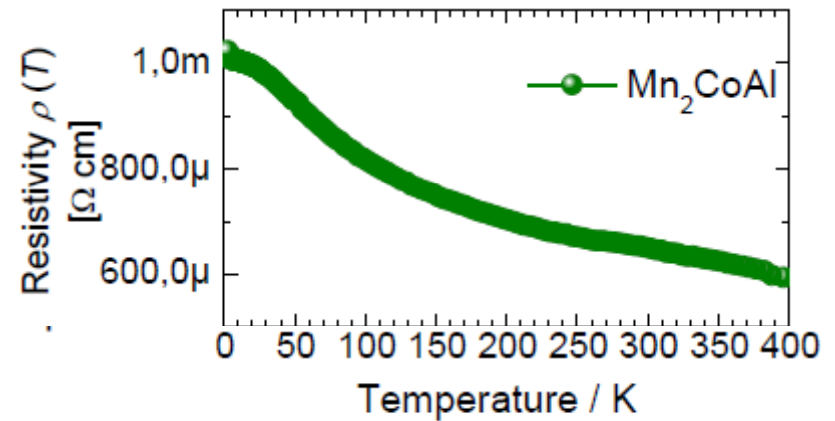


Magnetic Heusler compounds with and without inversion

26 Valence electrons



Zhijun Wang, et al., arXiv:1603.00479
Guoqing Chang et al., arXiv:1603.01255



Barth et al. PRB 81, 064404 2010

Ouardi et al., Phys. Rev. Lett. 110 (2013) 100401



AHE in half metallic ferromagnets

PHYSICAL REVIEW B **85**, 012405 (2012)

Berry curvature and the anomalous Hall effect in Heusler compounds

Jürgen Kübler^{1,*} and Claudia Felser²

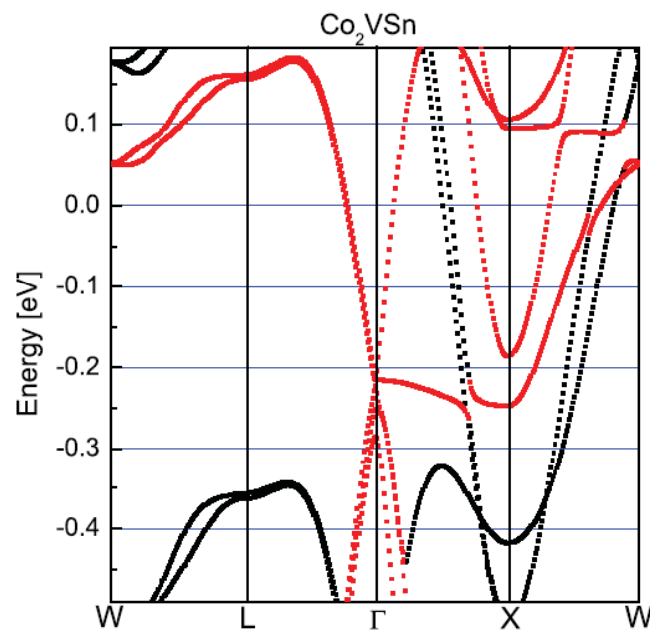


FIG. 4. (Color online) Band structure near the Fermi edge of Co_2VSn . Majority-spin electron states appear in red, minority-spin states in black. Note the Dirac cone at the Γ point at about -0.22 eV.

Compound ^a	N_V	a (nm)	M^{exp}	M^{calc}	σ_{xy}	P (%)
Co_2VGa	26	0.5779	1.92	1.953	66	65
Co_2CrAl	27	0.5727	1.7	2.998	438	100
Co_2VSn	27	0.5960	1.21	1.778	-1489	35
Co_2MnAl	28	0.5749	4.04	4.045	1800	75
Rh_2MnAl	28	0.6022		4.066	1500	94
Mn_2PtSn^b	28	0.4509 (1.3477)		6.66	1108	91
Co_2MnSn	29	0.5984	5.08	5.00	118	82
Co_2MnSi	29	0.5645	4.90	4.98	228	100

Kübler, Felser, PRB 85 (2012) 012405

Vidal et al Appl.Phys.Lett. 99 (2011) 132509

Kübler, Felser, Europhys. Lett. 114 (2016) 47005

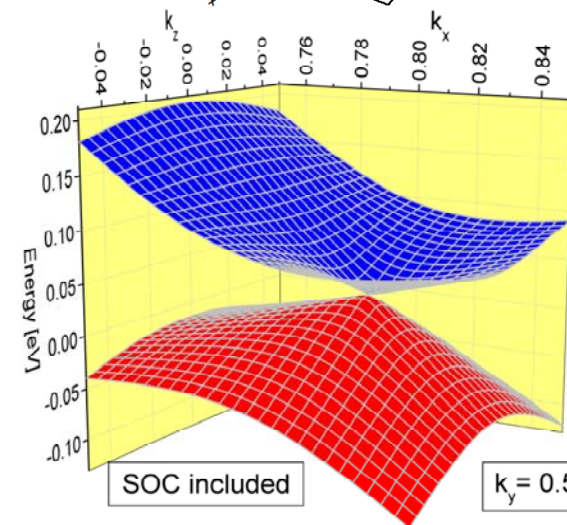
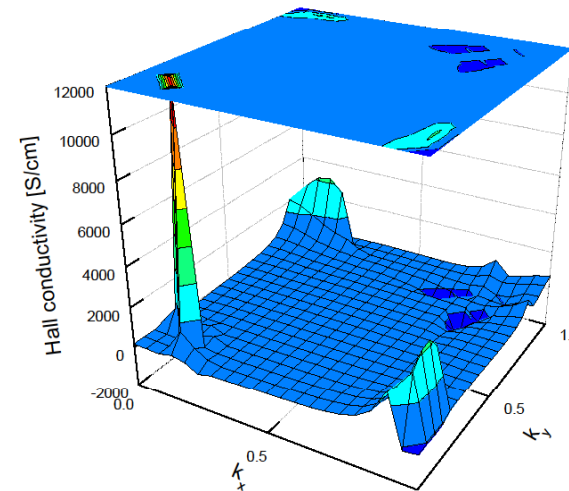
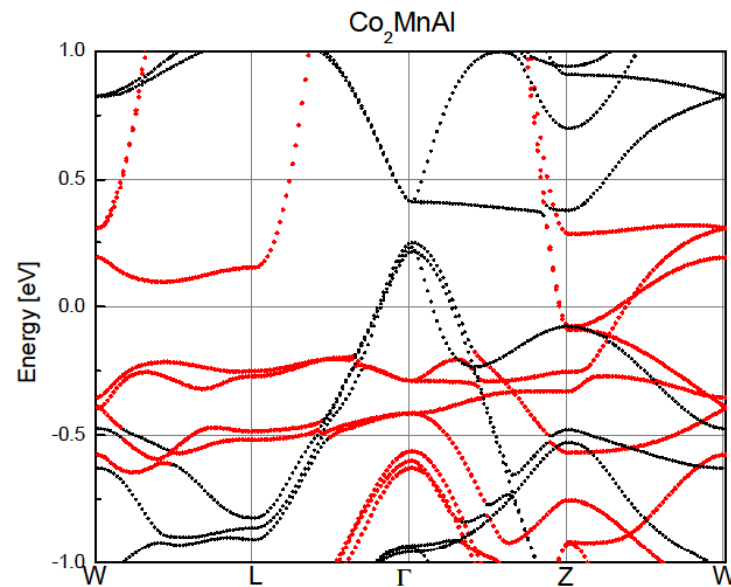


AHE in half metallic ferromagnets

Giant AHE in Co_2MnAl

$$\sigma_{xy} = 1800 \text{ S/cm calc.}$$

$$\sigma_{xy} \approx 2000 \text{ S/cm meas.}$$

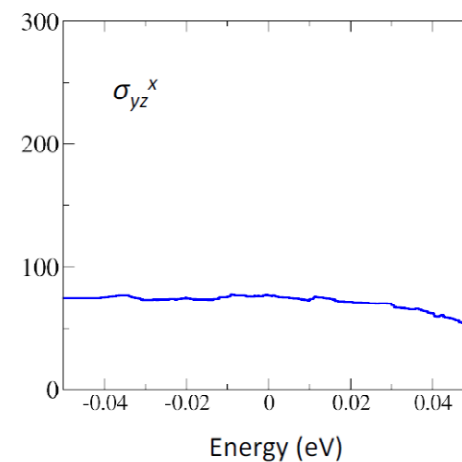
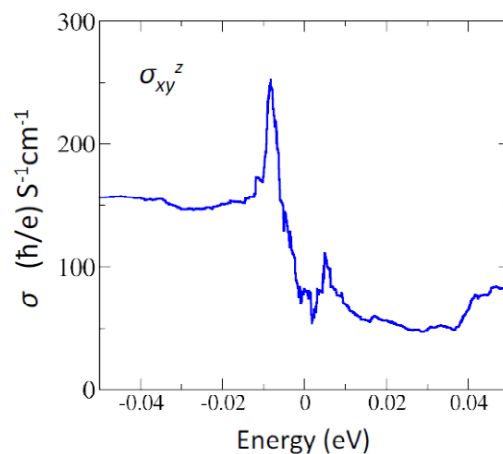
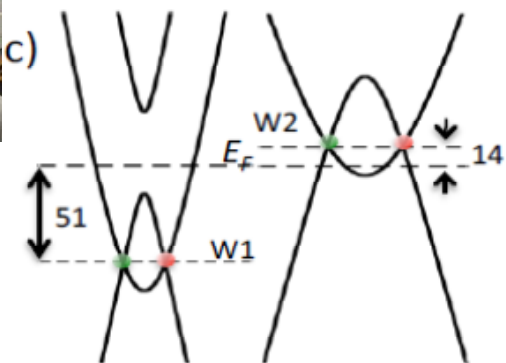


Weyl points are the origin for a large Berry phase and a Giant AHE

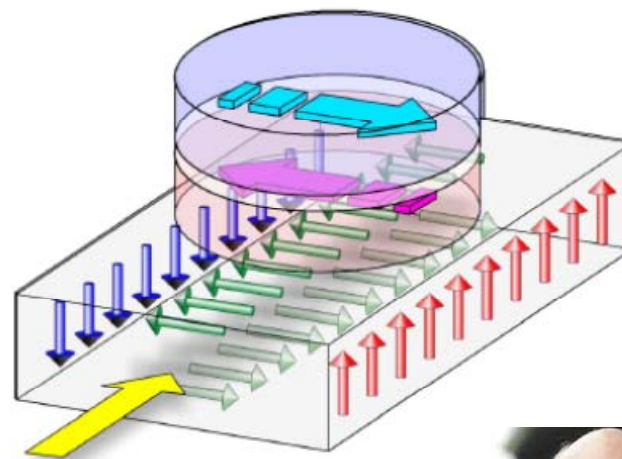
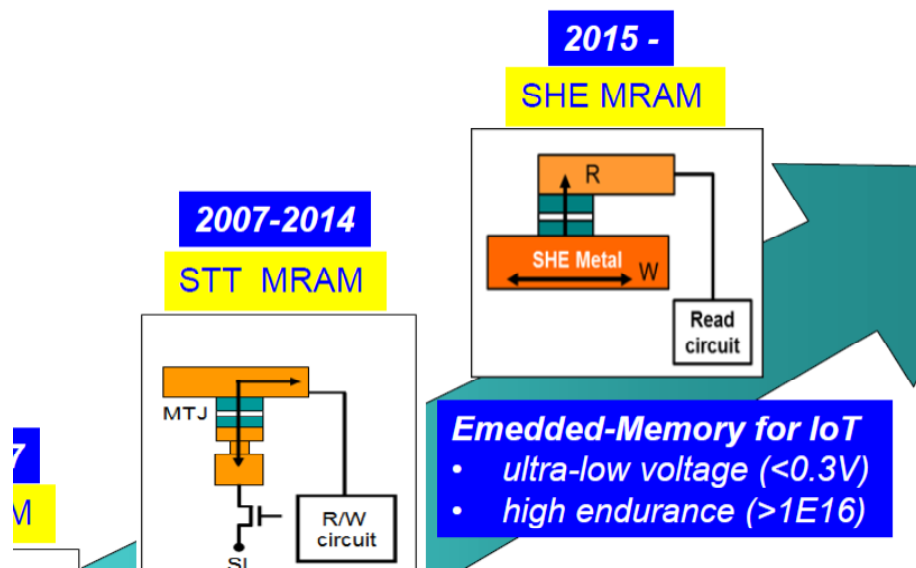
Kübler, Felser, PRB 85 (2012) 012405
Vidal et al Appl.Phys.Lett. 99 (2011) 132509
Kübler, Felser, Europhys. Lett. 114 (2016) 47005.



Application Spin Hall Effect



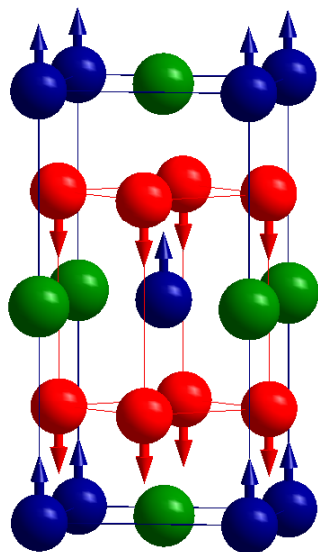
ITRI's MRAM Roadmap





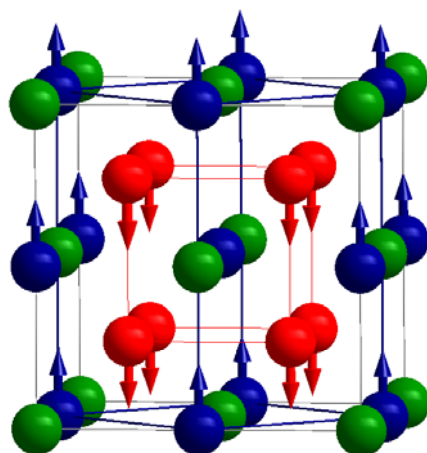
Structural distortion of Heusler

$I4/mmm$ ($D0_{22}$)



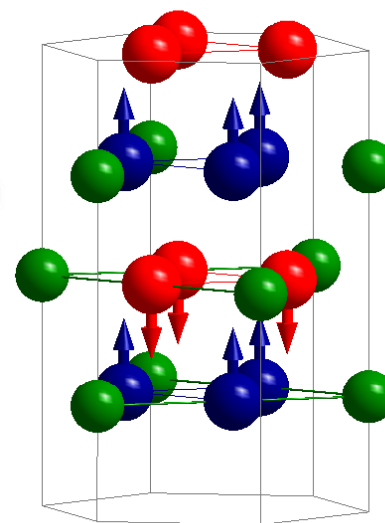
tetragonal

$Fm\bar{3}m$ ($L2_1$)



cubic

$P6_3/mmc$ ($D0_{19}$)



hexagonal





Hexagonal Antiferromagnet



epl A LETTERS JOURNAL EXPLORING
THE FRONTIERS OF PHYSICS

EPL, 108 (2014) 67001
doi: 10.1209/0295-5075/108/67001

December 2014

www.epljournal.org

Non-collinear antiferromagnets and the anomalous Hall effect

J. KÜBLER¹ and C. FELSER²

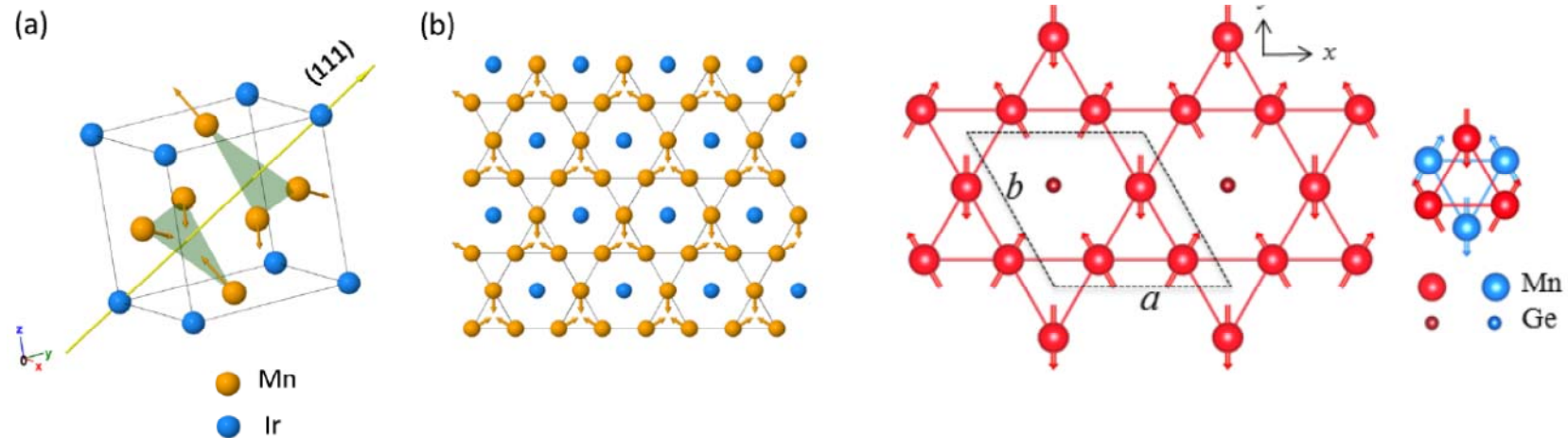
PRL 112, 017205 (2014)

PHYSICAL REVIEW LETTERS

week ending
10 JANUARY 2014

Anomalous Hall Effect Arising from Noncollinear Antiferromagnetism

Hua Chen, Qian Niu, and A. H. MacDonald



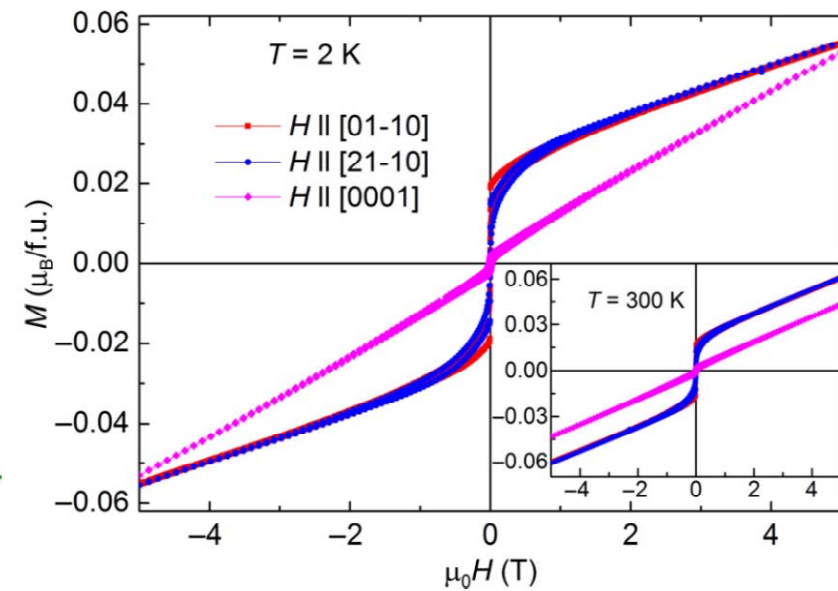
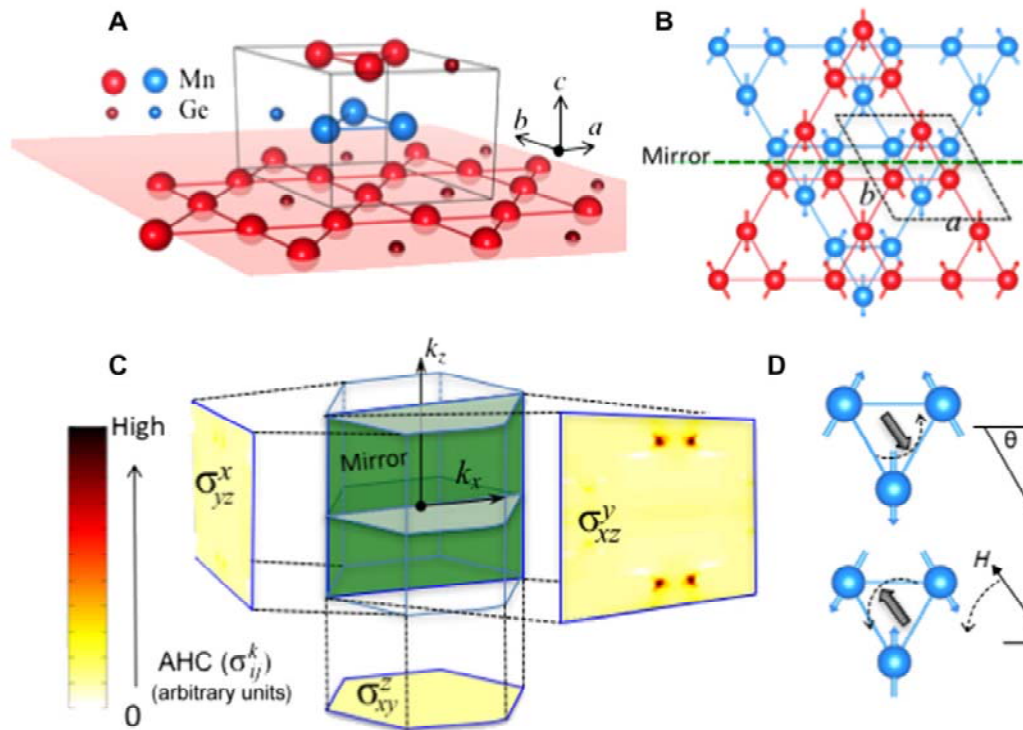
Chen, Niu, and MacDonald, Phys. Rev. Lett., 112 (2014) 017205

Kübler and Felser EPL 108 (2014) 67001



Non-collinear AFM in metallic Mn₃Ge

The anomalous Hall conductivities are normally assumed to be proportional to magnetization

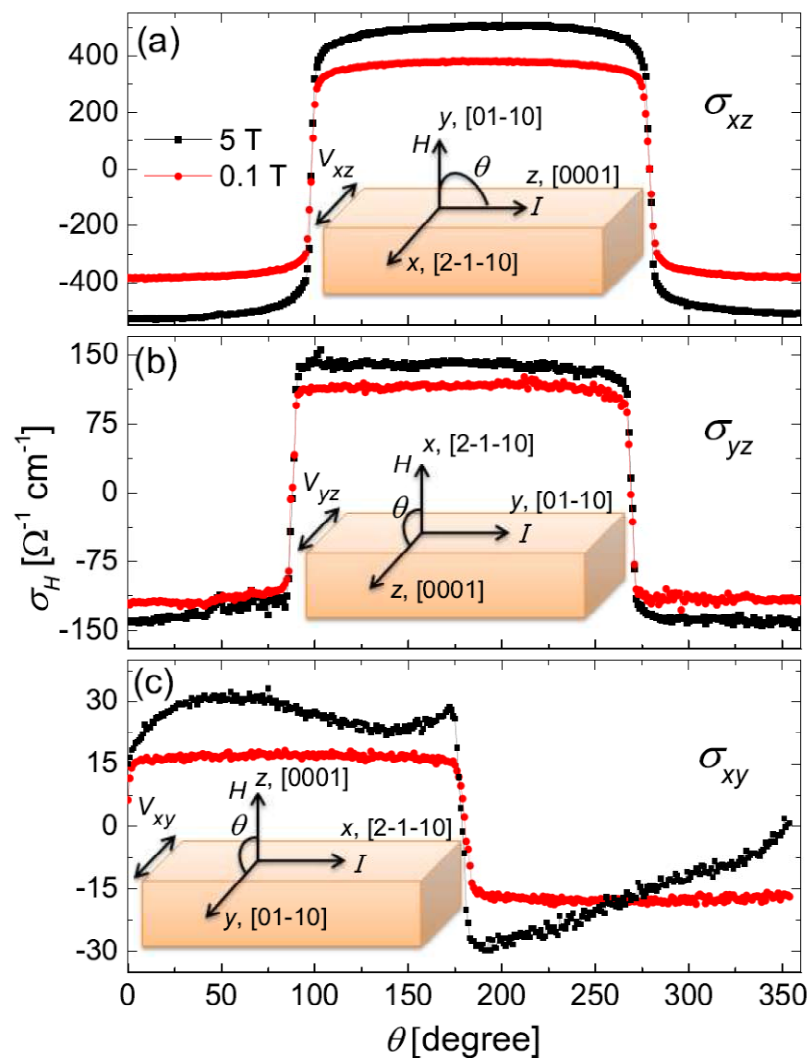




Non-collinear AFM Mn₃Ge/Mn₃Sn

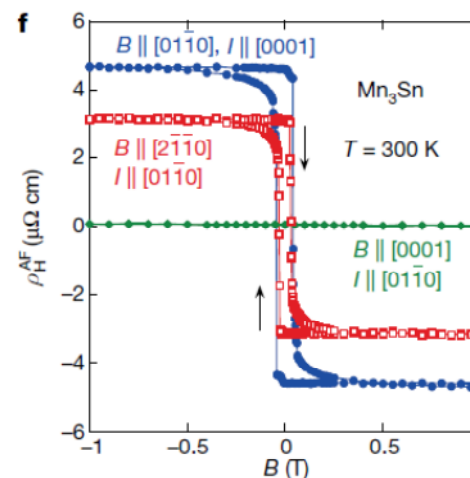
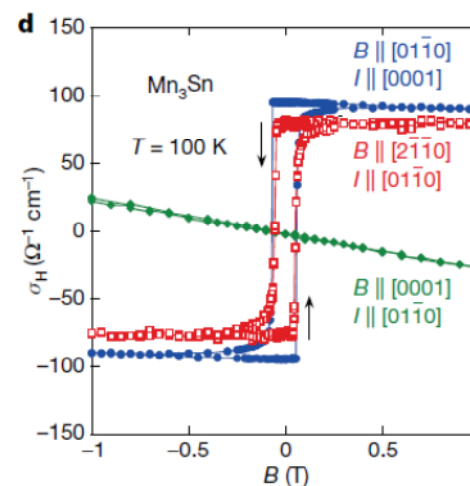
LETTER

doi:10.1038/nature15723



Large anomalous Hall effect in a non-collinear antiferromagnet at room temperature

Satoru Nakatsuji^{1,2}, Naoki Kiyohara¹ & Tomoya Higo¹

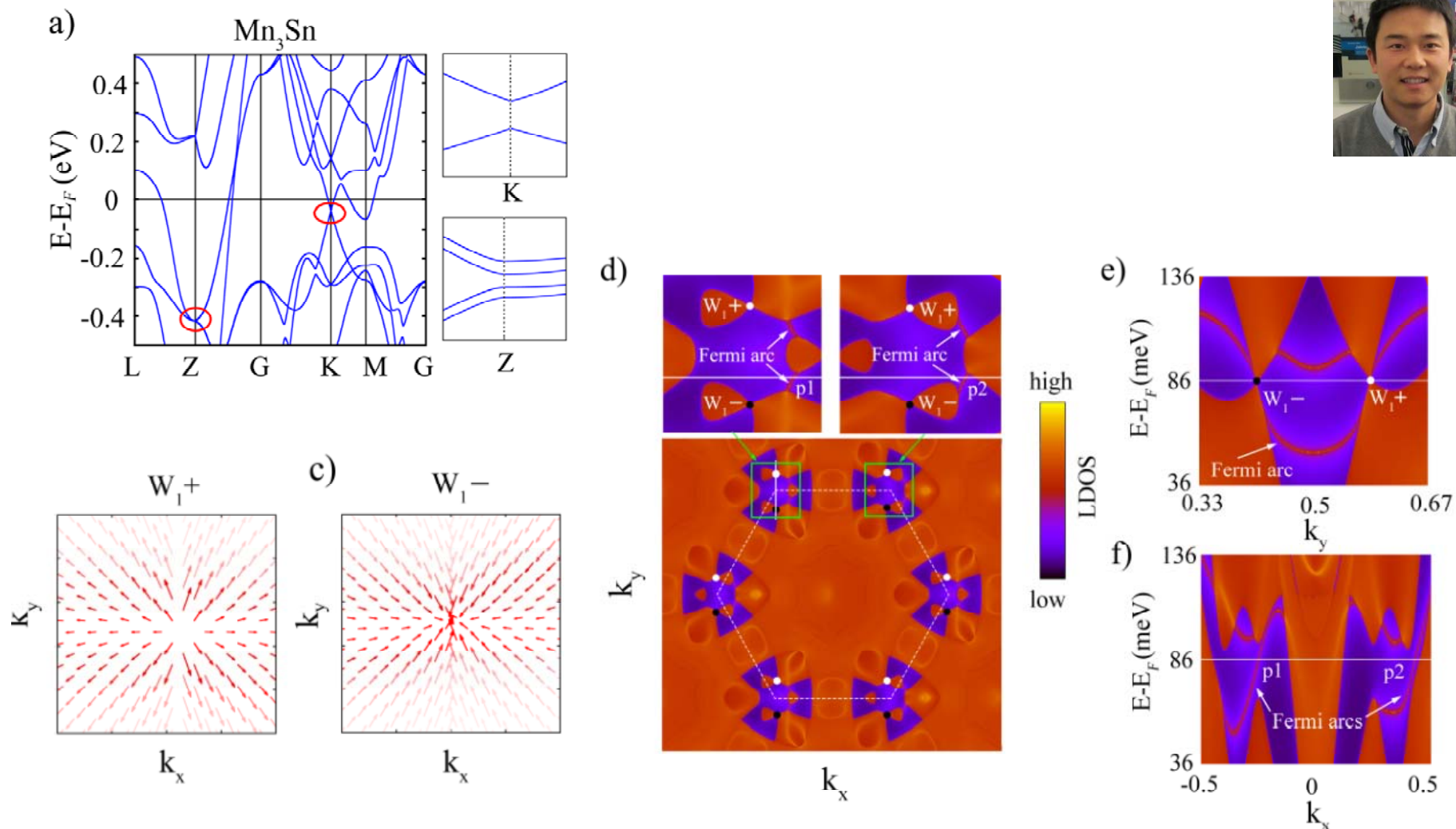
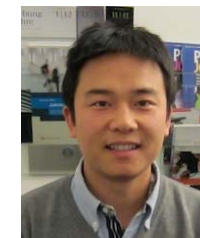


Nayak et al. preprint: arXiv:1511.03128, Science Advances in print
Kiyohara, Nakatsuji, preprint: arXiv:1511.04619,

Nakatsuji, Kiyohara, & Higo, Nature, doi:10.1038/nature15723



Fermiarcs in the Weyl AFM





Universe – applying a lattice



Bringing order to the expanding fermion zoo

Carlo Beenakker Commentary

Heisenberg (1930): We observe space as a continuum, but we might entertain the thought that there is an underlying lattice and that space is actually a crystal. Which particles would inhabit such a lattice world? Werner Heisenberg *Gitterwelt* (lattice world) hosted electrons that could morph into protons, photons that were not massless, and more peculiarities that compelled him to abandon “this completely crazy idea”



New Fermions

RESEARCH

RESEARCH ARTICLE SUMMARY

TOPOLOGICAL MATTER

Beyond Dirac and Weyl fermions: Unconventional quasiparticles in conventional crystals

Barry Bradlyn,* Jennifer Cano,* Zhijun Wang,* M. G. Vergniory, C. Felser, R. J. Cava, B. Andrei Bernevig†

Fermions in condensed-matter systems are not constrained by Poincare symmetry. Instead, they must only respect the crystal symmetry of one of the 230 space groups. Hence, there is the potential to find and classify free fermionic excitations in solid-state systems that have no high-energy counterparts.

What comes next? Magnetic Space groups

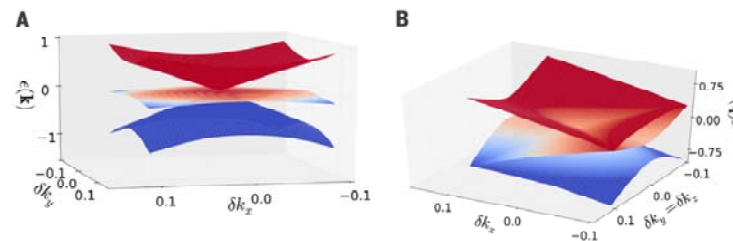
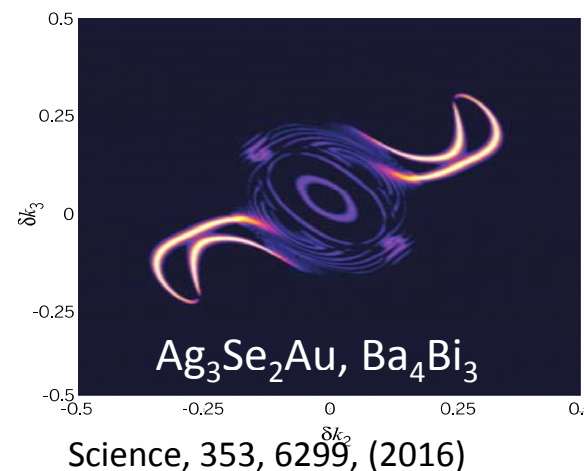
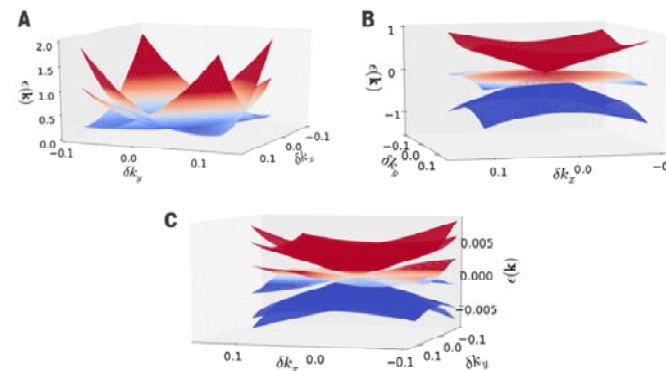


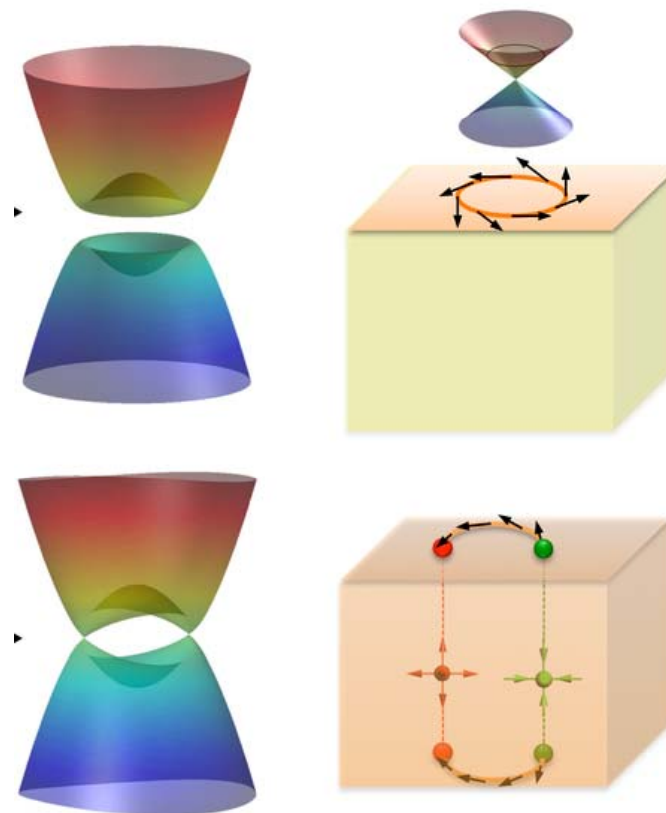
Fig. 1. Energy dispersion near a threefold degeneracy at the P point. (A and B) Shown are threefold degenerate points in (A) SGs 199 and 214 and (B) SG 220. In the latter case, pairs of bands remain degenerate in energy along the high-symmetry lines $|\delta k_x| = |\delta k_y| = |\delta k_z|$.





Can we do something useful- Catalysis

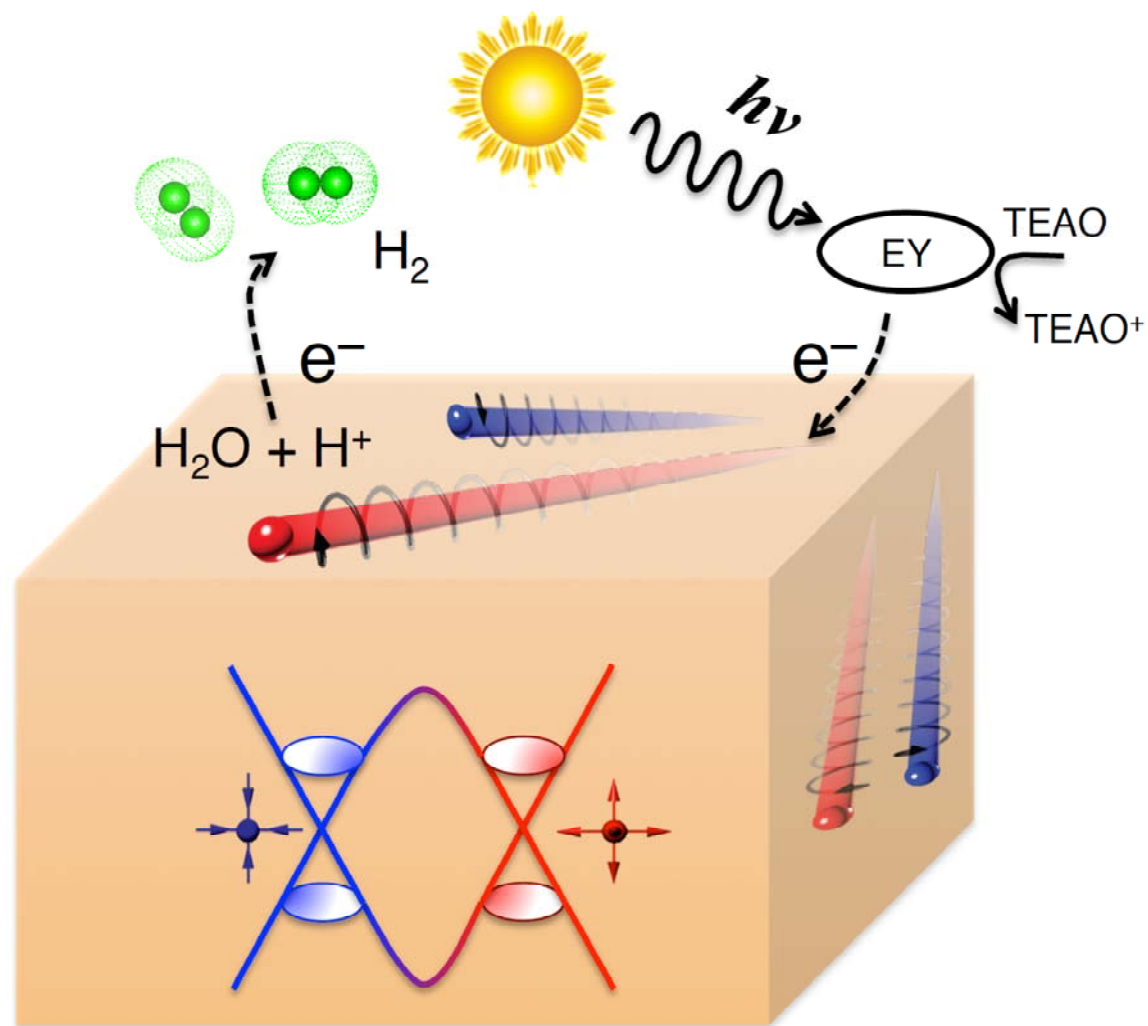
- Dirac and Weyl semimetals
 - Linear bands – electron and holes with **high mobilities**
 - High mobility of electrons and holes – reduces the probability of recombination of electron hole pairs in redox reaction
 - Topological connection between the two surfaces via Fermi arcs





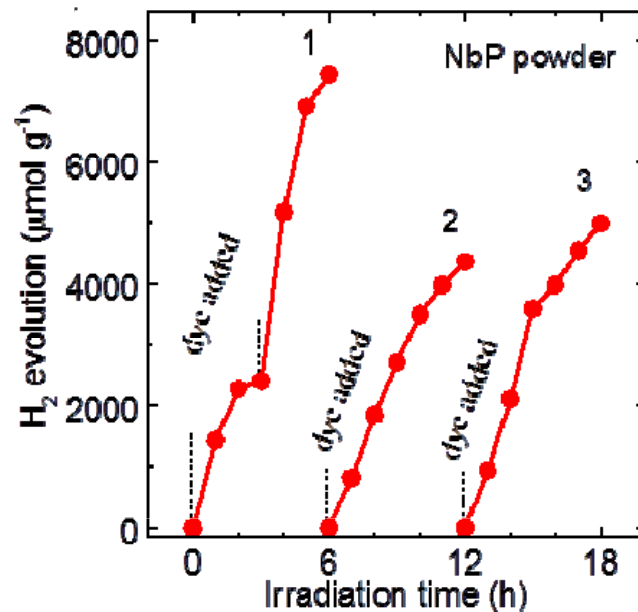
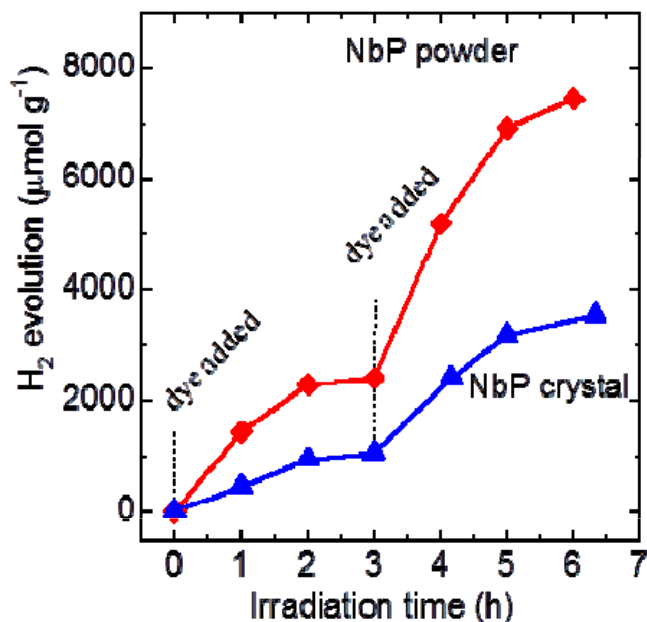
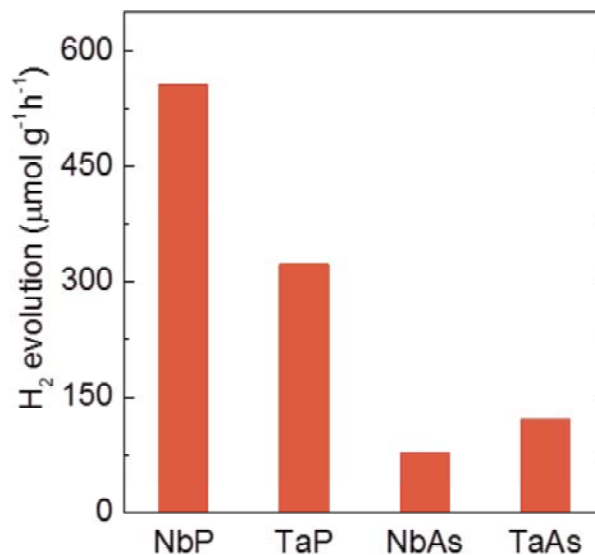
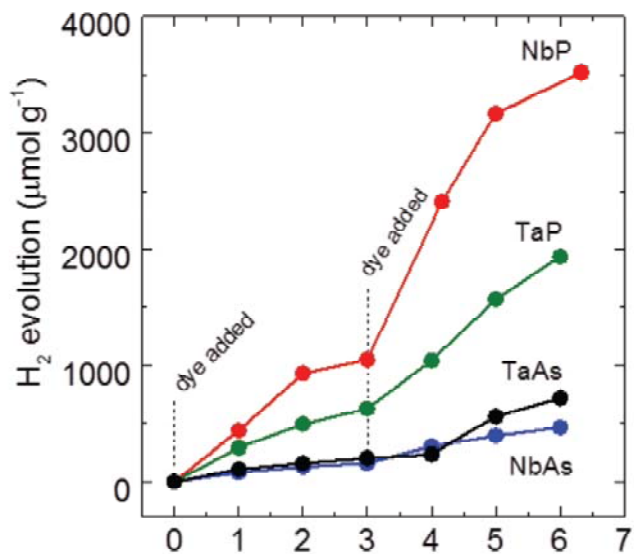
Catalysis

Hydrogen evolution reaction





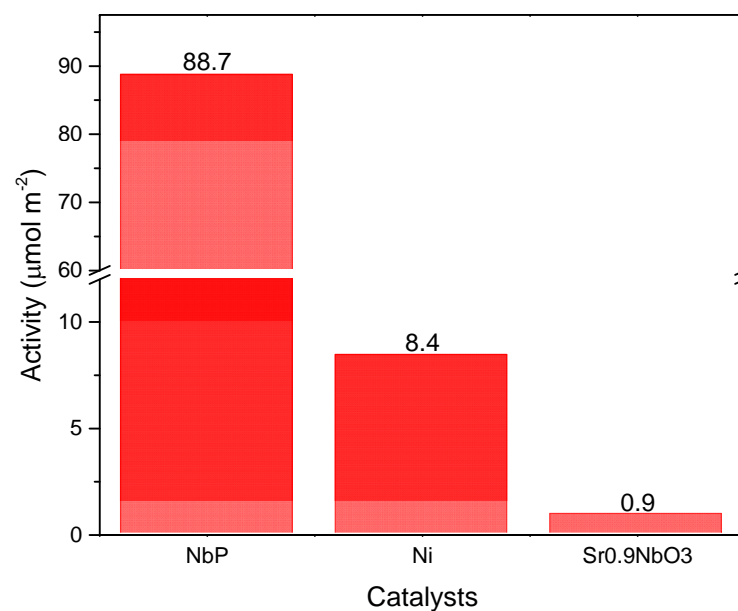
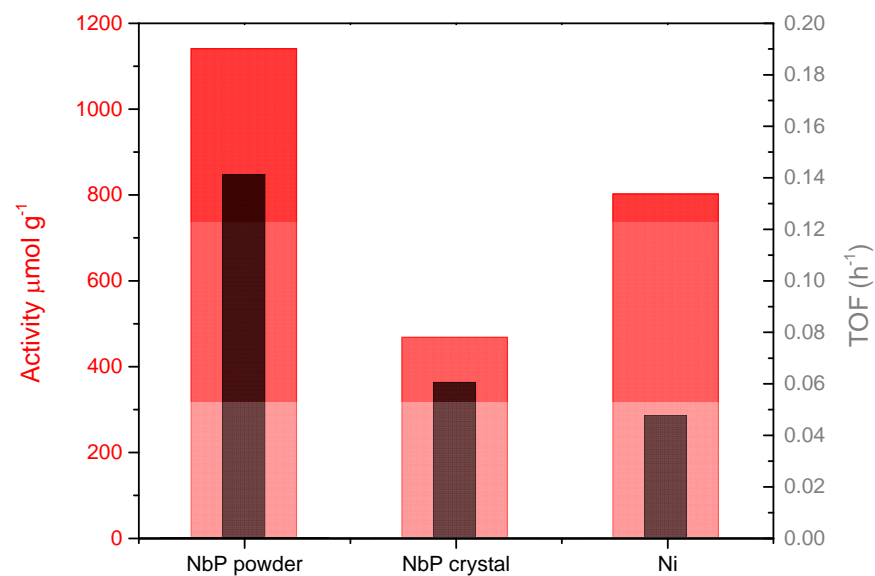
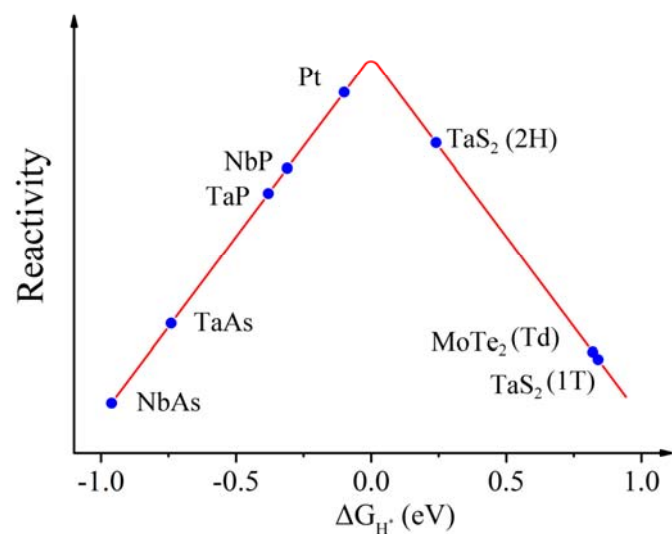
Weyl and catalysis





Comparison with other catalysts

Materials	Gibbs free energy (ΔG_H^* (eV))
NbP	-0.31
TaP	-0.38
TaAs	-0.74
NbAs	-0.96
Pt	-0.1
Ni (111)	-0.27
2H-TaS ₂	0.24
1T-TaS ₂	0.82
Td-MoTe ₂	0.84
2H-MoS ₂	2.19





Summary

Solid State Chemistry can have an impact on topological effects

- Topological insulators (Oxides, correlated systems)
- Weyl and Dirac semimetals
- ..

Applications in

- Electronics AHE SHE QAHE
- chemistry (catalysis)

