Topological Materials

MAX-PLANCK-GESELLSCHAFT

Claudia Felser

the revolution

- Non-trivial Phenomena captured by **Single-Particle Picture**
  $\rightarrow$ predictive design of novel materials and functionalities
- Novel Transport Phenomena determined by **Global Properties**
  - quantized transport from topological protection
  - giant responses

    …
- Vision:
  - Quantum effects at room temperature, spintronics
  - Catalysis, energy conversion
  - …

How does a materials scientist find topological materials?

outline

- Introduction
- Topological insulators
- Weyl semimetals – broken symmetry
- Magnetic Weyl semimetals
- New Fermions
- Outlook – axion insultors and beyond

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- Introduction
- Topological insulators
- Weyl semimetals – broken symmetry
- Magnetic Weyl semimetals
- New Fermions
- Outlook – axion insultors and beyond

the predictions

ARTICLE

doi:10.1038/nature23268

Topological quantum chemistry

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

https://doi.org/10.1038/s41586-019-0954-4

A complete catalogue of high-quality topological materials

M. G. Vergniory[1,2,3,11], L. Elcoro[4,11], Claudia Felser[5], Nicolas Regnault[6], B. Andrei Bernevig[7,8,9*] & Zhijun Wang[7,10*]

https://doi.org/10.1038/s41586-019-0937-5

Comprehensive search for topological materials using symmetry indicators

Feng Tang[1,2], Hoi Chun Po[3,4], Ashvin Vishwanath[3] & Xiangang Wan[1,2*]

https://doi.org/10.1038/s41586-019-0944-6

Catalogue of topological electronic materials

Tiantian Zhang[1,2,9], Yi Jiang[1,2,9], Zhida Song[1,2,9], He Huang[3], Yuqing He[2,3], Zhong Fang[1,4], Hongming Weng[1,5,6,7,8*] & Chen Fang[1,4,6,7,8*]

http://topologicalquantumchemistry.org/

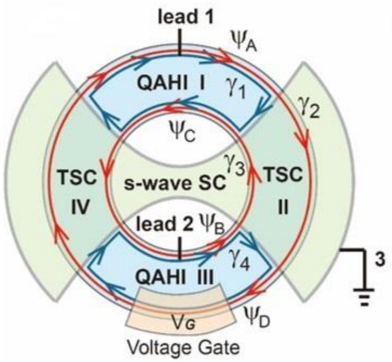
Compound Contains Only these elements ☐ Exclude ICSD Number

e.g. Bi1 Se2 Ge | eg. O1 N | - or - | eg. 123456 | Search

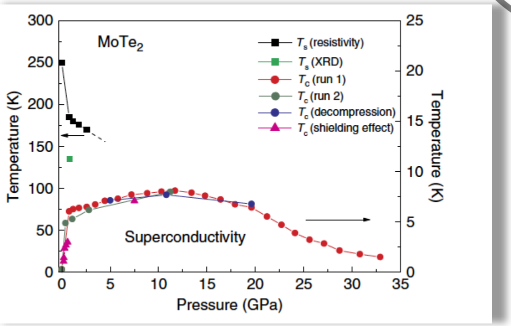
Show Advanced Search

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

the concept



Lian, et al., PNAS 2018



Qi et al. Nat. Com. (2016)

predictive materials design

synthesis

verification of electronic structure

emergent phenomena

control/ functionality

new concepts for topological classes:

magnetic
correlated
higher order ...

Topological quantum chemistry
Bradlyn, et al., Nature 2017
1807.10271, 1807.08756

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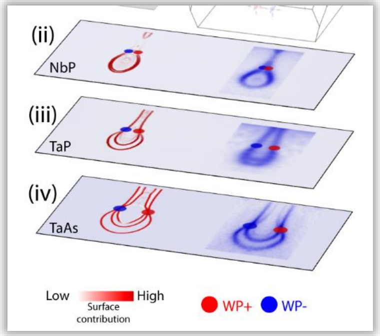
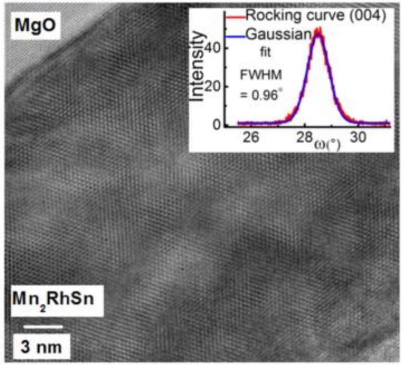
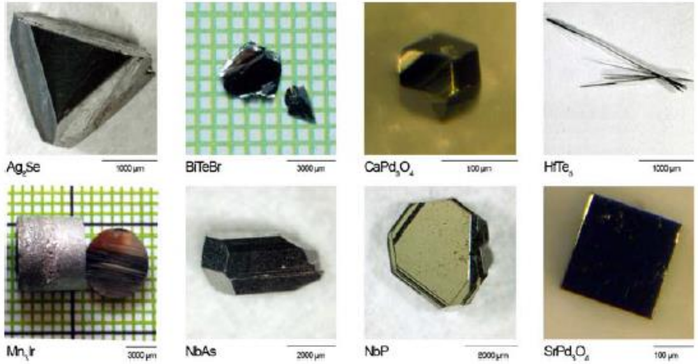


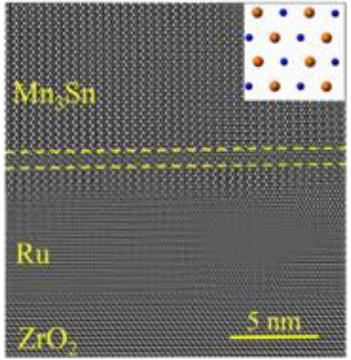
Liu et al. Nat. Mat. (2016)

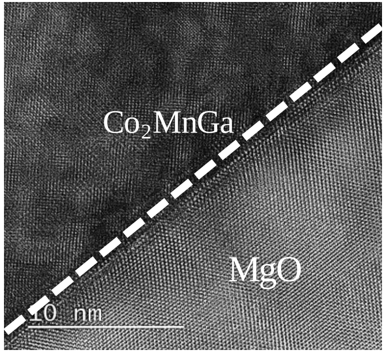
the materials

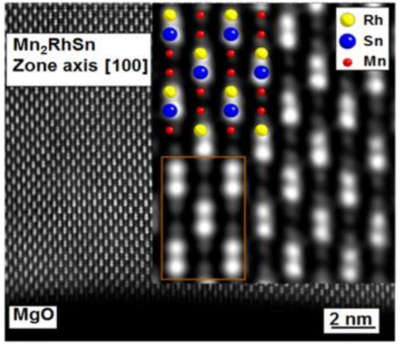
- **explorative search for new materials** & **predictive design**
- high quality **single crystal growth**
- **epitaxial growth** of ultrathin films and heterostructures
- **2D materials and micro/nano structures**



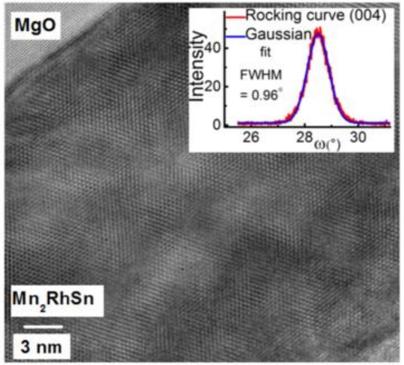


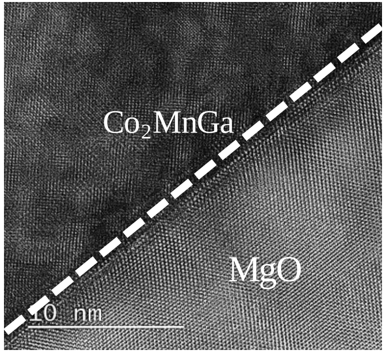


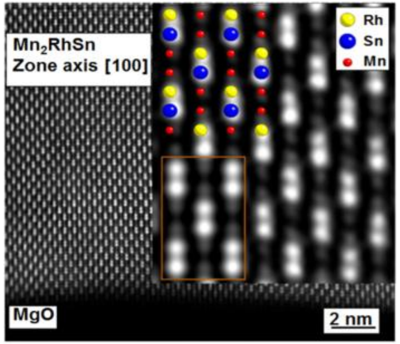




the materials

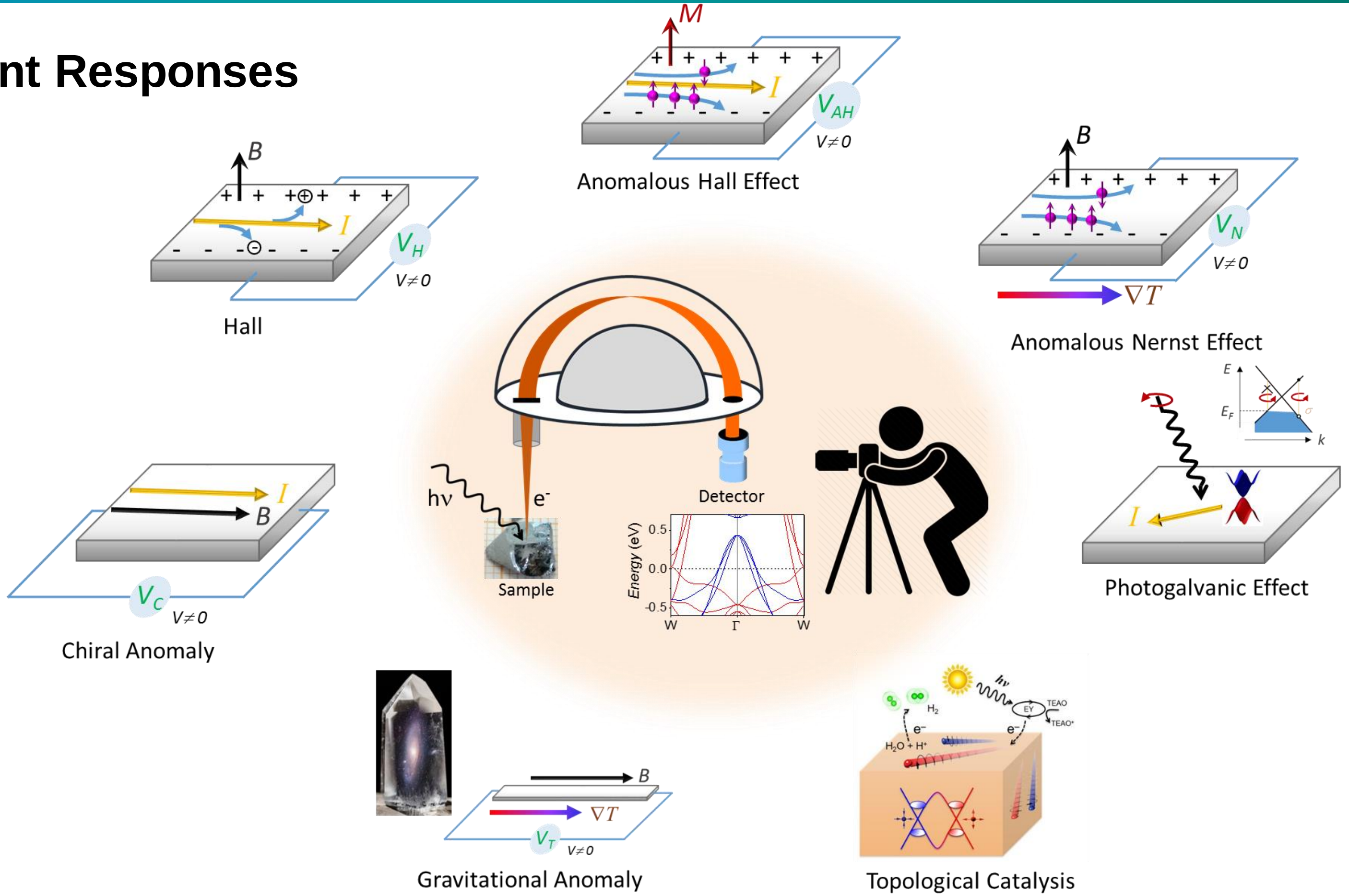




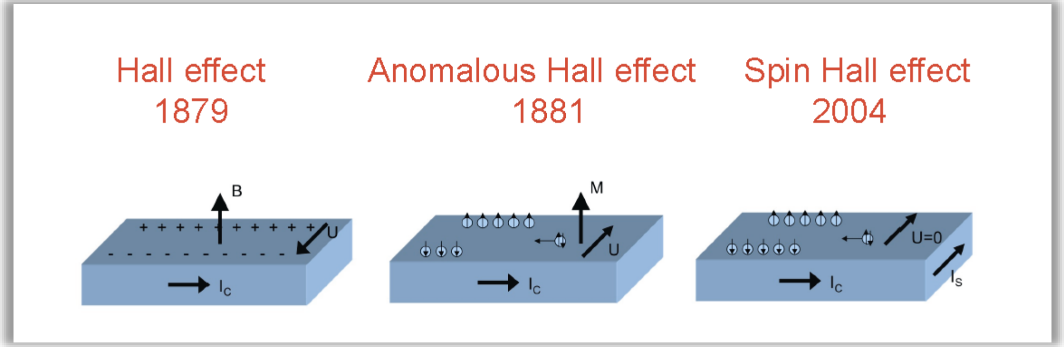


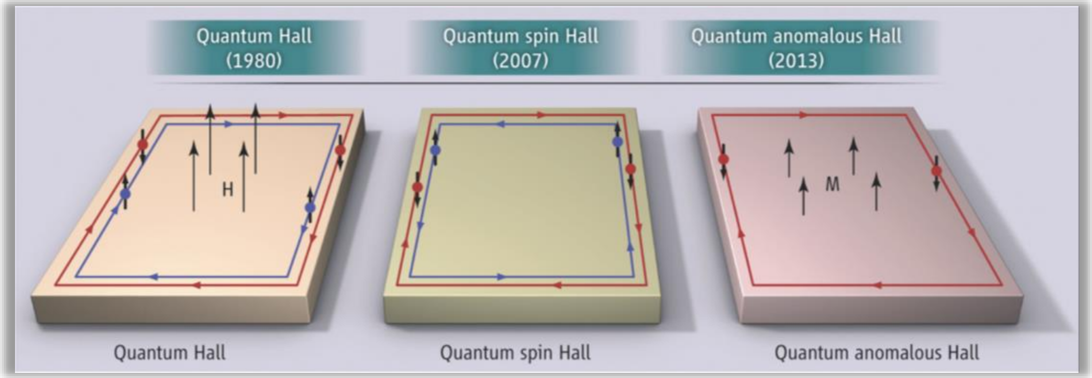
the measurements

Giant Responses



family of quantum Hall effects



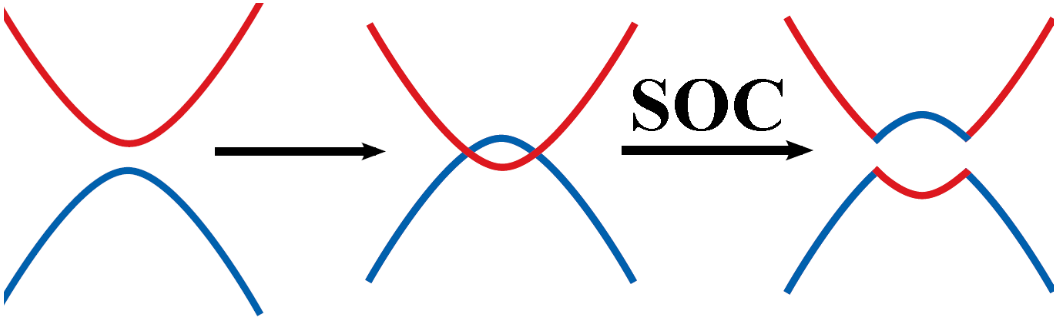


1985
Klaus von Klitzing
1998
Horst Ludwig Störmer and Daniel Tsui
2010
Andre Geim and Konstantin Novoselov

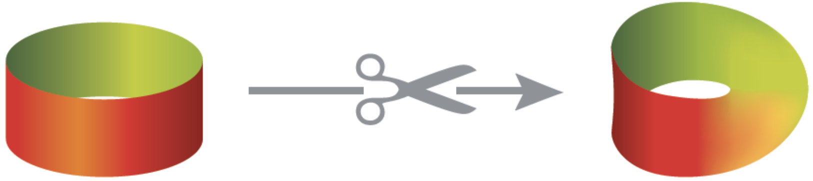
S Oh Science 340 (2013) 153

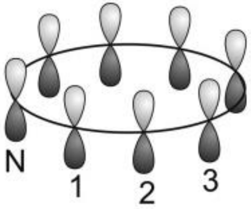
2016
David Thouless, Duncan Haldane und Michael Kosterlitz

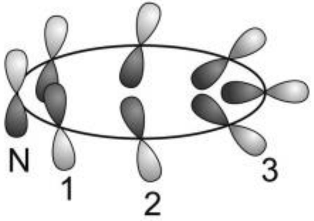
topology in the electronic structure



topology in the electronic structure







Magic electron numbers

Hückel:

4n+2 aromatic

4n antiaromatic

Möbius:

4n aromatic

4n+2 antiaromatic

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.

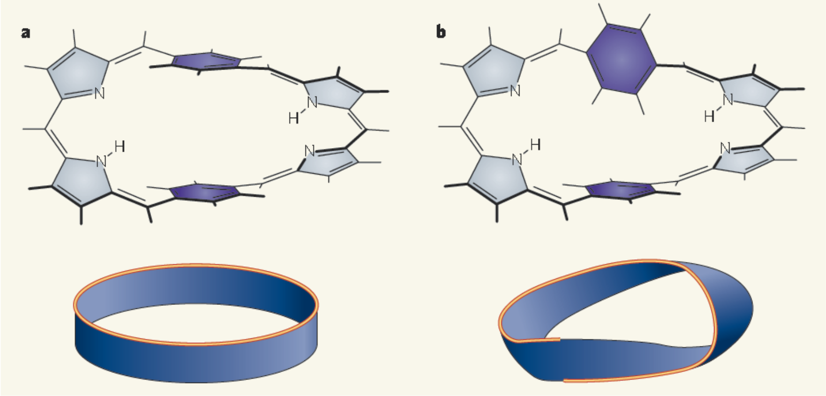
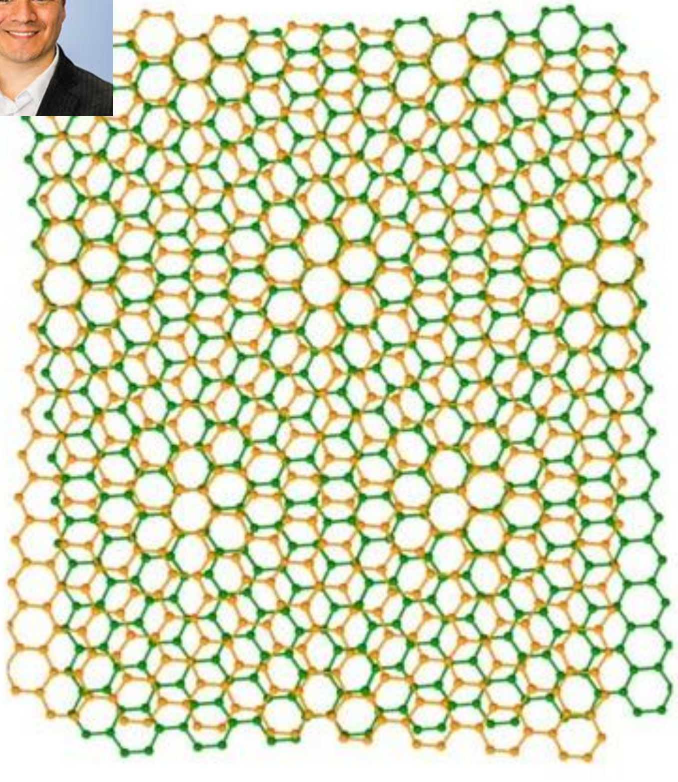


Figure 2 | A molecular topological switch. Latos-Grażyński and colleagues[1] have made a compound that is antiaromatic in nonpolar solvents, but not in polar solvents. **a**, In nonpolar solvents, the two benzene rings (purple) in the molecule are parallel, and the molecule is a two-sided, non-twisted 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.

topology in the electronic structure



VIP Nanographenes Very Important Paper

International Edition: DOI: 10.1002/anie.201808178
German Edition: DOI: 10.1002/ange.201808178

Undecabenzo[7]superhelicene: A Helical Nanographene Ribbon as a Circularly Polarized Luminescence Emitter

*Carlos M. Cruz, Silvia Castro-Fernández, Ermelinda Maçôas, Juan M. Cuerva, and Araceli G. Campaña**

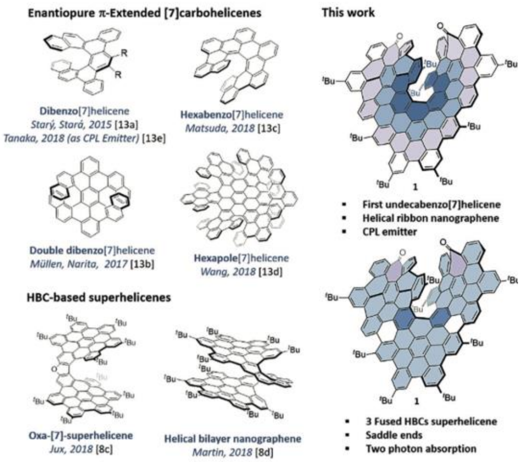
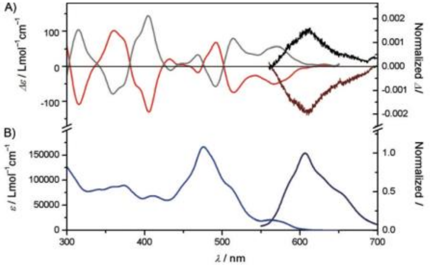


Figure 1. Background and novel structural features of compound **1**.



igure 3. a) Experimental ECD (left) and CPL (right, λ_{exc} = 490 nm) of M) (red and scarlet) and (P) (gray and black) enantiomers of **1** in CH_2Cl_2 at ca. 5×10^{-6} M. b) Experimental UV/Vis (blue) and fluores-ence (navy, λ_{exc} = 490 nm) spectra of **1** in CH_2Cl_2 at ca. 5×10^{-6} M.

outline

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- Magnetic Weyl semimetals
- New Fermions
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topological insulators – quantum spin Hall

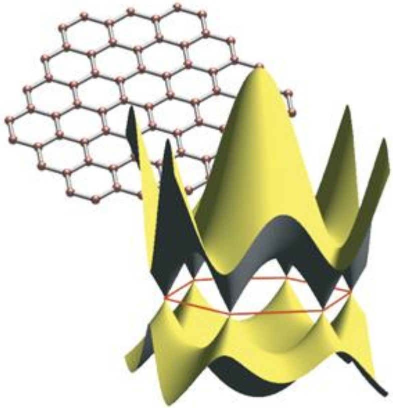
Z_2 Topological Order and the Quantum Spin Hall Effect

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 state with a bulk electronic band gap that supports the transport of charge and spin in gapless edge states. We show that this phase is associated with a novel Z_2 topological invariant, which distinguishes it from an ordinary insulator. The Z_2 classification, which is defined for time reversal invariant Hamiltonians, is analogous to the Chern number classification of the quantum Hall effect. We establish the Z_2 order of the QSH phase in the two band model of graphene and propose a generalization of the formalism applicable to multiband and interacting systems.

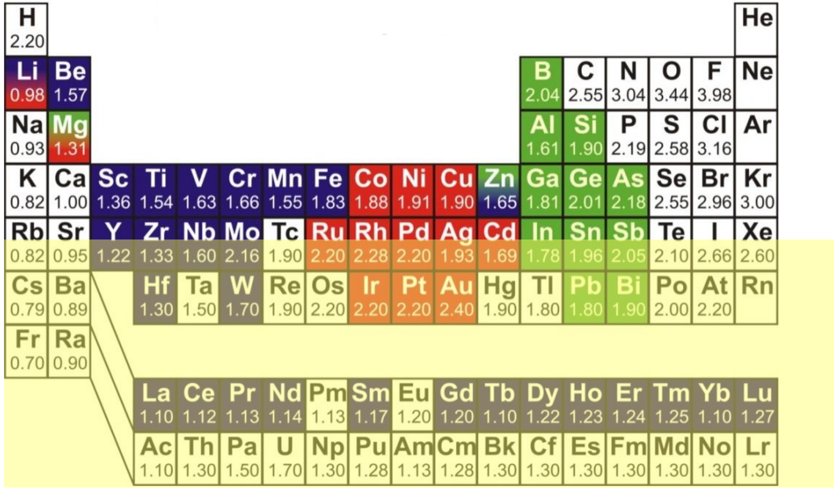


First prediction in graphene by Kane

Kane and Mele, PRL 95, 146802 (2005)

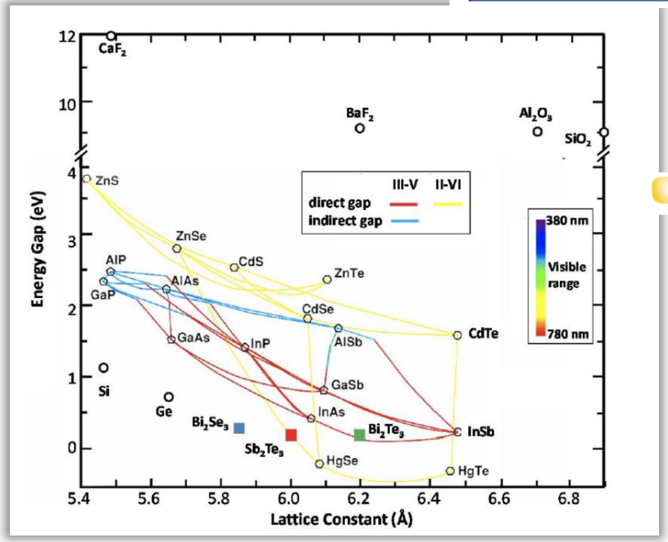
Heavy insulating elements?

Strained α-Sn and Bi-bilayer

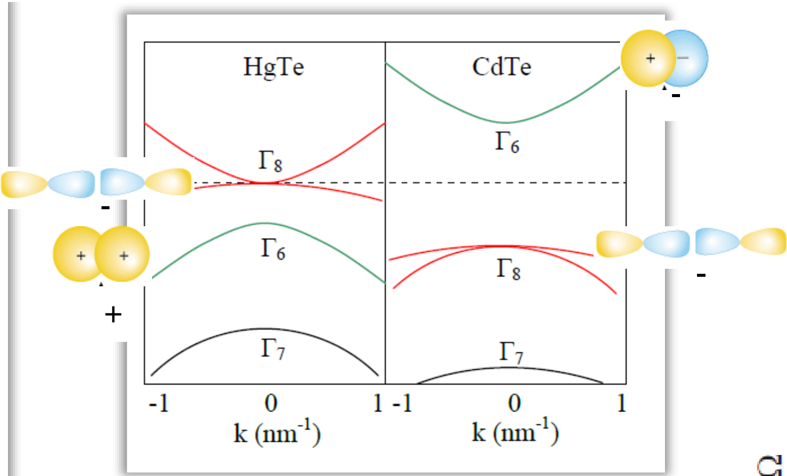


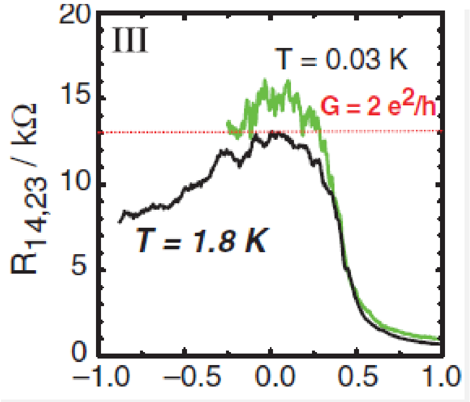
$\lambda_{SOC} \sim Z^2$ **for valence shells**

topological insulators – quantum spin Hall

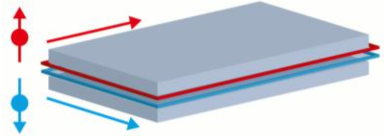


Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells
B. Andrei Bernevig, *et al.*
Science **314**, 1757 (2006);
DOI: 10.1126/science.1133734





Inert pair effect



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)

topological insulators – quantum spin Hall

Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells
B. Andrei Bernevig, *et al.*
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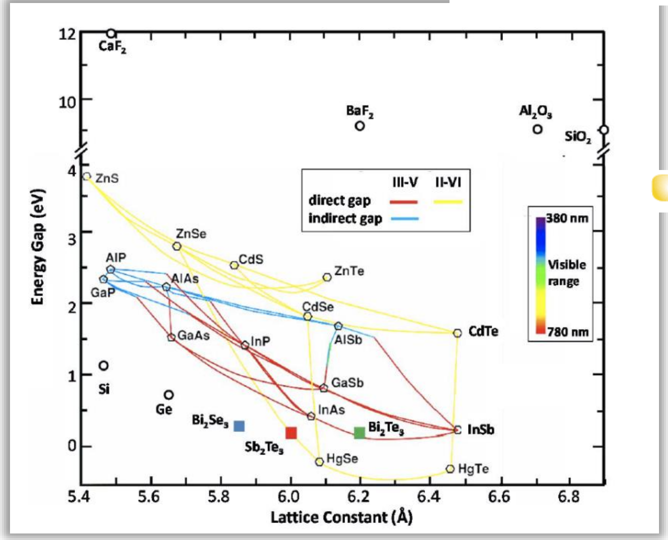
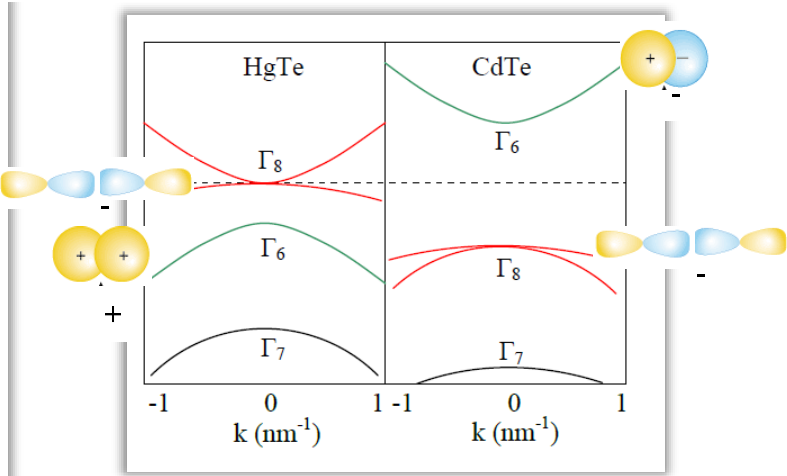
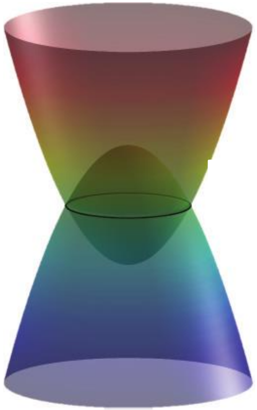
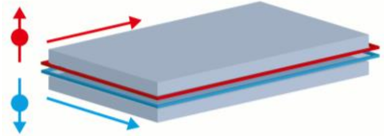






Band inversion

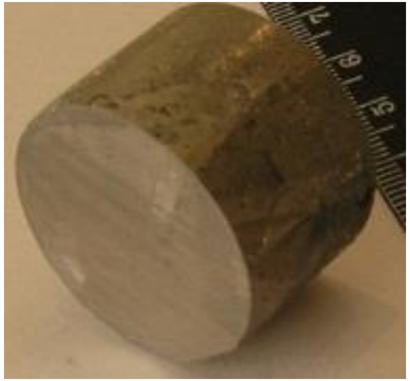
Inert pair effect

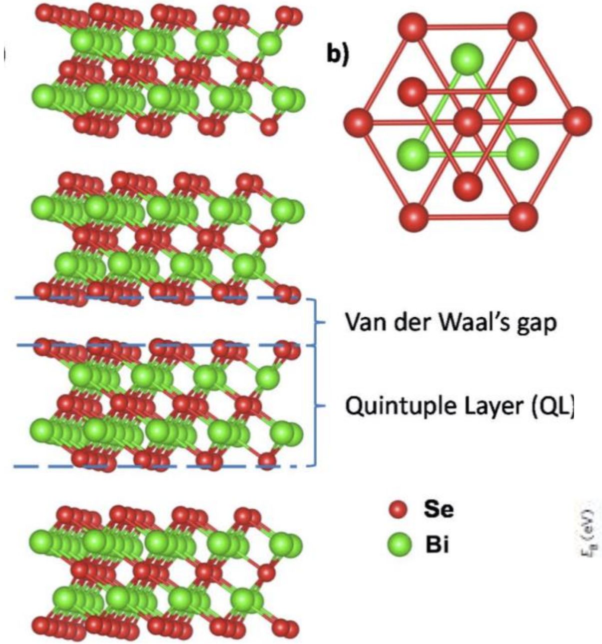


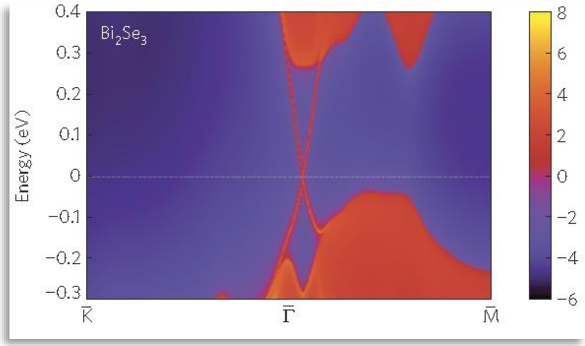
Kane and Mele, PRL 95, 146802 (2005)
Bernevig, et al., Science 314, 1757 (2006)
Bernevig, S.C. Zhang, PRL 96, 106802 (2006)
König, et al. Science 318, 766 (2007)

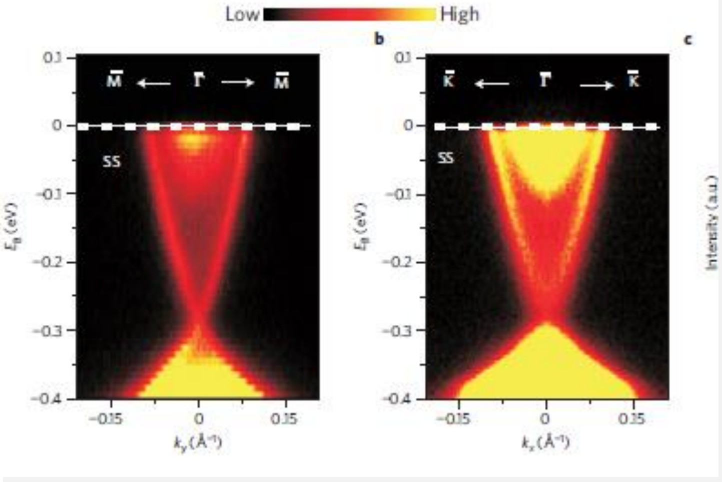
topological insulators

Starting with Bismuth
Bi-Sb Legierungen
Bi2Se3 und verwandte Strukturen



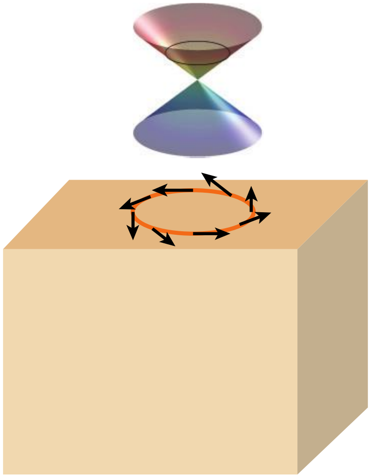


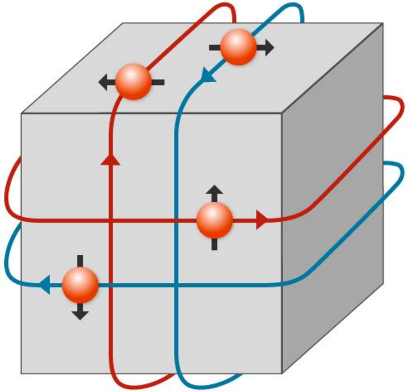


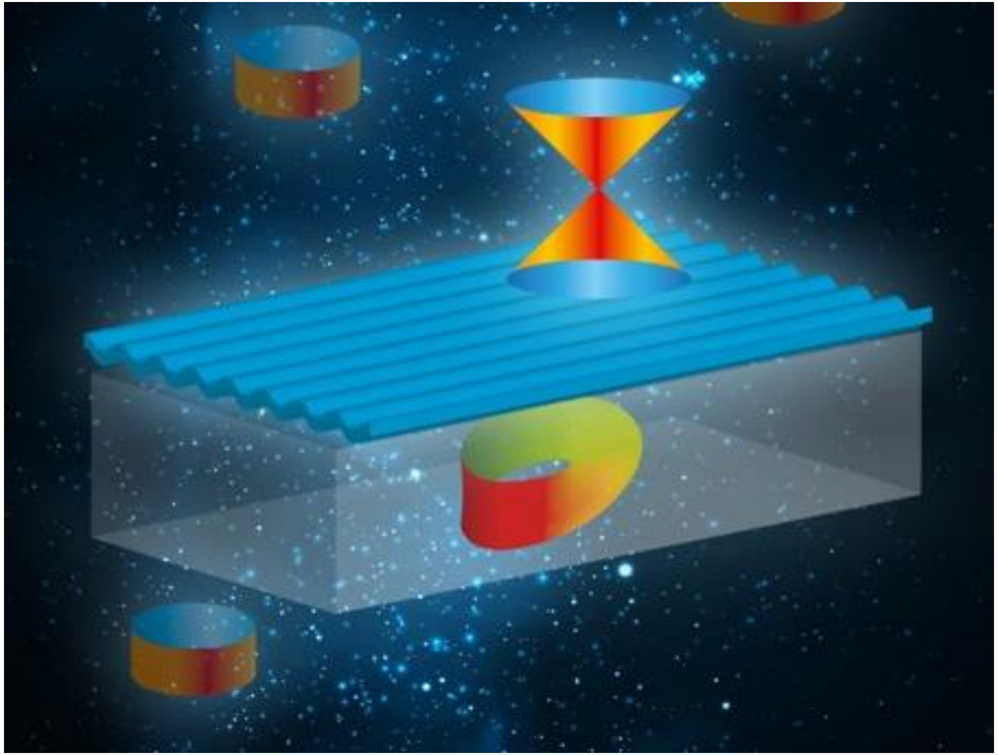


Moore and Balents, PRB 75, 121306(R) (2007)
Fu and Kane, PRB 76, 045302 (2007)
Murakami, New J. Phys. 9, 356 (2007)
Hsieh, et al., Science 323, 919 (2009)
Xia, et al., Nature Phys. 5, 398 (2009); Zhang, et al., Nature Phys. 5, 438 (2009)

topological insulators

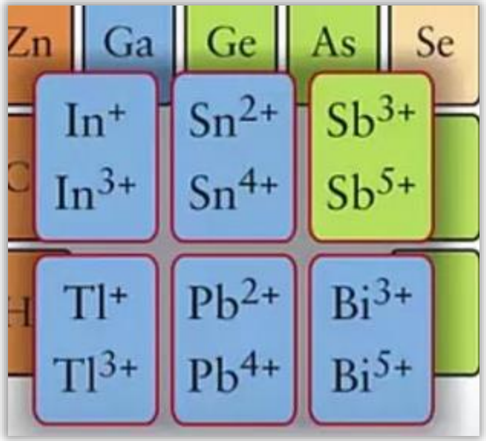






chemistry

Table I. Proposed topological insulator materials grouped into several different material classes.[4,12,13,19,23–29]							
HgTe-type	**Bi_2Se_3-type**	**Honey Comb Lattice**	**Bismuth-Alloys**	**NaCl Structure**	**Oxides**	**Correlated Materials**	**Super-conductors**
HgTe	Bi_2Se_3, Bi_2Te_3, and Sb_2Te3	Graphene	Bi-Sb	SnTe PbTe	Doped $BaBiO_3$	Iridates	$Cu_xBi_2Se_3$
Half-Heuslers such as LaPtBi	Bi_2Te_2Se	LiAuTe		PuTe AmN	Iridates	SmB_6	LaPtBi YPtBi LuPtBi
α-Sn, HgSe β-HgS	$(Bi_xSb_{1-x})_2Te_3$					YbPtBi	$TlBiSe_2$ $TlBiTe_2$
Chalco-pyrites	$TlBiSe_2$ and $TlBiTe_2$					Skutterudites	
AlSb/InAs/GaSb	$Bi_{14}Rh_3I_9$					PuTe, AmN	

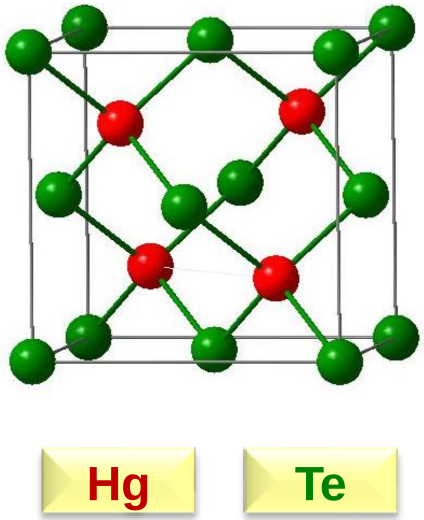


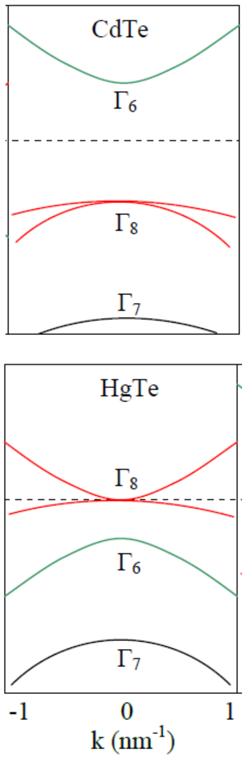
Claudia Felser and Xiao-Liang Qi , Guest Editors, MRS Bull. 39 (2014) 843.

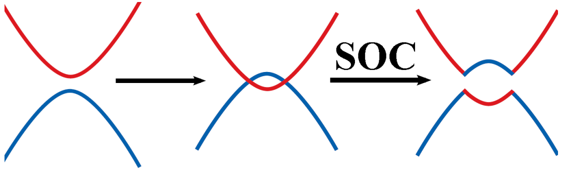
Tl^{+1} Sn^{2+} Bi^{+3}

inert pair effect

predicting topological insulators



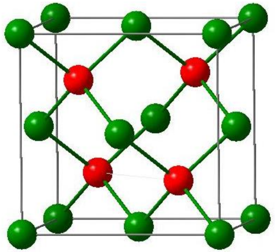


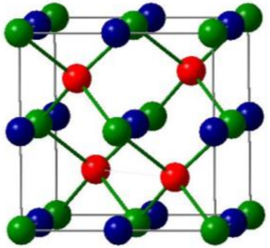


Bernevig et al., Science 314, 1757 (2006), König et al., Science 318 (2007) 766.

1, 2, 3, …

ZnS **Heusler XYZ $C1_b$**





Zr **Ni** **Sn**

4 + 10 + 4 = 18

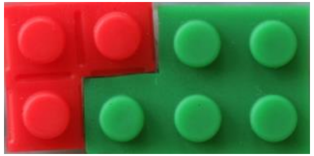
Ga **As**

3 + 5 = 8

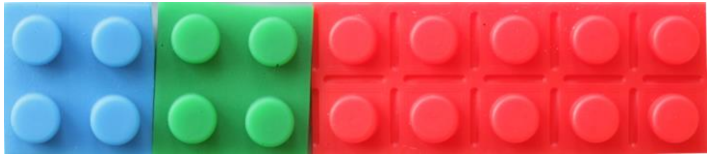
Li **Mg** **As**

1 + 2 + 5 = 8

2s +6p electrons

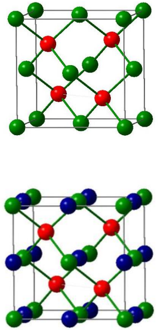


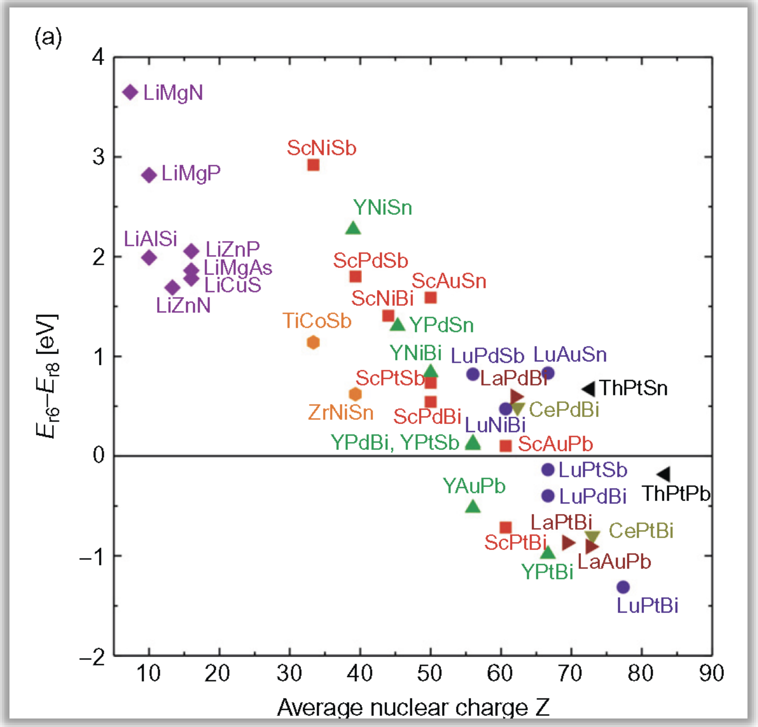
2s +6p+10d electrons

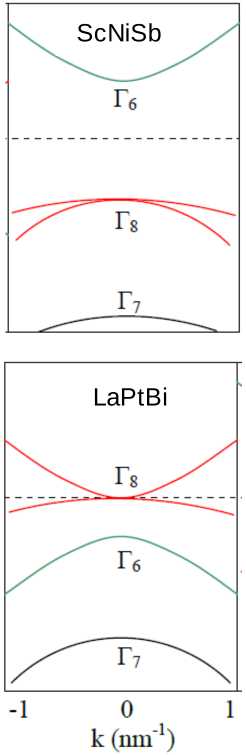


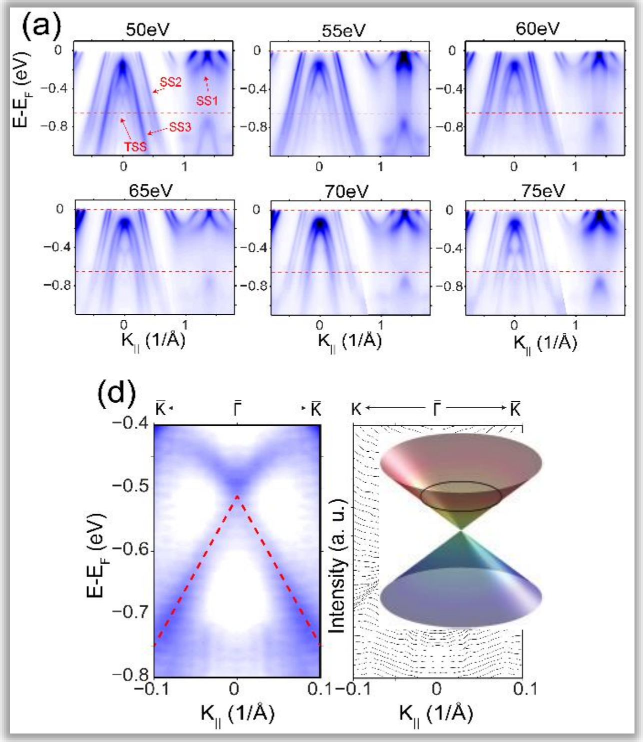
Graf, Felser, Parkin, IEEE TRANSACTIONS ON MAGNETICS 47 (2011) 367
Graf, Felser, Parkin, Progress in Solid State Chemistry Chemistry 39 (2011) 1

predicting topological insulators





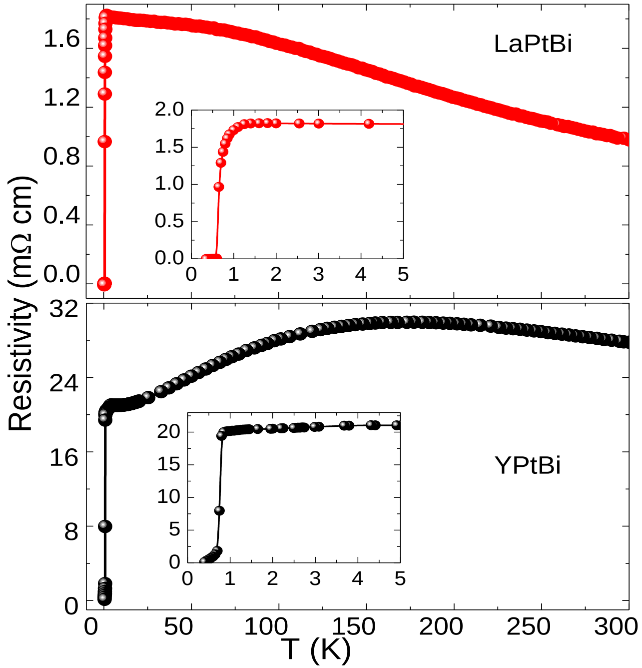


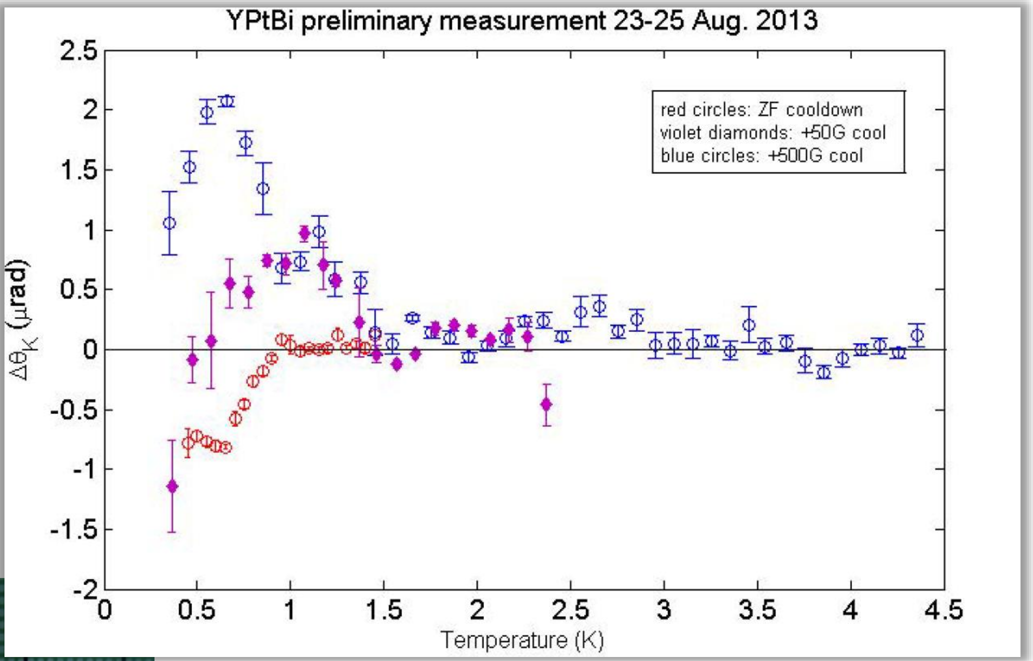


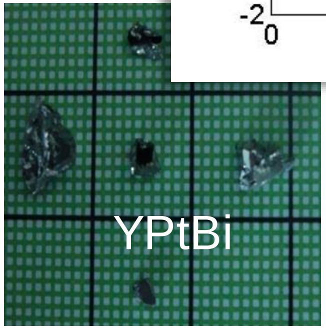
Chadov, et al., Nature Mat. 9 (2010) 541

Lin et al., Nature Mat. 9 (2010) 546

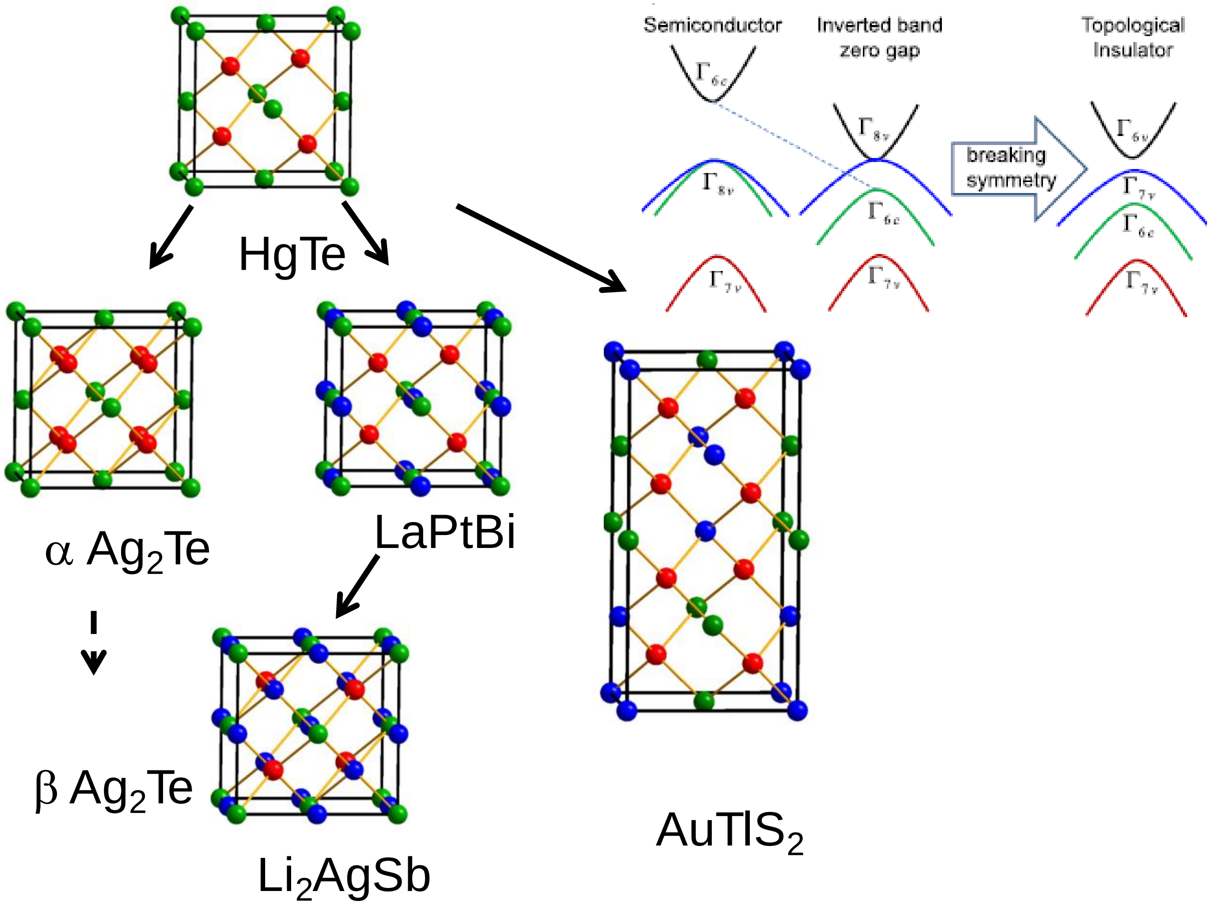
unconventional superconductors





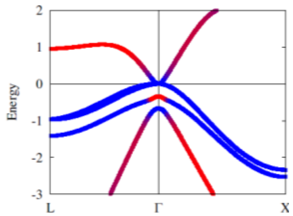


distorted structure to property

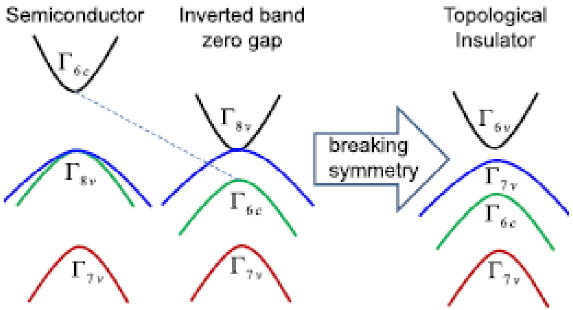


distorted structure to property

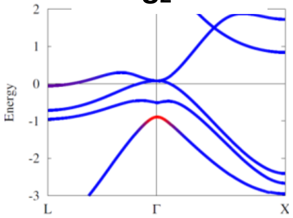
HgTe



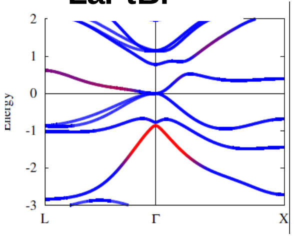
From 2D to 3D



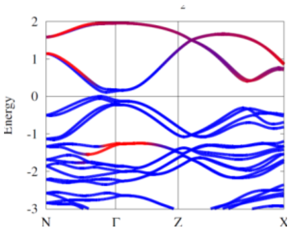
α Ag_2Te

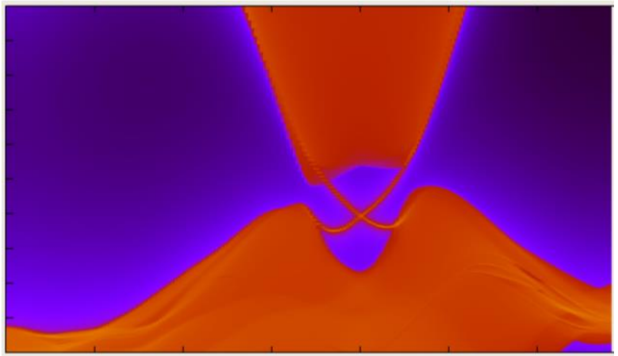


LaPtBi

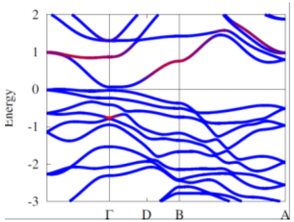


$AuTlS_2$

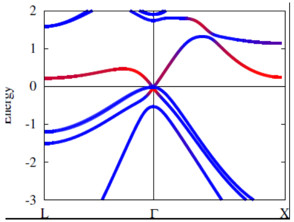




β Ag_2Te



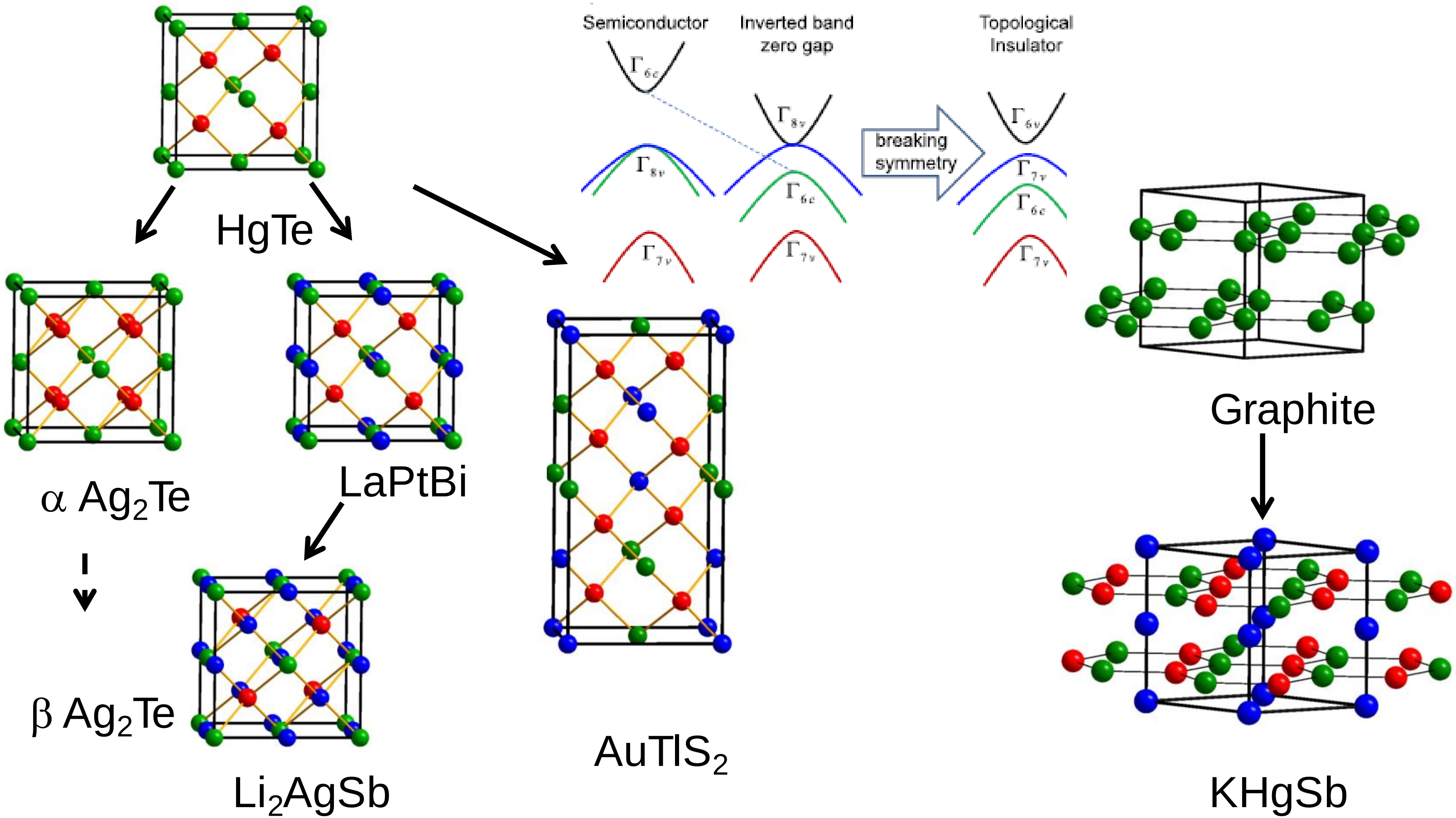
Li_2AgSb

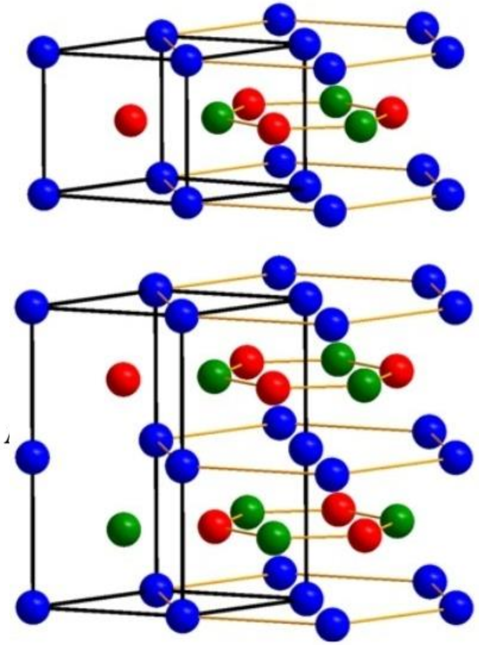


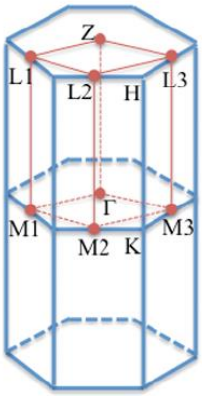
Nature Mat. 9 (2010) 541
Nature Mat. 9 (2010) 546
arXiv:1004.0999v1
PRL 106, 016402 (2011)
PRL 106, 156808 (2011)
arXiv:1104.0335v1

Müchler, Zhang, Chadov, Yan, Kübler, Zhang, Felser, Angewandte Chemie 2012

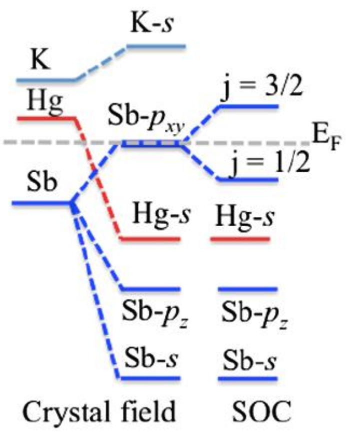
distorted structure to property



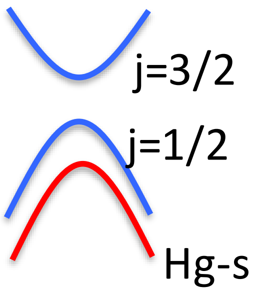




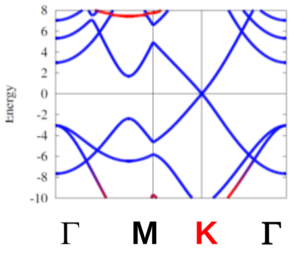
(c)



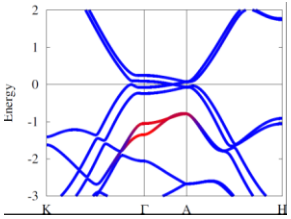
(d)



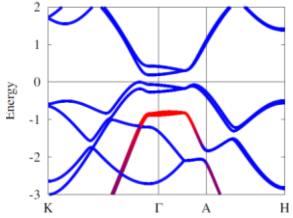
Graphite



LiAuSn



KHgSb

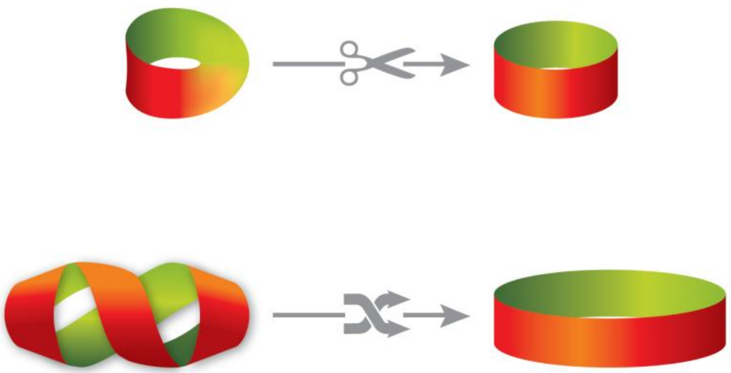


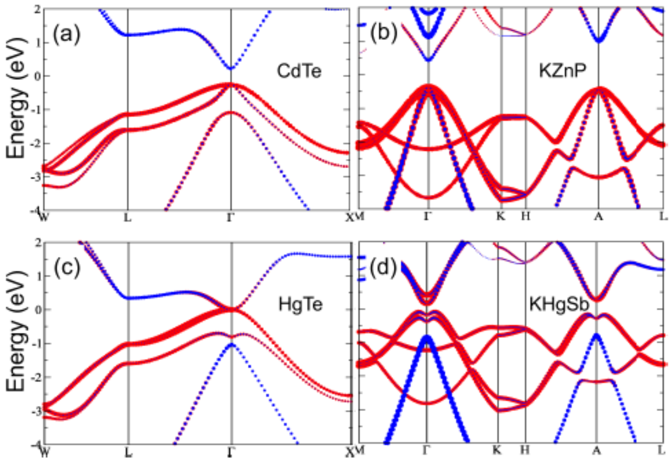
Yan, Müchler, Felser, Phys. Rev. Lett. 109 (2012) 116406

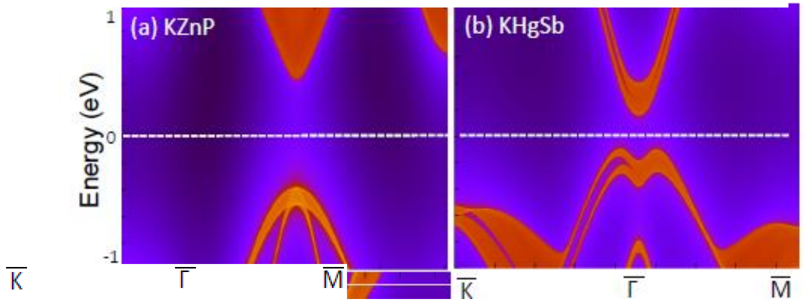
Zhang, Chadov, Müchler, Yan, Qi, Kübler, Zhang, Felser, Phys. Rev. Lett. 106 (2011) 156402

honeycomb from sp3 to sp2

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

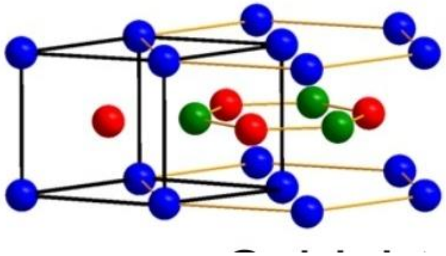




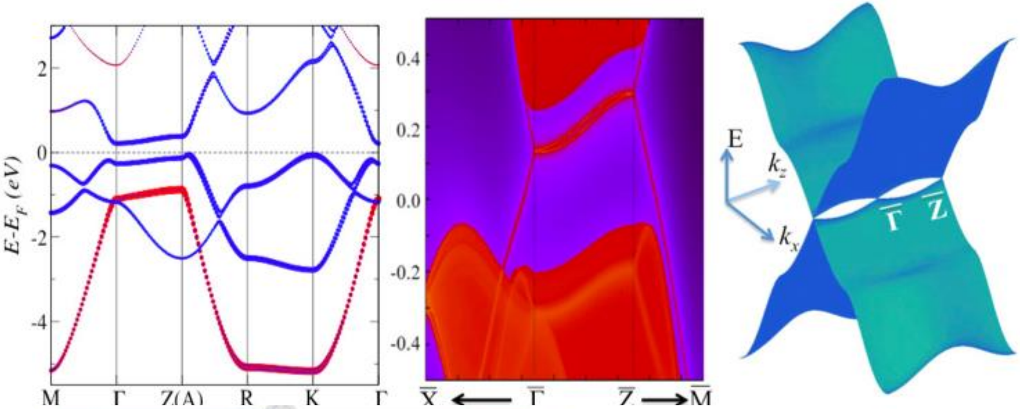


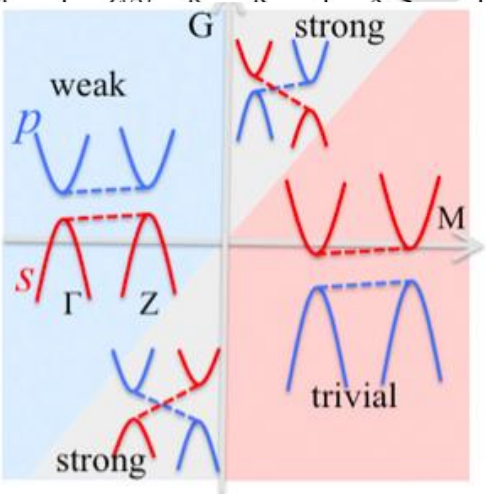
Zhang, Chadov, Müchler, Yan, Qi, Kübler, Zhang, Felser, Phys. Rev. Lett. 106 (2011) 156402 arXiv:1010.2195v1

honeycomb from sp3 to sp2



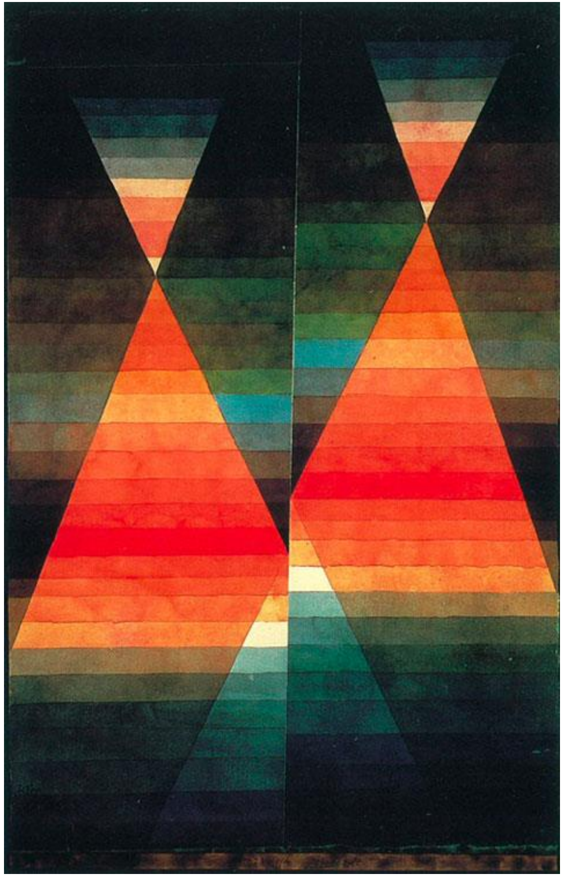
Yan, Müchler, Felser, Phys. Rev. Lett. 109 (2012) 116406





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

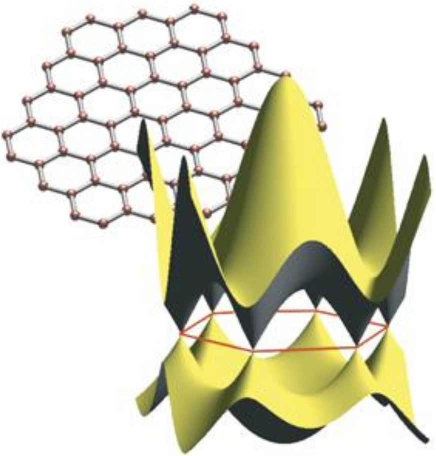
KAuTe	KAuSe
NaAuTe	NaAuSe
LiAuTe	LiAuSe
KAgTe	KAgSe
NaAgTe	NaAgSe
LiAgTe	LiAgSe

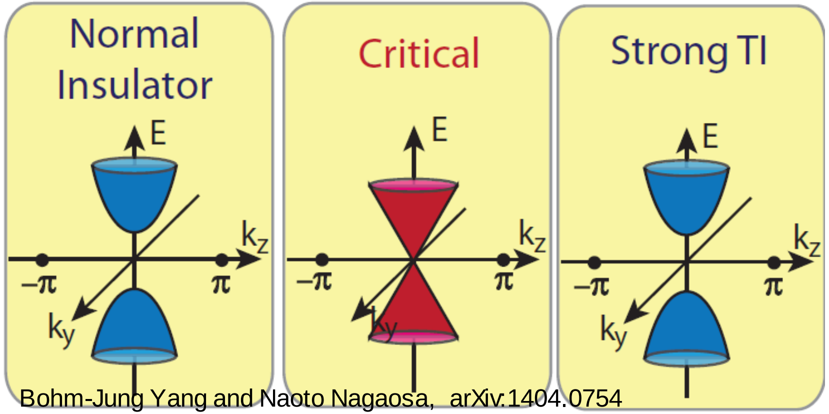


Weyl semimetals

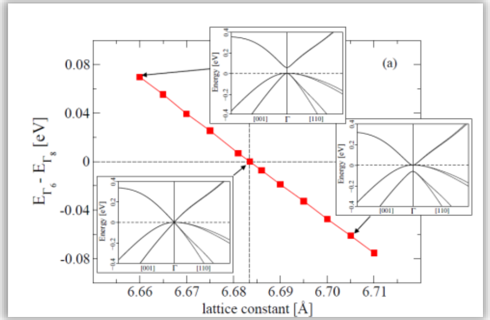
Breaking inversion symmetry

Dirac semimetals





Bohm-Jung Yang and Naoto Nagaosa, arXiv:1404.0754



nature COMMUNICATIONS

ARTICLE

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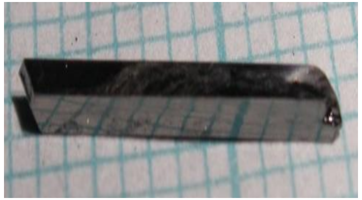
DOI: 10.1038/ncomms4786

Observation of a three-dimensional topological Dirac semimetal phase in high-mobility Cd_3As_2

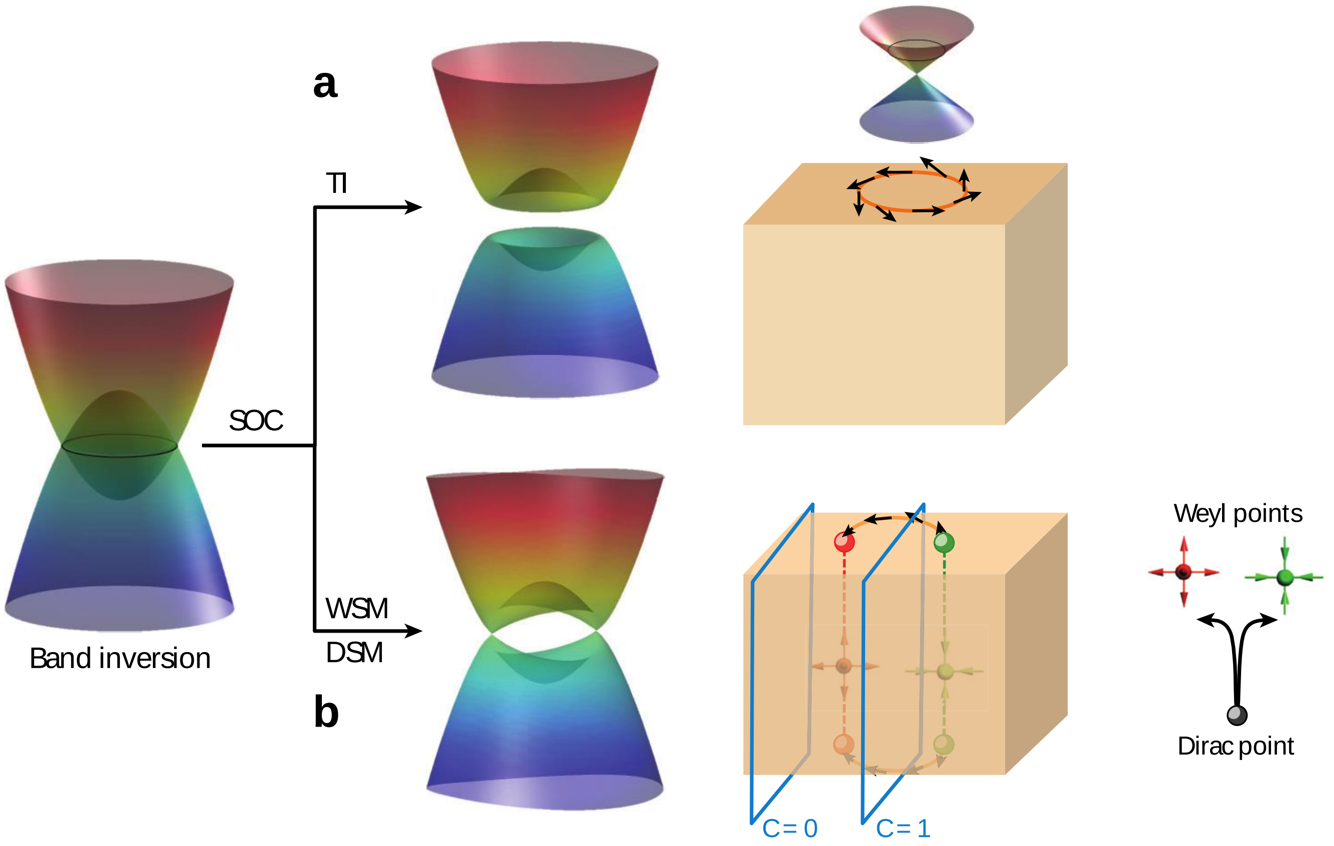
Madhab Neupane[1,*], Su-Yang Xu[1,*], Raman Sankar[2,*], Nasser Alidoust[1], Guang Bian[1], Chang Liu[1], Ilya Belopolski[1], Tay-Rong Chang[3], Horng-Tay Jeng[3,4], Hsin Lin[5], Arun Bansil[6], Fangcheng Chou[2] & M. Zahid Hasan[1,7]



Science AAAS

Observation of Fermi arc surface states in a topological metal
Su-Yang Xu *et al.*
Science **347**, 294 (2015);
DOI: 10.1126/science.1256742

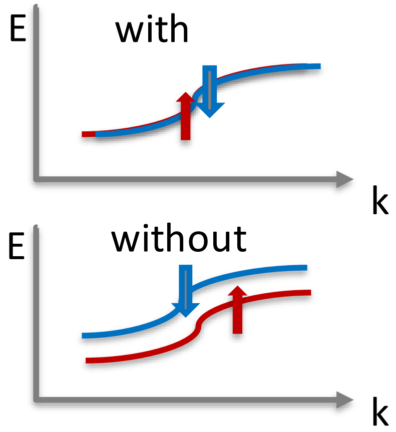
Weyl semimetals



Binghai Yan and Claudia Felser, Annual Review in Condensed Matter 8 (2017) 337

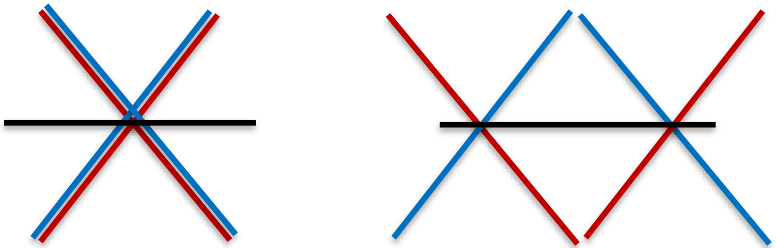
Weyl semimetals

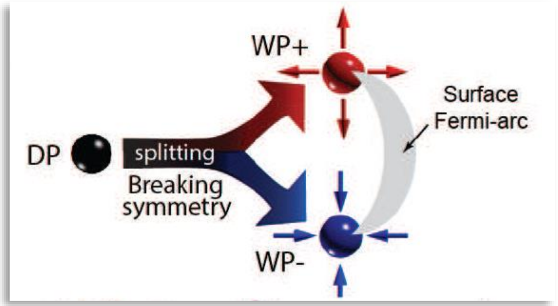
- Breaking symmetry
  - Inversion symmetry (Structural distortion)



- Breaking time reversal symmetry
  - Magnetic field

Dirac points are at high symmetry points
Weyl points are not at high symmetry points





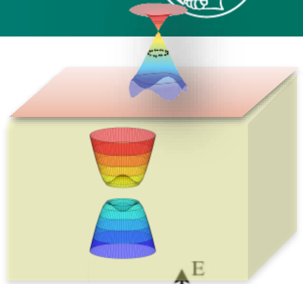
the materials

Topological materials

Topological Insulators

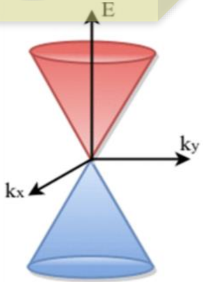
$RPtBi$, $RPdBi$, $RPtSb$

Bi_2Se_3, Bi_2Te_3 , Sb_2Te_3 Bi_2Te_2Se, Sb_2Te_2Se $TlBiTe_2$ $TlBiSe_2$, $TlBiSSe_2$



Topological Dirac semimetals

Cd_3As_2, Na_3Bi, ZrSiS, HfSiS, LaBi, LaSb, $PtSe_2$, $PtTe_2$, MA_3 (M=V, Nb, Ta; A=Al, Ga, In), CuMnAs, $HfTe_5$

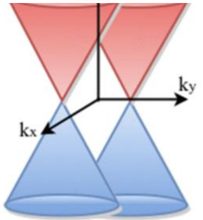


Topological Weyl semimetals

NbP,TaP,NbAs,TaAs,WTe_2, Td-$MoTe_2$

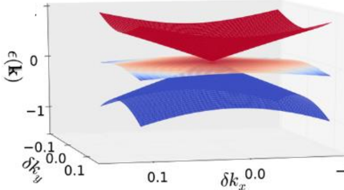
Co_2TiX (X=Si, Ge, Sn)

Mn_3Ge, Mn_3Sn, Mn_3Ir, Mn_3Ga, RPtBi, WP_2, MoP_2



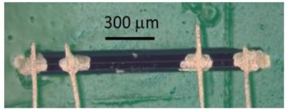
Beyond-Topological Dirac and Weyl

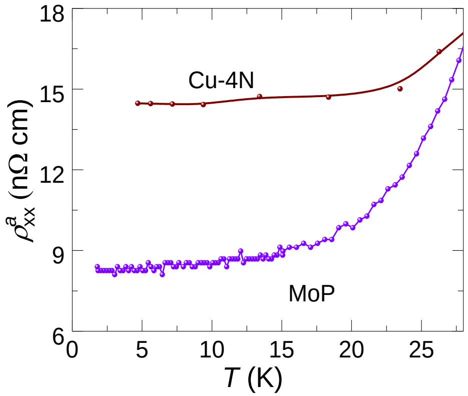
MoP, $PdSb_2$, La_4Bi_3, Mg_3Ru_2, Ta_3Sb, Nb_3Bi, CoSi, RhSi, AlPt, PdGa

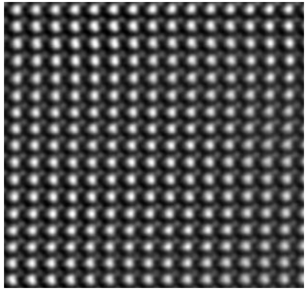


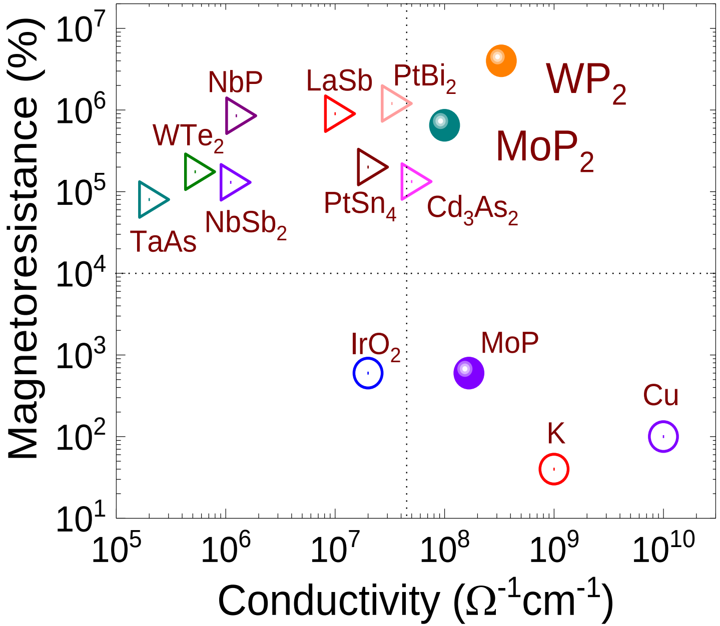
high quality materials

- large **mean free path**, high mobility
- large magneto resistance, quantum oscillations
- low defect density
- high conductivity









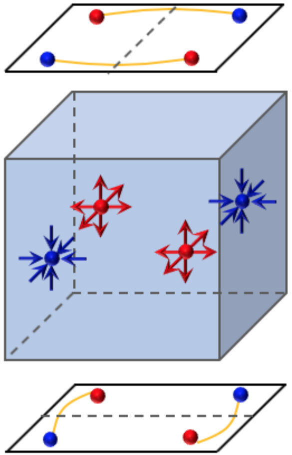
Hydrodynamic flow of electrons

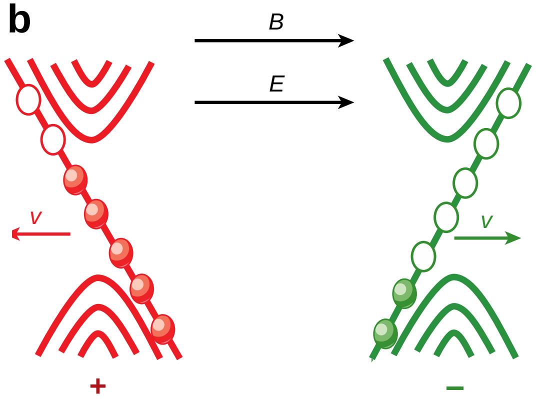
C. Shekhar et al. Nat. Phys. 2015, N. Kumar et al. Nat. Commun 2017, J. Gooth et al. Nat. Commun. 2018, Gooth Nature 2017

Weyl semimetals

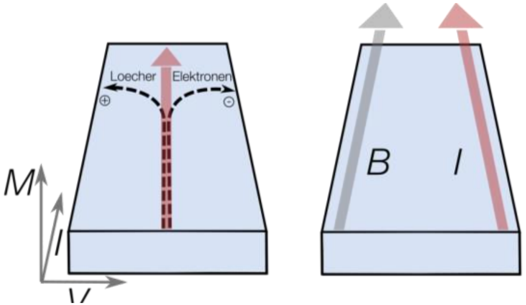
3D topological Weyl in transport measurement:

1. Fermi arc
2. Intrinsic anomalous Hall effect
3. Planar Hall effect
4. Chiral anomaly
5. Axial gravitational anomaly



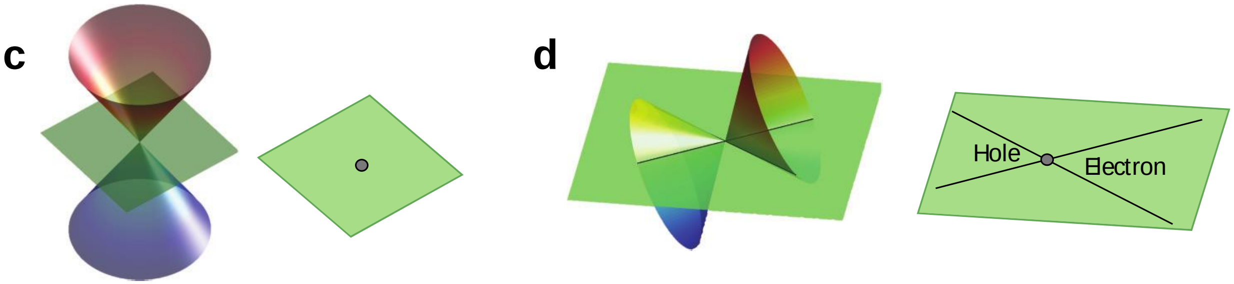


$$\partial_\mu j^\mu_\chi = -\chi \frac{e^3}{4\pi^2\hbar^2}\boldsymbol{E}\cdot\boldsymbol{B}$$



AA Burkov, L Balents, PRL 107 12720 (2012)
AA Burkov, arXiv:1704.05467v2
AA Burkov, J. Phys.: Condens. Matter 27 (2015) 113201

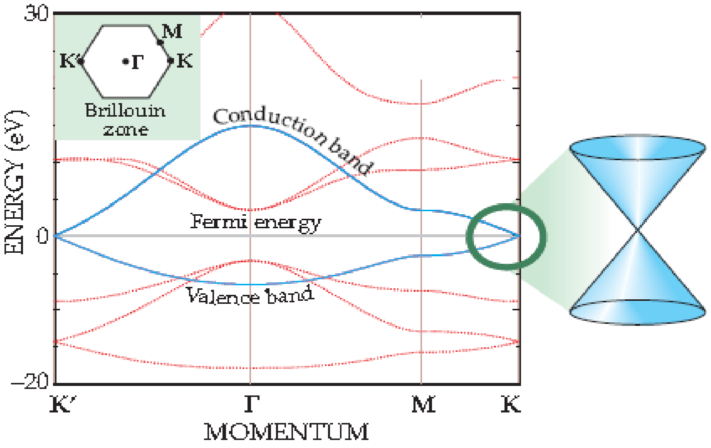
type I or II

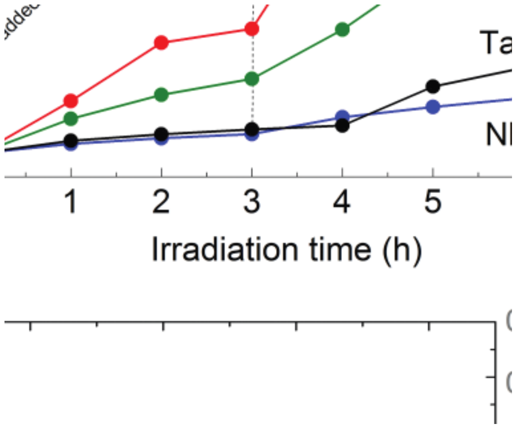


Type-I WSM

Type-II WSM

Graphene



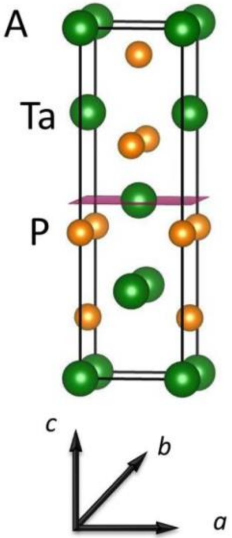


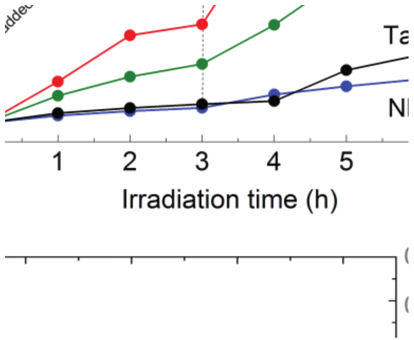
A. K. Geim, A. H. MacDonald Physics Today, 08.(2007), 35-41

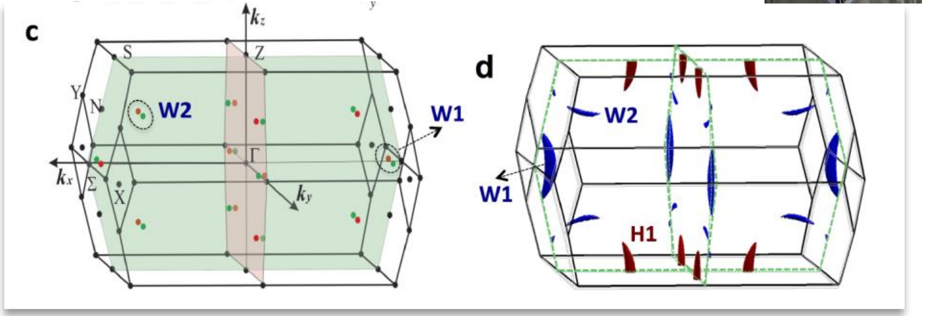
Shekhar Chandra, et al. , Nature Physics 11 (2015) 645

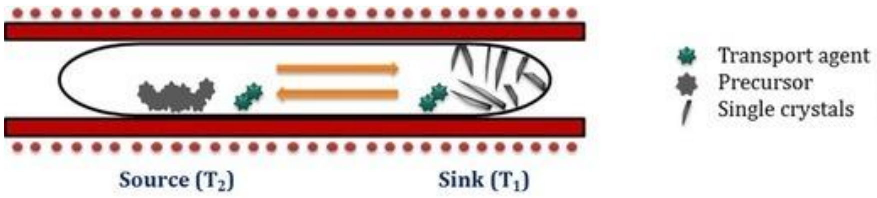
Weyl semimetals in non-centro NbP

NbP, NbAs, TaP, TaAs







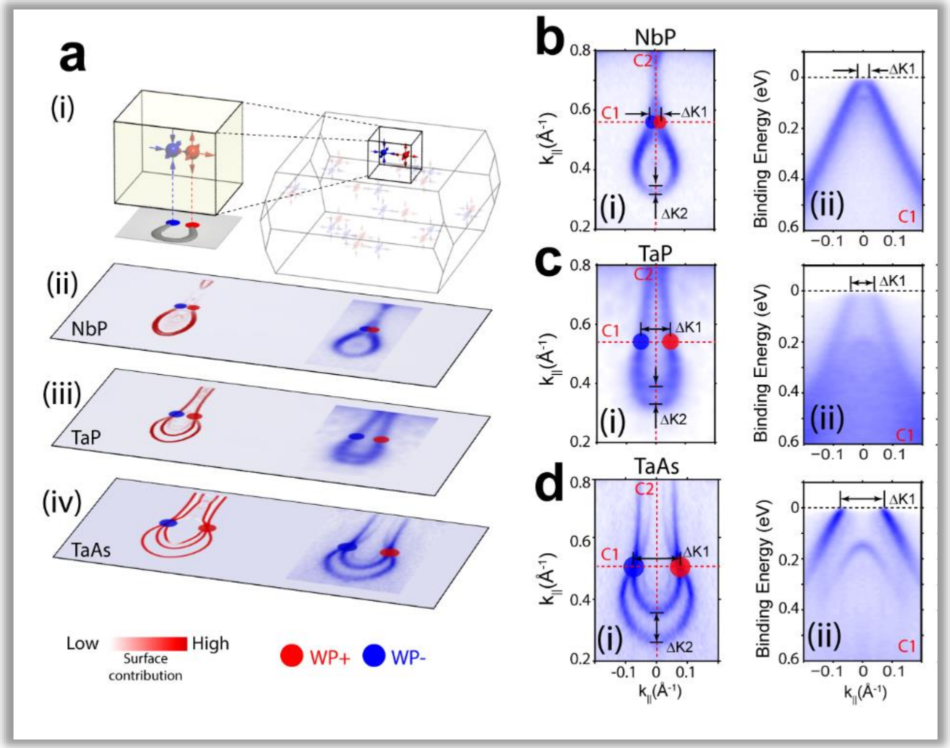


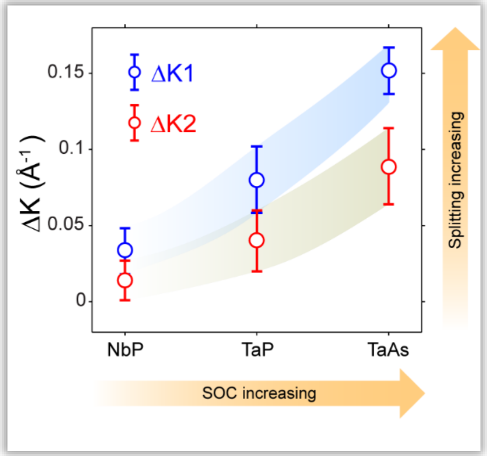
Shekhar, et al. , Nature Physics 11 (2015) 645,
Arnold, et al., Nature Communication 7 (2016) 11615

Weng, et al. Phys. Rev. X 5, 11029 (2015)
Huang et al. preprint arXiv:1501.00755

Fermi arcs

Increasing spin orbit coupling increases – heavier elements
Distance between the Weyl points increases



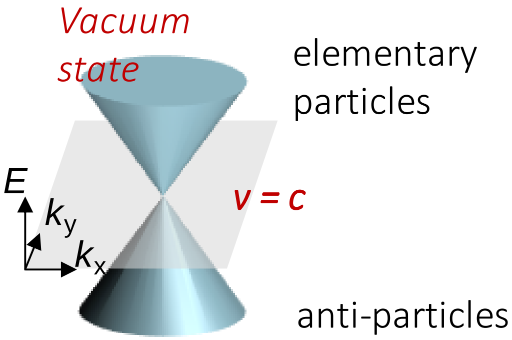


Liu et al., Nature Mat. 15 (2016) 27
Yang, et al. Nature Phys. 11 (2015) 728

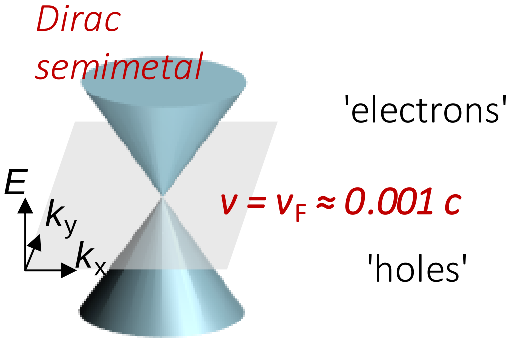
chiral anomaly

- Chiral anomaly is the **anomalous non-conservation** of a chiral current.
- A sealed box with equal number of positive and negative charged particles, its found when it is opened to have more positive than negative particles, or vice-versa.
- Events are expected to be prohibited according to classical conservation laws, must be ways they can be broken, because the observable **universe contains more matter than antimatter**

Wikipedia



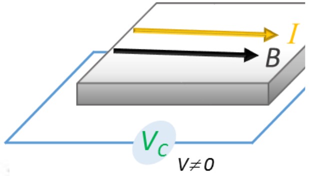
vacuum dispersion



band structure

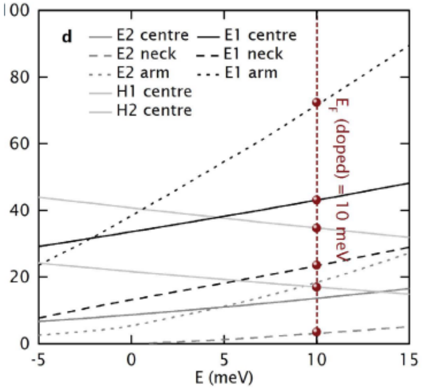
S. L. Adler, Phys. Rev. 177, 2426 (1969)
J. S. Bell and R. Jackiw, Nuovo Cim. A60, 47 (1969)
AA Zyuzin, AA Burkov - Physical Review B (2012)

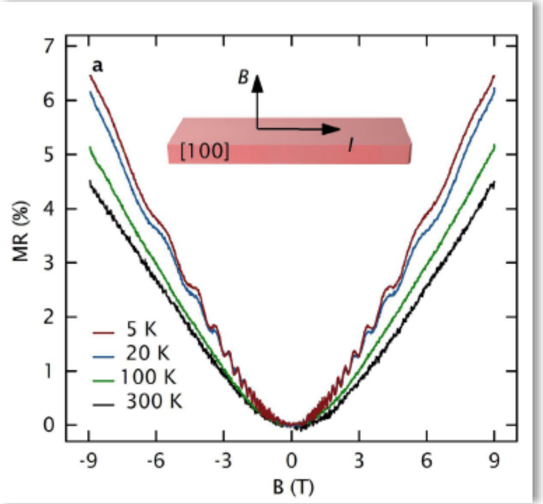
chiral anomaly

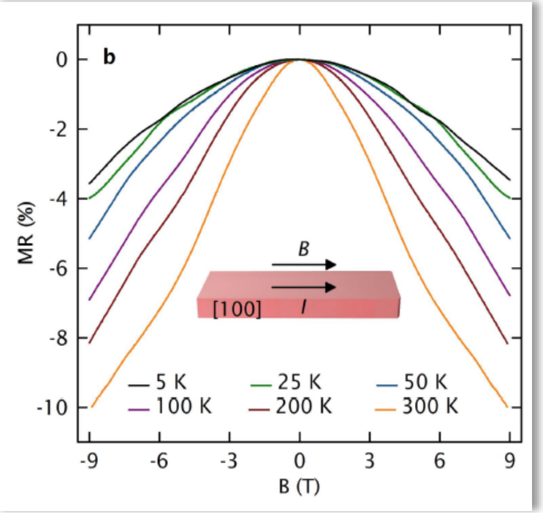


Chiral Anomaly

$$\sigma_a = \frac{e^3 v_f^3}{4\pi^2 \hbar \mu^2 c} B^2, \qquad \partial_\mu j_\chi^\mu = -\chi \frac{e^3}{4\pi^2 \hbar^2} \boldsymbol{E} \cdot \boldsymbol{B}$$





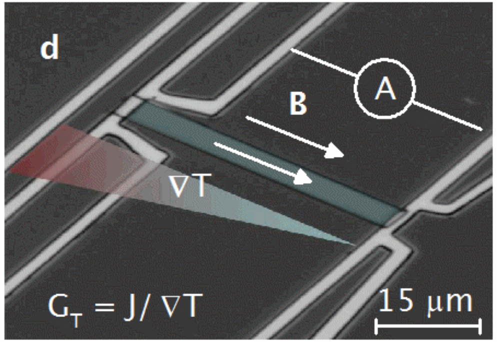


Ga-doping relocate the Fermi energy in NbP close to the W2 Weyl points
Therefore we observe a negative MR as a signature of the chiral anomaly the, NMR survives up to room temperature

Niemann, et al. Scientific Reports 7 (2017) 43394 doi:10.1038/srep4339 preprint arXiv:1610.01413

axial-gravitational anomaly

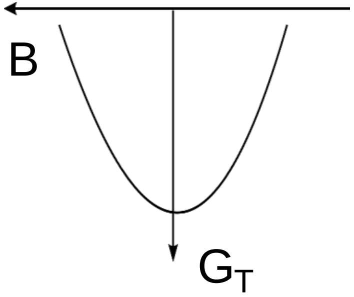
Experimental signatures for the mixed axial-gravitational anomaly in Weyl semimetals



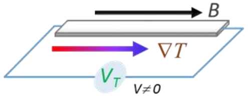
- In solid state physics, mixed axial-gravitational anomaly can be identified by a positive magneto-thermoelectric conductance (PMTG) for ΔT ll B.

  - Low fields: quadratic

$$G_T = d_{\mathrm{th}} + c_2 a_\chi a_g B_\parallel^2$$



  - High fields: deminishes

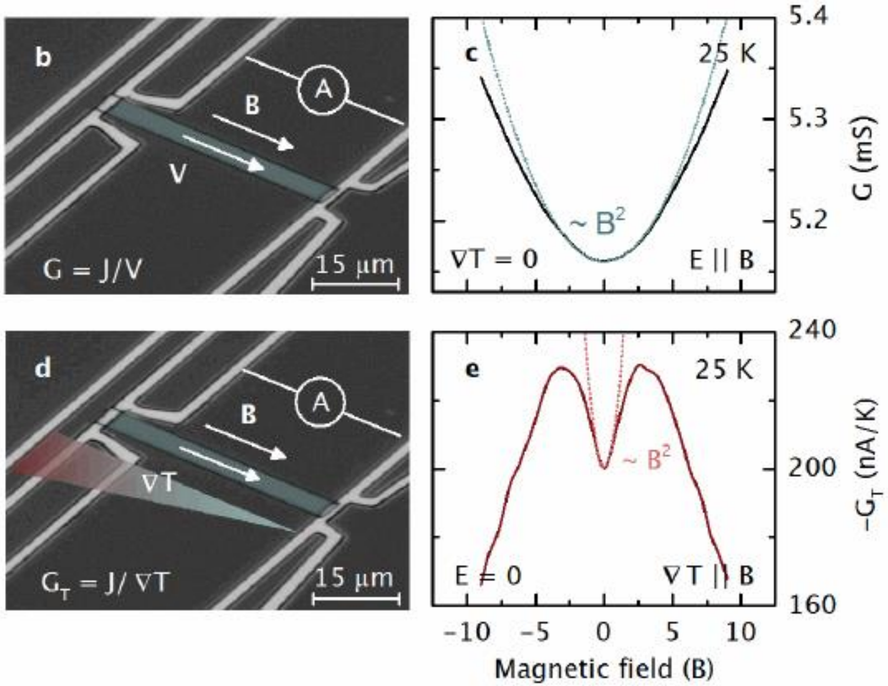


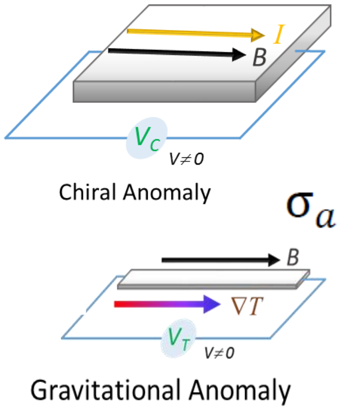
Gravitational Anomaly

  - ΔT ll B dictates sensitivity on alignement of B and ΔT.

[Lucas, et al. Proceedings of the National Academy of Sciences **113,** 9463 (2016)]

gravitational anomaly





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

- Landsteiner K., et al. Gravitational anomaly and transport phenomena. Phys. Rev. Lett. 107, 021601 (2011). URL
- Jensen, et al. Thermodynamics, gravitational anomalies and cones. Journal of High Energy Physics 2013, 88 (2013).
- Lucas, A., Davison, R. A. & Sachdev, S. Hydrodynamic theory of thermoelectric transport and negative magnetoresistance in weyl semimetals. PNAS 113, 9463–9468 (2016).

A positive longitudinal magneto-thermoelectric conductance (PMTC) in the Weyl semimetal NbP for collinear temperature gradients and magnetic fields that vanishes in the ultra quantum limit.

Gooth et al., Nature 547 (2017) 324 arXiv:1703.10682

universe – in a crystal

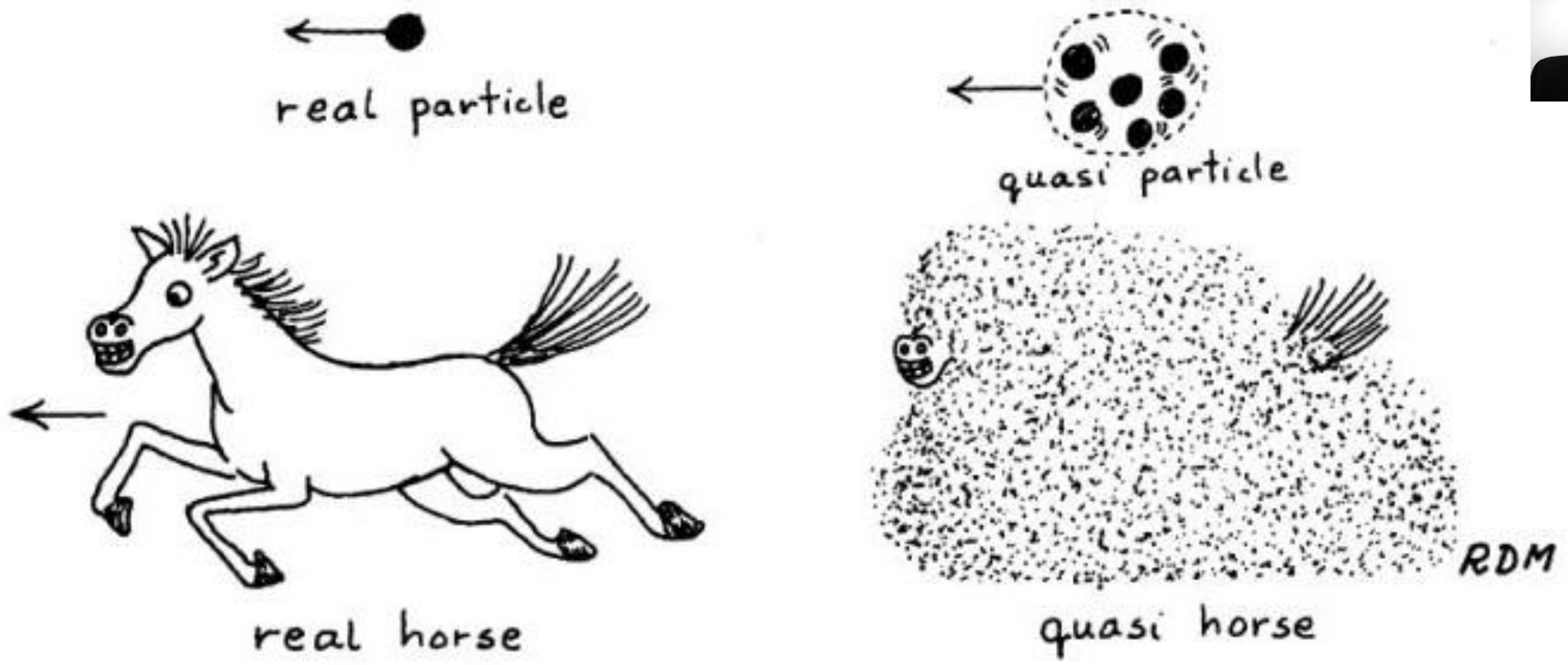
The New York Times | https://nyti.ms/2vCMCGi

SCIENCE

An Experiment in Zurich Brings Us Nearer to a Black Hole's Mysteries

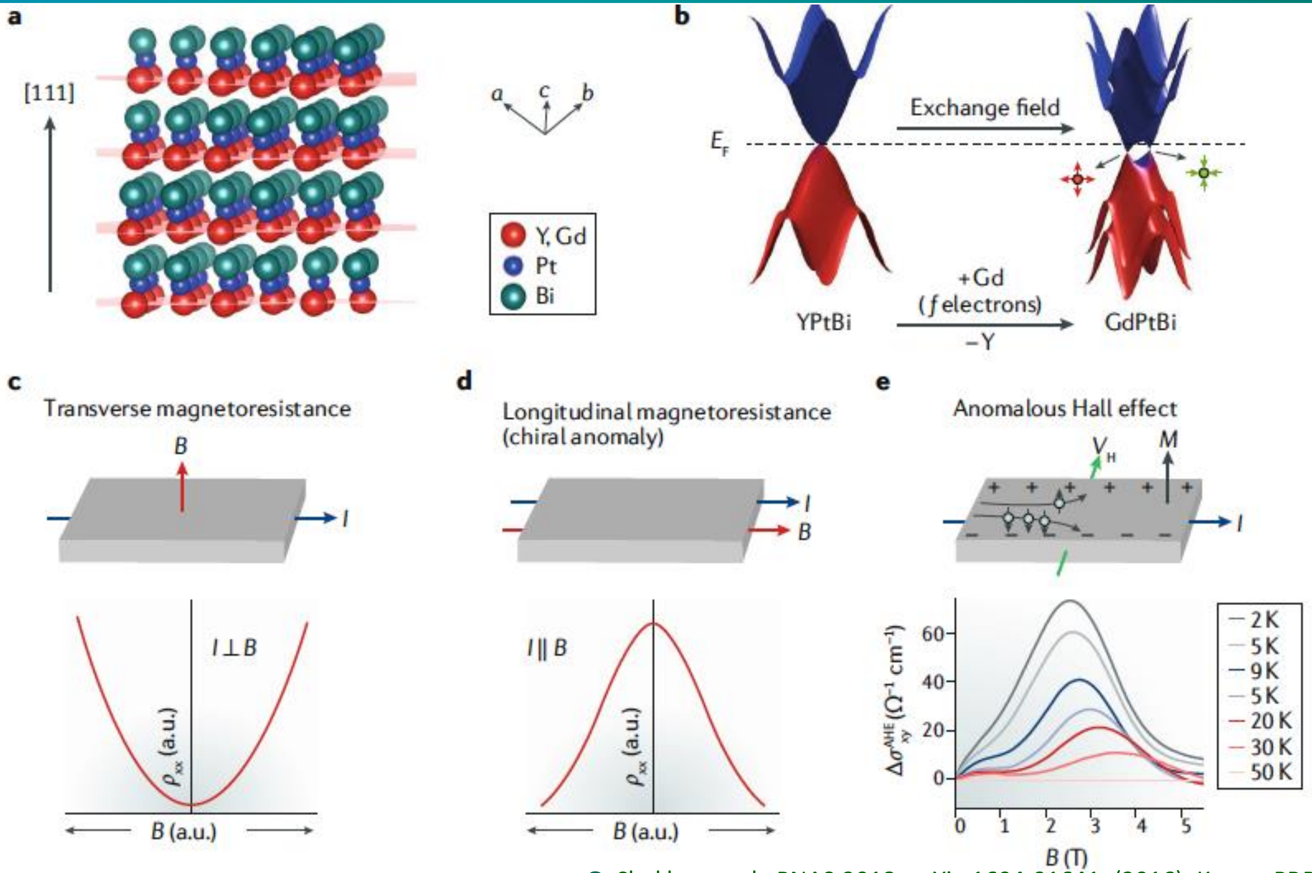
By KENNETH CHANG JULY 19, 2017

particles and quasi particles



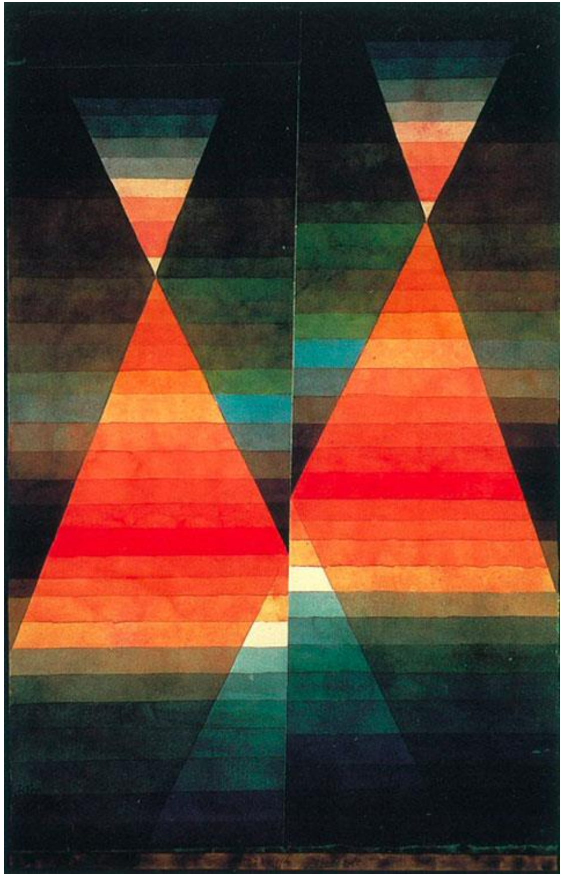
Mattuck, “A Guide to Feynman Diagrams in the Many-Body Problem” (1967)

GdPtBi – an ideal Weyl



C. Shekhar et al., PNAS 2018, arXiv:1604.01641, (2016), Kumar PRB 2018, Kaustuv Nat. Mat. Rev. (2019).

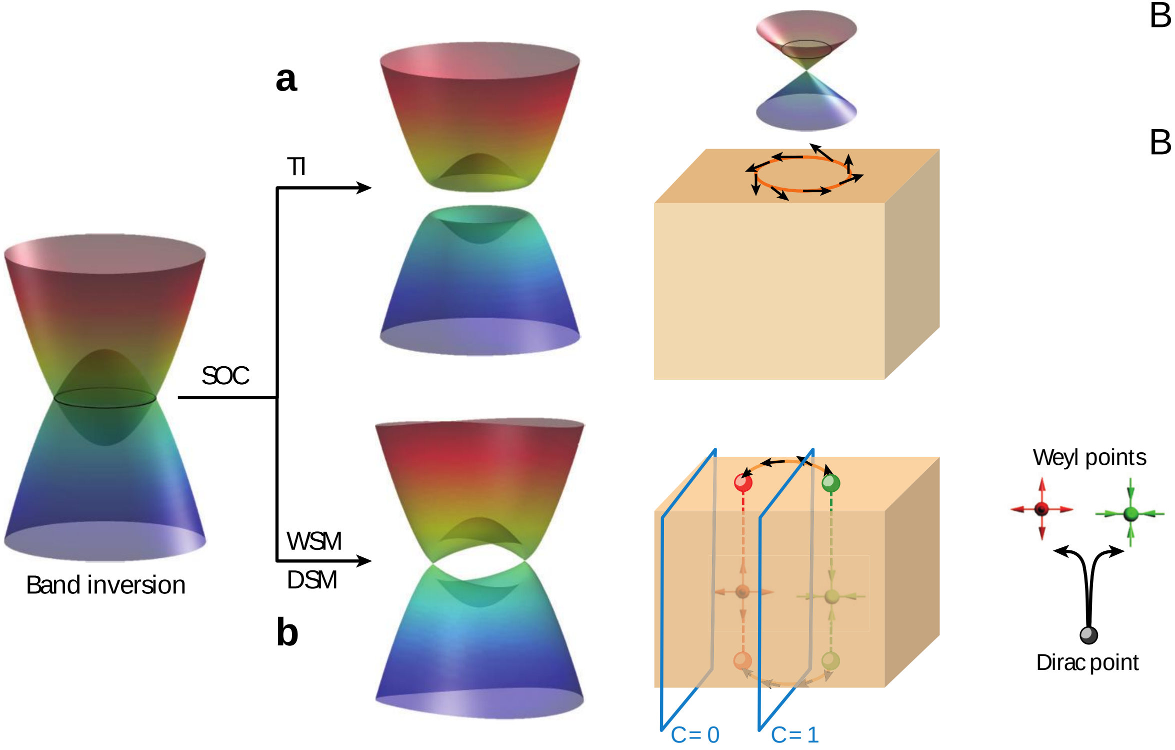
M. Hirschberger et al.,. Nature Mat. Online arXiv:1602.07219, (2016).



Weyl semimetals

Breaking time reversal symmetry

Weyl semimetals

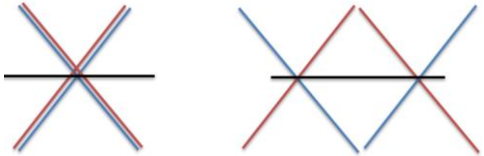


Breaking symmetry

- Inversion symmetry (Strain)

Breaking time reversal symmetry

- Magnetic field

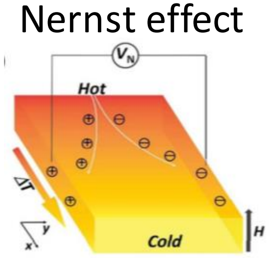


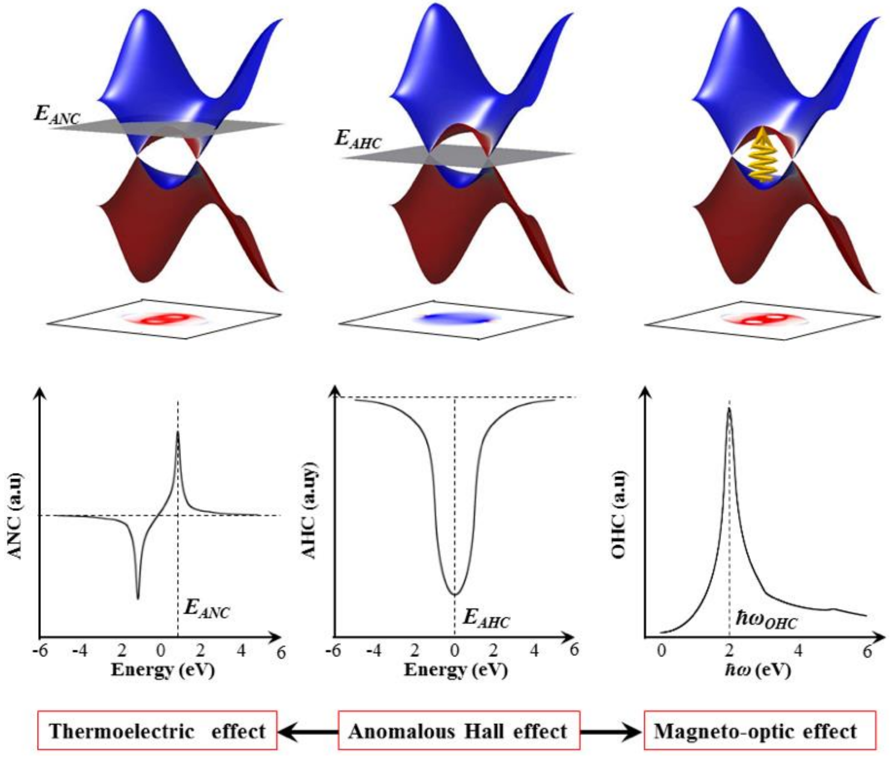
- **Dirac points at high symmetry**
- **Weyl points at low symmetry**
- **All crossings in ferromagnets: Weyl points**

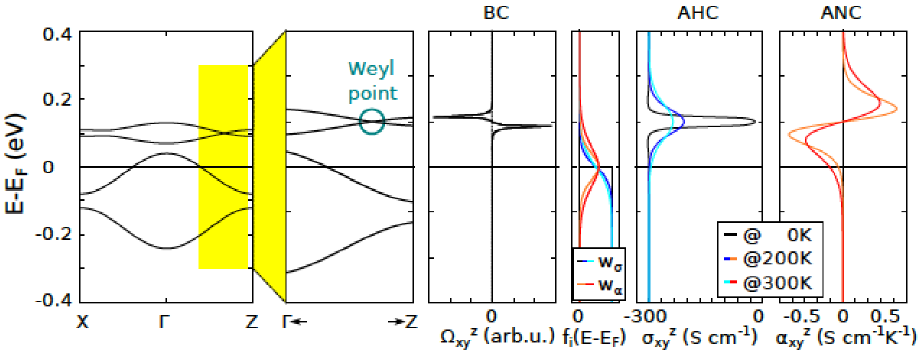
Binghai Yan and Claudia Felser, Annual Review in Condensed Matter 8 (2017) 337

Berry curvature design

Berry curvature design
- giant spin Hall
- giant anomalous Hall
- giant topological Hall
- giant anomalous Nernst







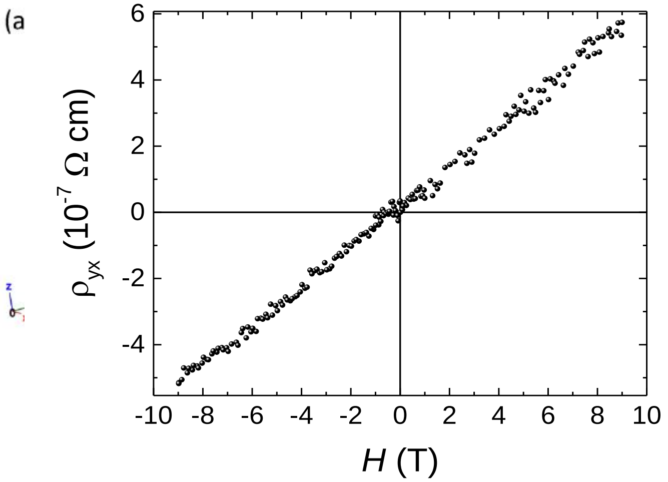
J. Noky et al., Phys. Rev. B 98, 241106(R) (2018), arXiv:1807.07843, arXiv:1806.06753

Heusler, Weyl and Berry

PRL **112,** 017205 (2014) PHYSICAL REVIEW LETTERS week ending 10 JANUARY 20

Anomalous Hall Effect Arising from Noncollinear Antiferromagnetism

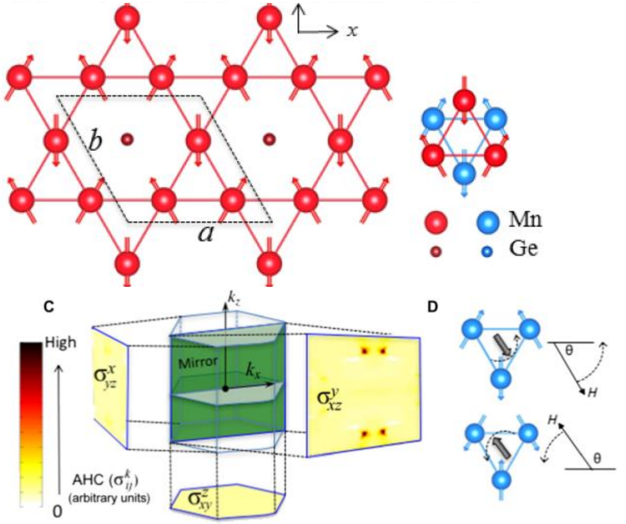
Hua Chen, Qian Niu, and A. H. MacDonald



epl A Letters Journal Exploring the Frontiers of Physics December 2014
EPL, **108** (2014) 67001 www.epljournal.org
doi: 10.1209/0295-5075/108/67001

Non-collinear antiferromagnets and the anomalous Hall effect

J. Kübler[1] and C. Felser[2]



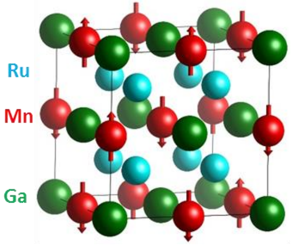
For the planar cases the AHC is connected with Weyl points in the energy- band structure.

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

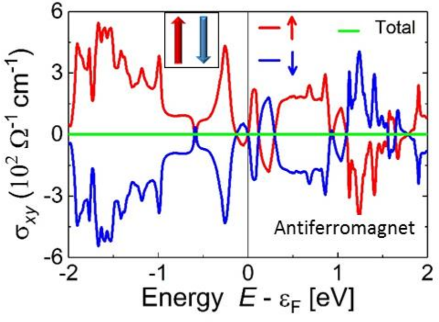
Kübler and Felser EPL 108 (2014) 67001

Heusler, Weyl and Berry

$$\sigma_{xy}^{A}(\mu) = ie^2 \left(\frac{1}{2\pi}\right)^3 \int_k dk \sum_{E(n,k)<\mu} f(n,k,\mu)\Omega_{n,xy}(k),$$

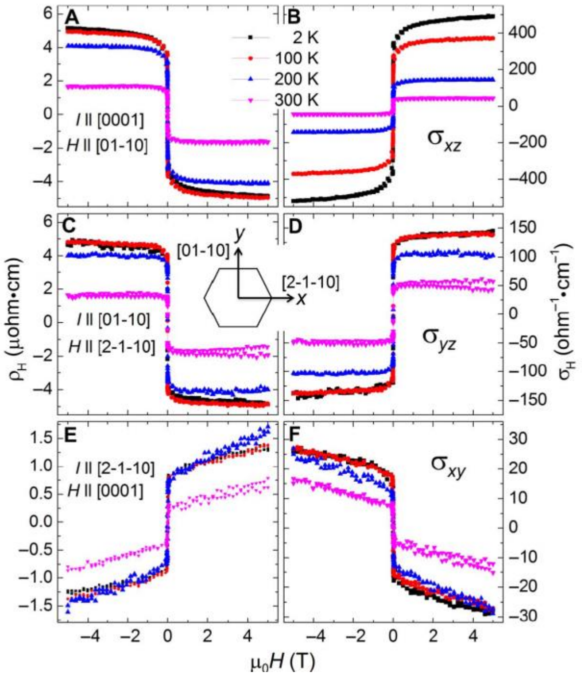


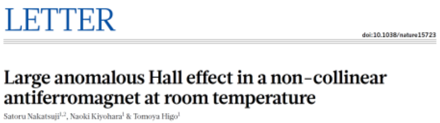
[Ru_2MnSi]

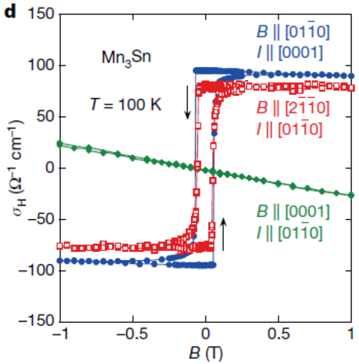


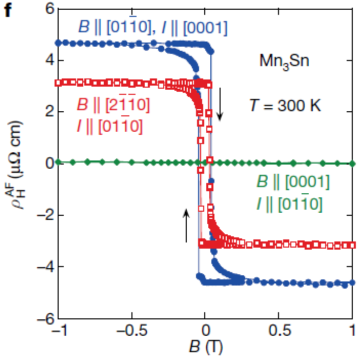
The anomalous Hall conductivity in an antiferromagnetic metal is zero

Mn_3Ge
Mn_3Sn









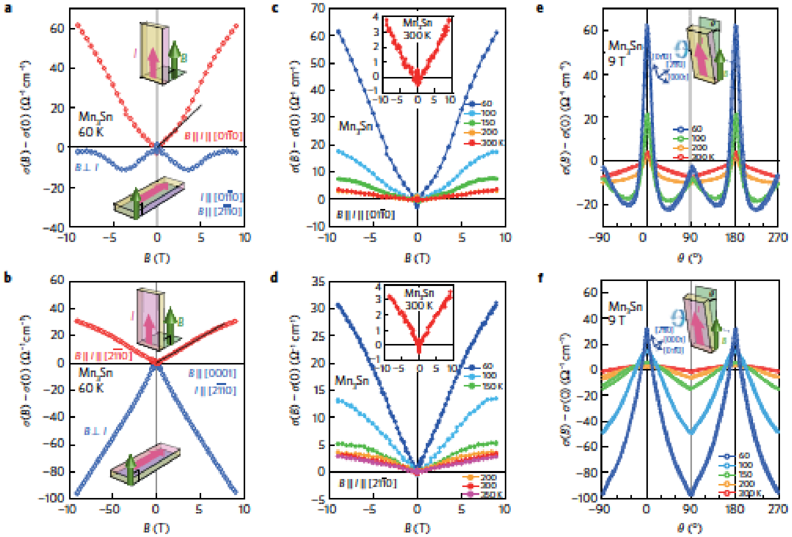
Nayak et al. arXiv:1511.03128, Science Advances 2 (2016) e1501870
Kiyohara, Nakatsuji, preprint: arXiv:1511.04619
Nakatsuji, Kiyohara, & Higo, Nature, doi:10.1038/nature15723

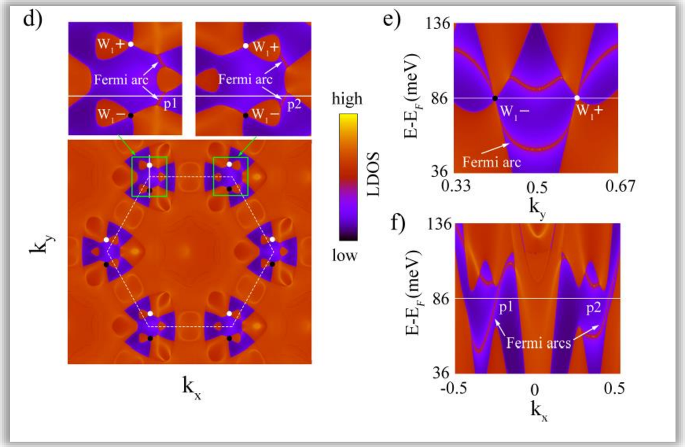
Fermiarcs and chiral anomaly in the Weyl AFM

nature materials | LETTERS
PUBLISHED ONLINE: 25 SEPTEMBER 2017 | DOI: 10.1038/NMAT4987

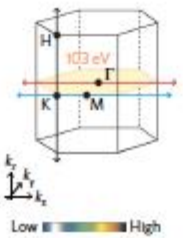
Evidence for magnetic Weyl fermions in a correlated metal

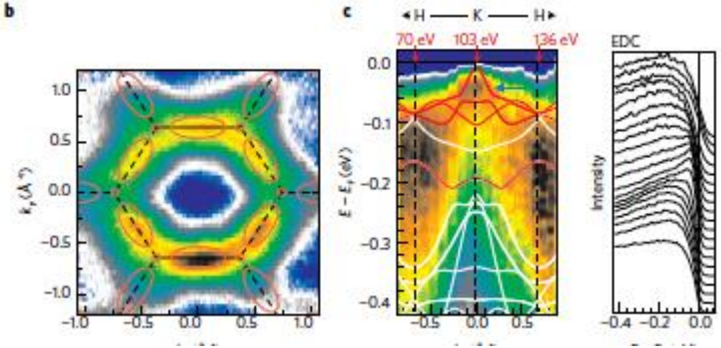
K. Kuroda[1†], T. Tomita[1,2†], M.-T. Suzuki[2,3], C. Bareille[1], A. A. Nugroho[1,4], P. Goswami[5,6], M. Ochi[7], M. Ikhlas[1,2], M. Nakayama[1], S. Akebi[1], R. Noguchi[1], R. Ishii[1], N. Inami[8], K. Ono[8], H. Kumigashira[8], A. Varykhalov[9], T. Muro[10], T. Koretsune[2,3], R. Arita[2,3], S. Shin[1], Takeshi Kondo[1] and S. Nakatsuji[1,2*]





Hao Yang, et al. New J. Phys. 19 (2017) 015008,



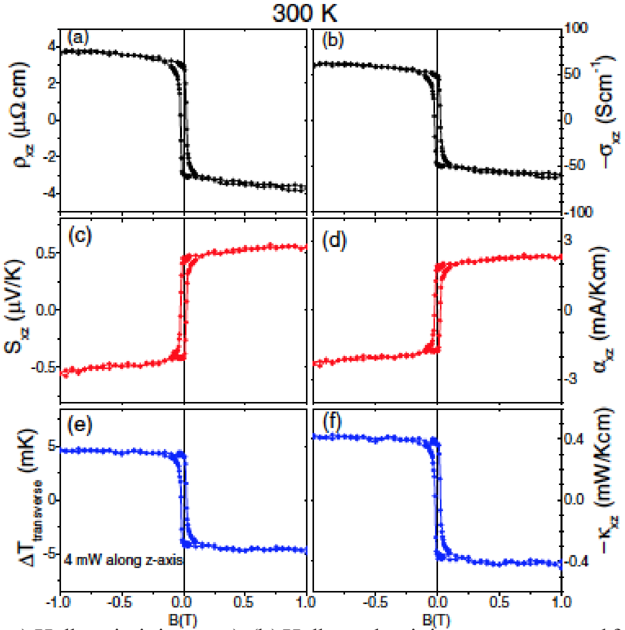


Nernst effect in Mn_3Sn

PRL 119, 056601 (2017) PHYSICAL REVIEW LETTERS week ending 4 AUGUST 2017

Anomalous Nernst and Righi-Leduc Effects in Mn_3Sn: Berry Curvature and Entropy Flow

Xiaokang Li,[1] Liangcai Xu,[1] Linchao Ding,[1] Jinhua Wang,[1] Mingsong Shen,[1] Xiufang Lu,[1] Zengwei Zhu,[1,*] and Kamran Behnia[1,2,†]

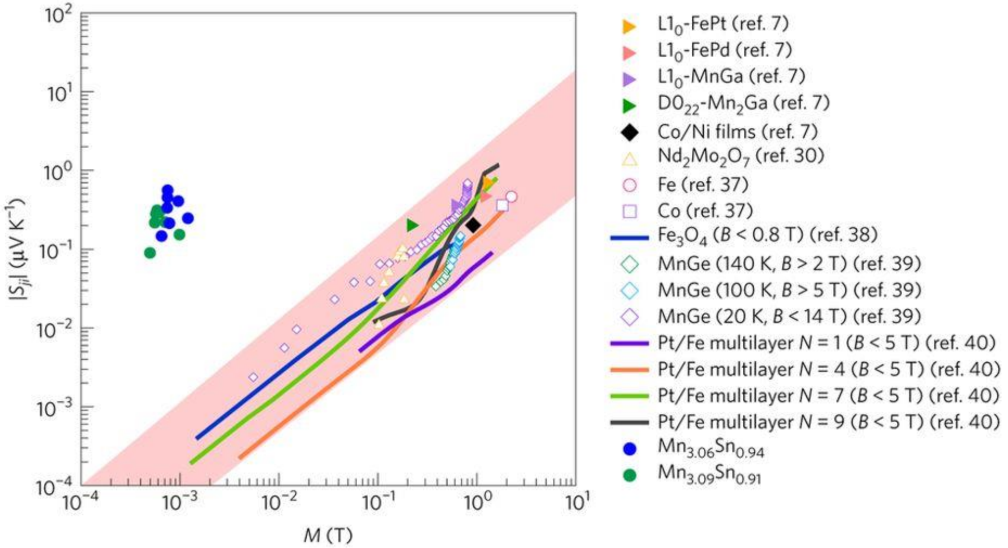


a) Hall resistivity, ρxz); (b) Hall conductivity, σxz, extracted from ρxz, ρxx, and ρzz; (c) Nernst signal, Sxz; (d) Transverse thermoelectric conductivity, αxz,

nature physics LETTERS
PUBLISHED ONLINE: 24 JULY 2017 | DOI: 10.1038/NPHYS4181

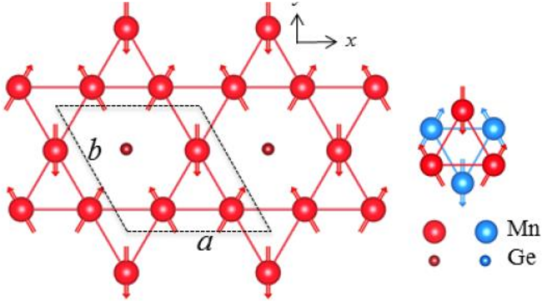
Large anomalous Nernst effect at room temperature in a chiral antiferromagnet

Muhammad Ikhlas[1†], Takahiro Tomita[1†], Takashi Koretsune[2,3], Michi-To Suzuki[2], Daisuke Nishio-Hamane[1], Ryotaro Arita[2,4], Yoshichika Otani[1,2,4] and Satoru Nakatsuji[1,4*]



Magnetization dependence of the spontaneous Nernst effect for ferromagnetic metals and Mn_3Sn

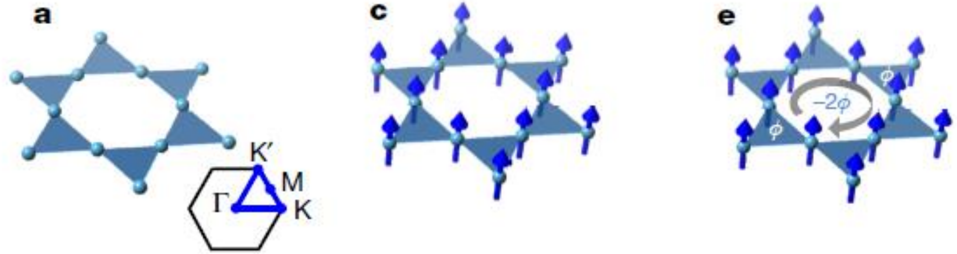
Kagome lattice



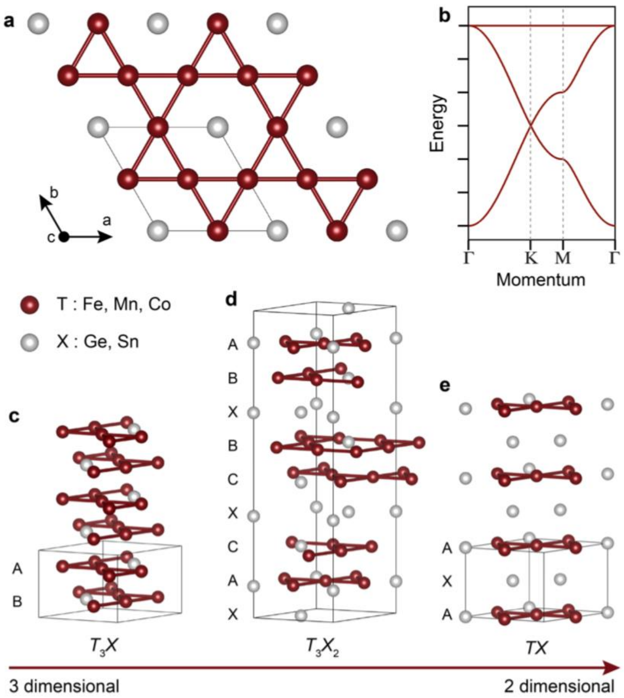
LETTER

doi:10.1038/nature25987

Massive Dirac fermions in a ferromagnetic kagome metal



Mn,Fe,Co



Nature, 2018, doi:10.1038/nature25987

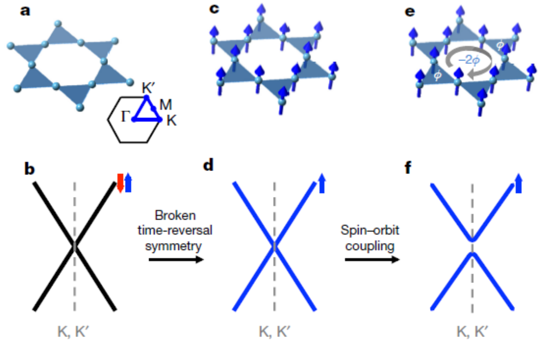
Kang et al., preprint arXiv:1906.02167

Kagome lattice

LETTER

doi:10.1038/nature25987

Massive Dirac fermions in a ferromagnetic kagome metal

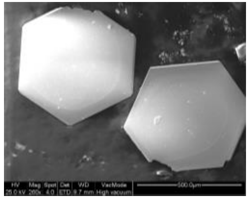


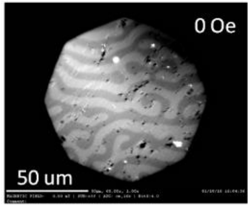
Fe_3Sn_2

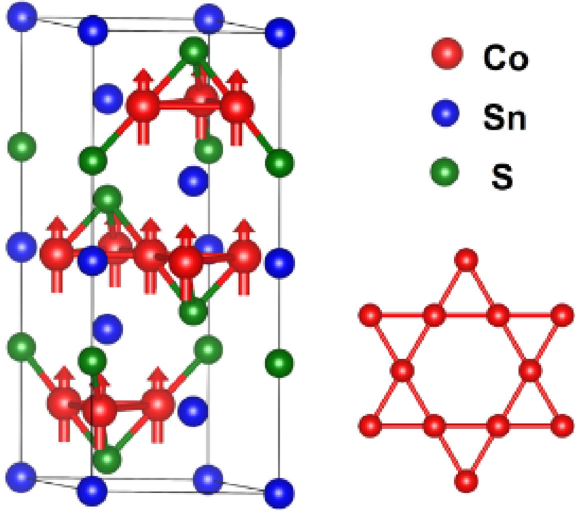
Nature, 2018, doi:10.1038/nature25987

Looking for Weyl fermions on a ferromagnetic Kagomé lattice with out of plane magnetisation.

$Co_3Sn_2S_2$

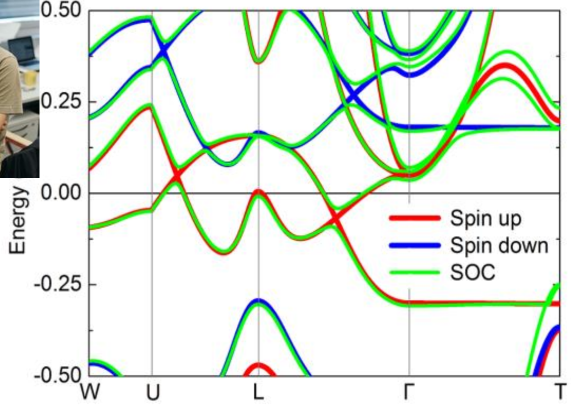


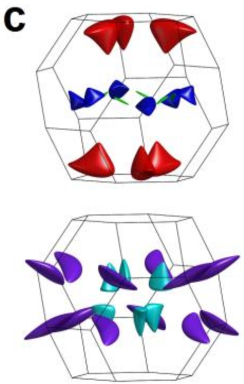




Enke Liu, et al. Nature Physics 14 (2018) 1125 , preprint arXiv:1712.06722

Weyl and Berry

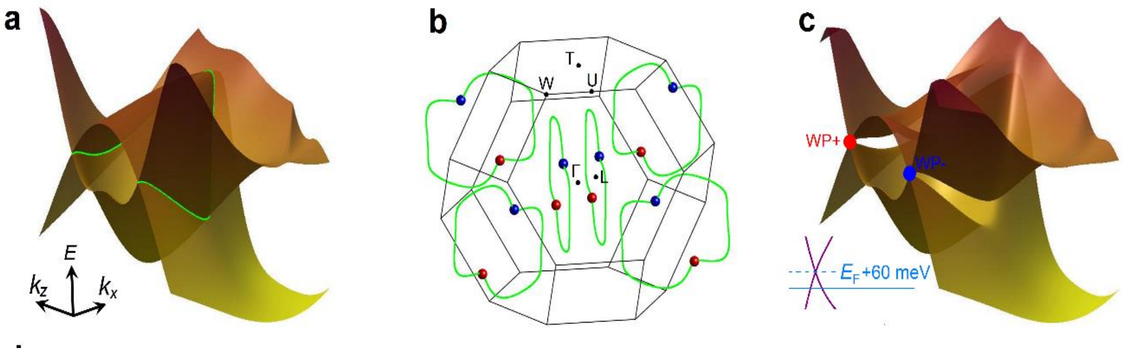


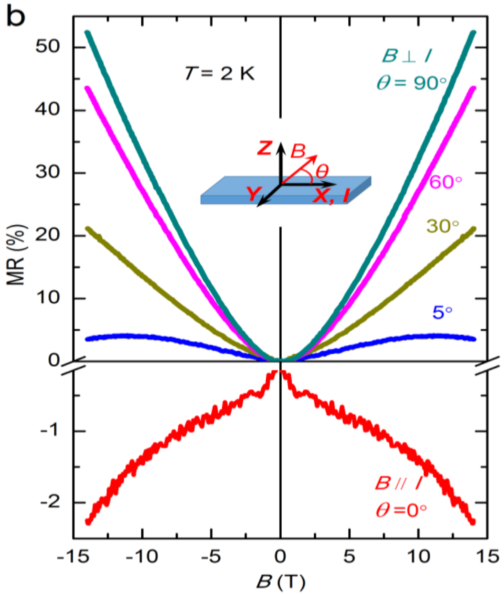


$Co_3Sn_2S_2$

Weyl points are close to EF
Hard magnetic behaviour

transport: chiral anomaly



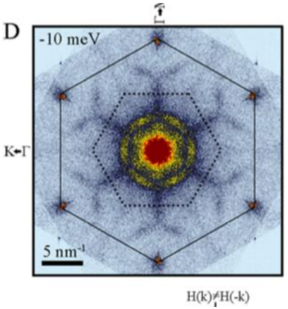


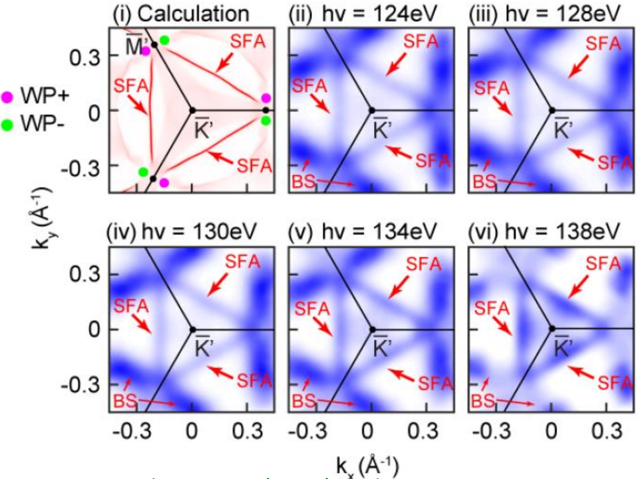
D. F. Liu, et al., Science (2019) under review

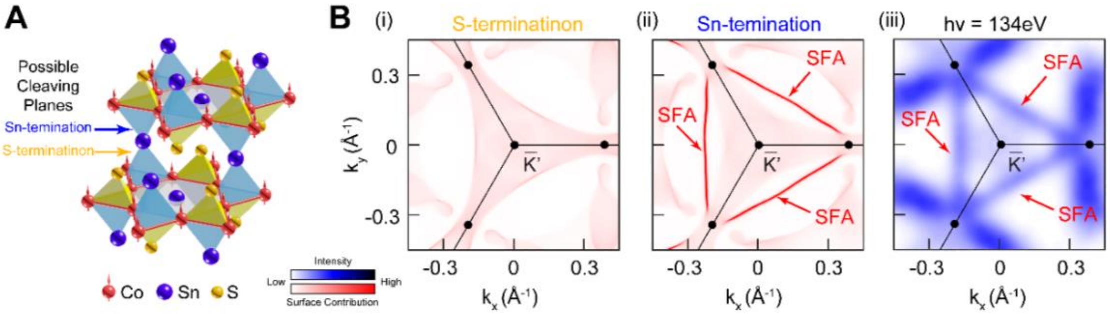
Liu, et al. Nature Physics 14 (2018) 1125 , preprint arXiv:1712.06722

Weyl and Berry

STM and ARPES confirms Weyl and Fermiarcs





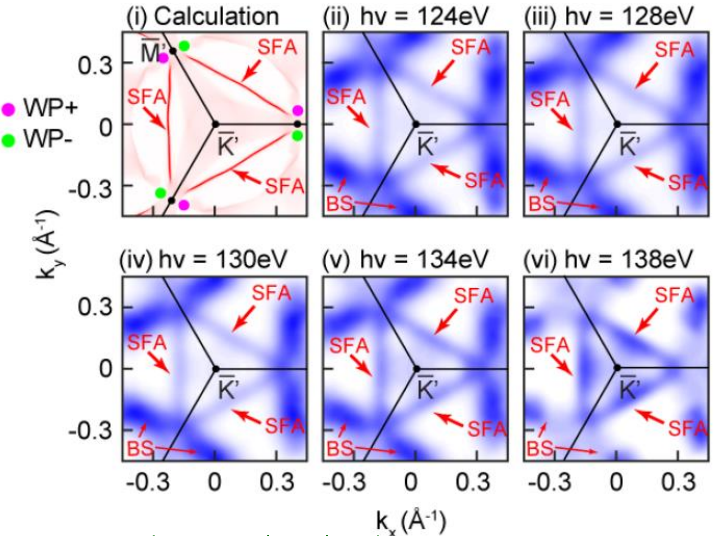


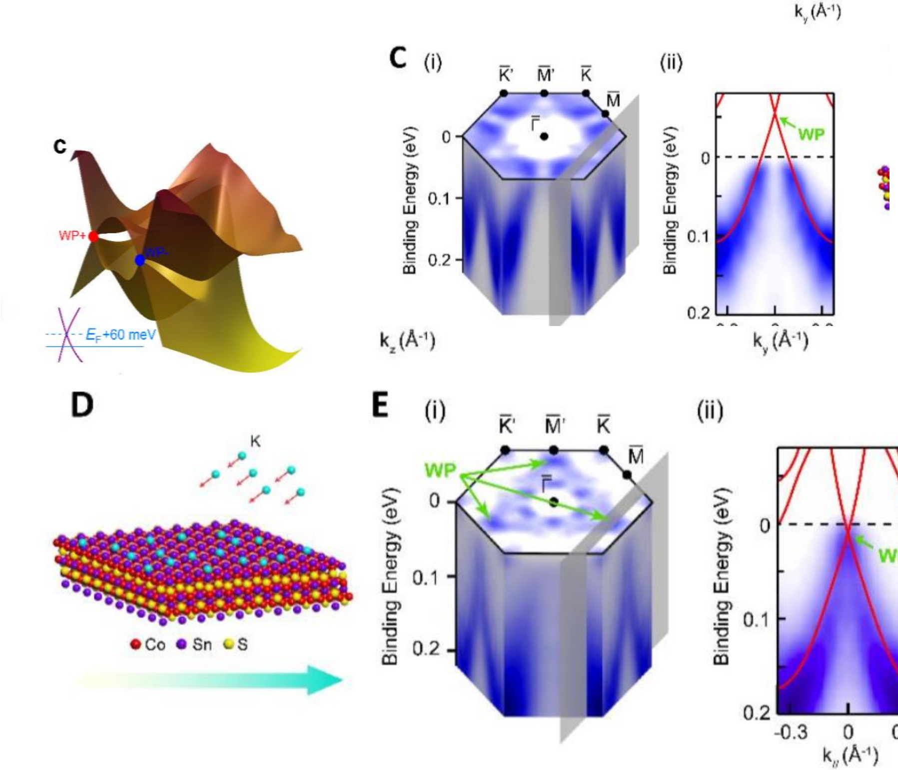
D. F. Liu, et al., Science (2019) under review

Morali et al., Science accepted , preprint arXiv:1903.00509

Weyl and Berry

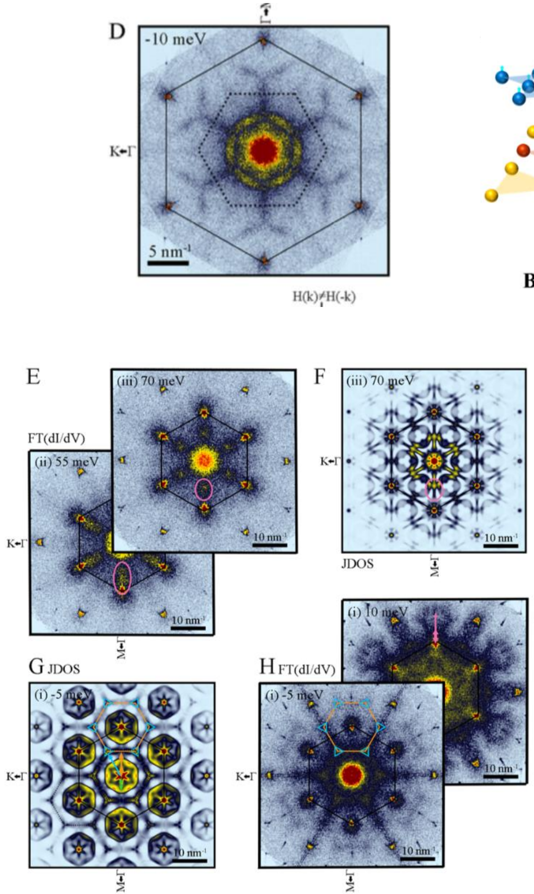
ARPES confirms Weyl and Fermiarcs

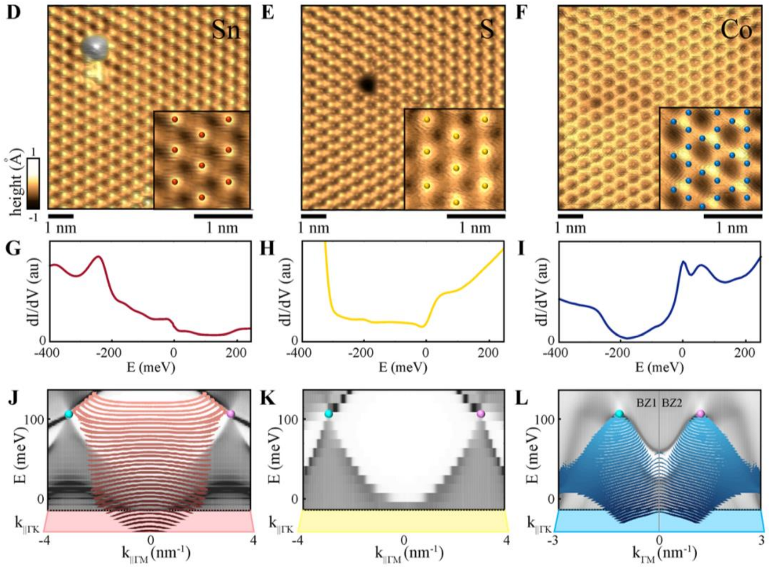




D. F. Liu, et al., Science (2019) under review

Weyl and Berry





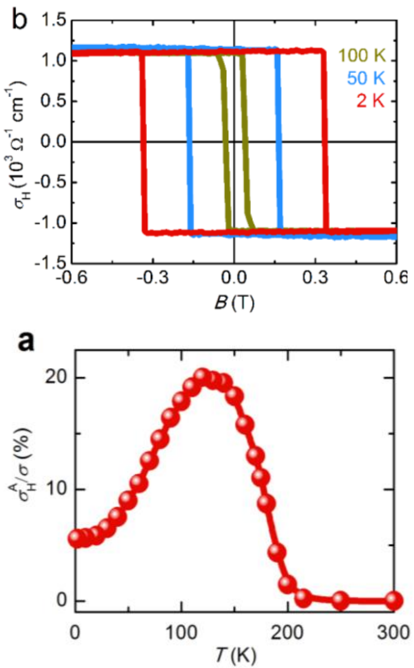
Morali et al., Science accepted , preprint arXiv:1903.00509

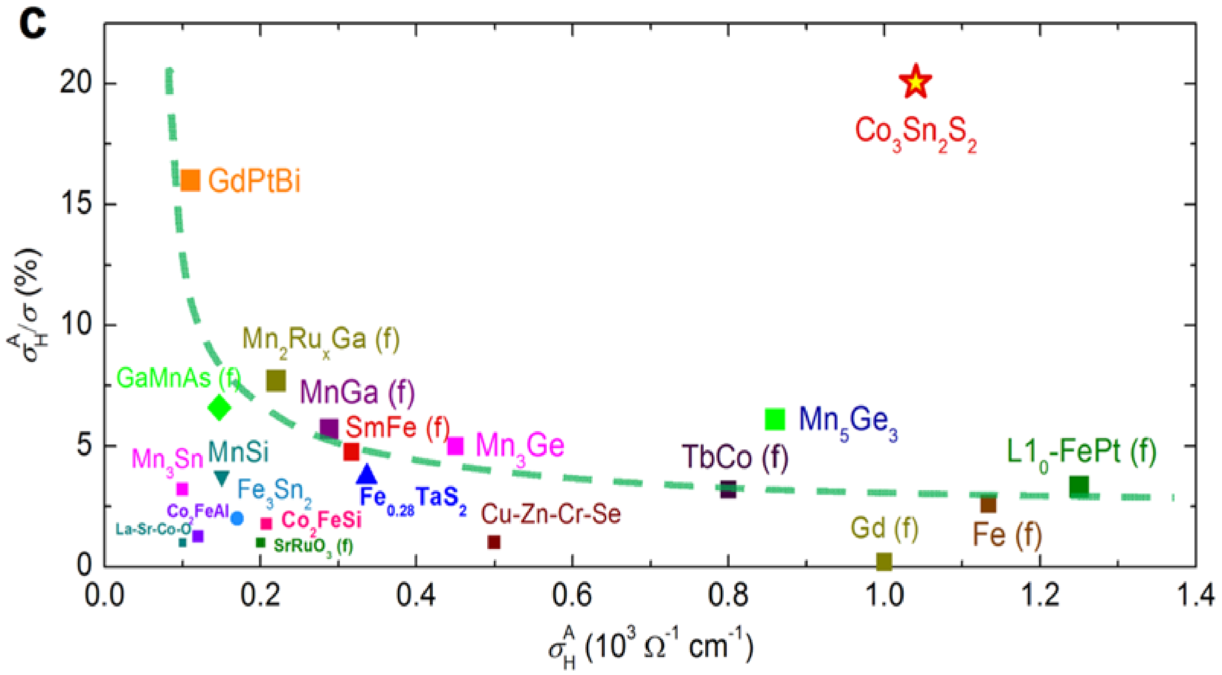
new transport properties

Berry curvature design
- giant anomalous Hall
- giant anomalous Nernst

$Co_3Sn_2S_2$
Mn_3Sn

Giant Hall Angle 20%



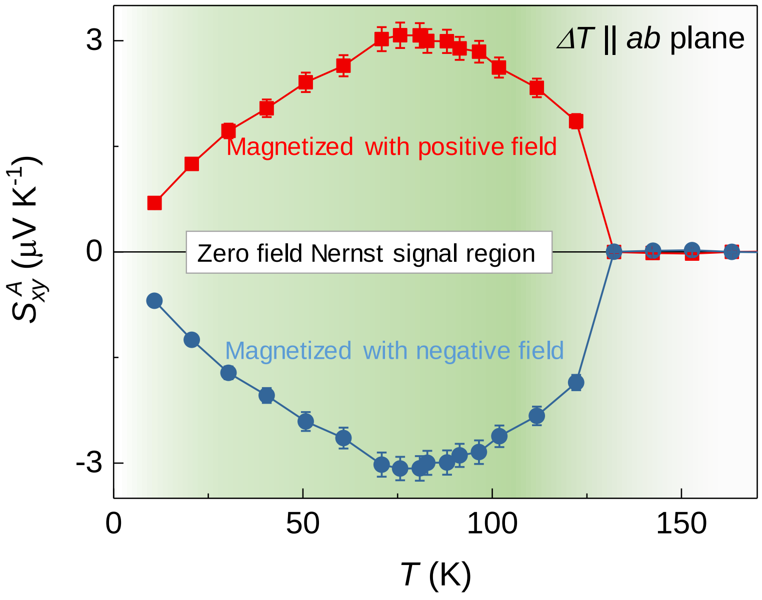


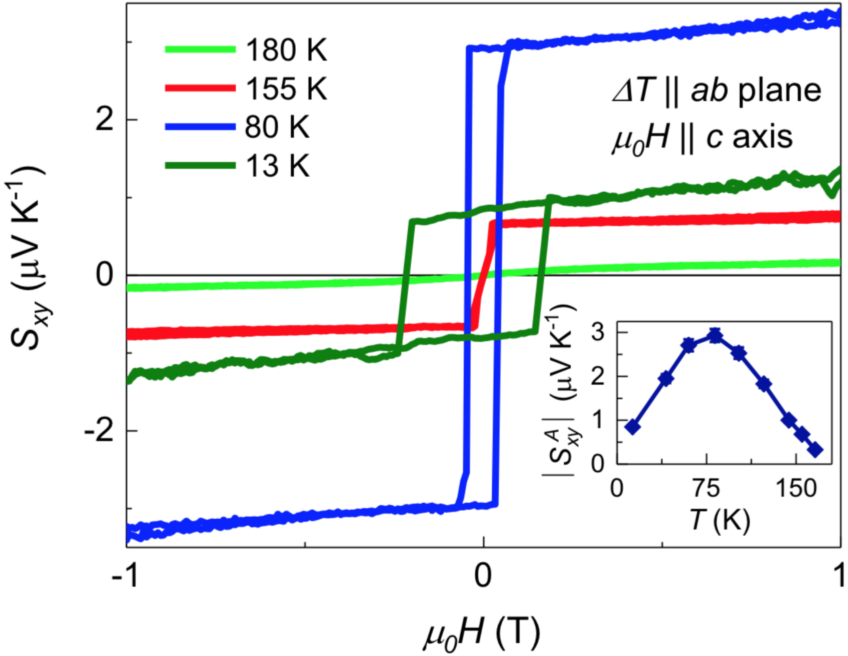
Liu, et al. Nature Physics 14 (2018) 1125 , Guin, et al. Adv. Mater. 2019, 1806622, arXiv:1712.06722, arXiv:1807.07843, arXiv:1806.06753

new transport properties

Berry curvature design
- giant anomalous Hall
- giant anomalous Nernst

Co_2MnGa
$Co_3Sn_2S_2$
Mn_3Sn



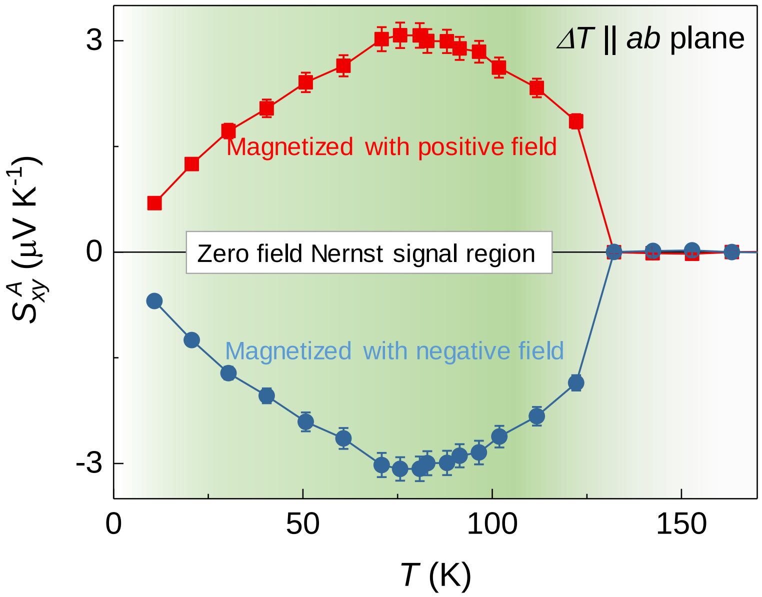


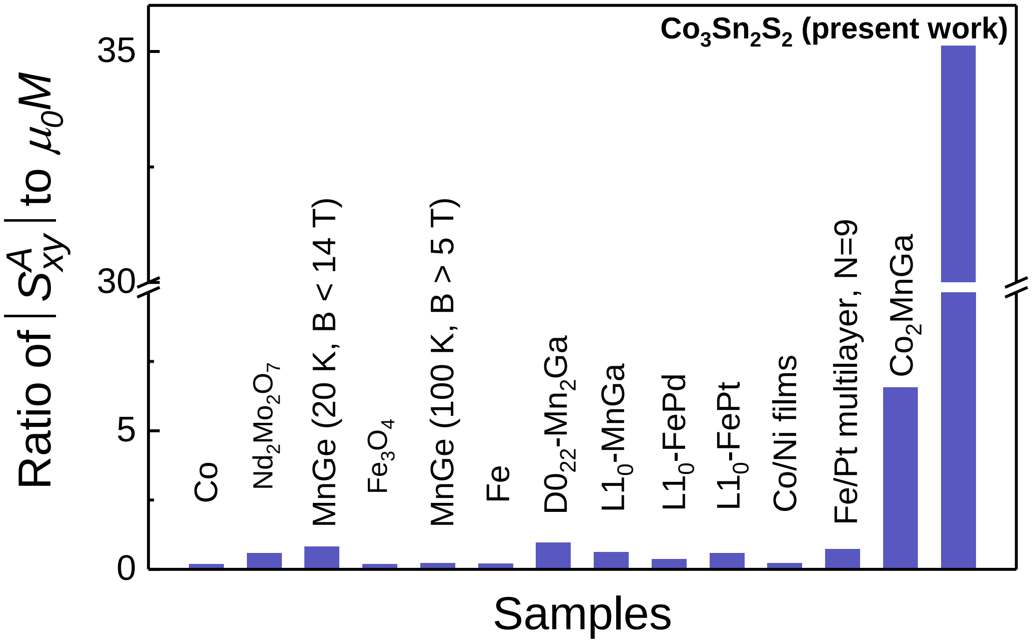
Guin, et al. Adv. Mater. 2019, 1806622, arXiv:1712.06722, arXiv:1807.07843, arXiv:1806.06753

new transport properties

Berry curvature design
- giant anomalous Hall
- giant anomalous Nernst

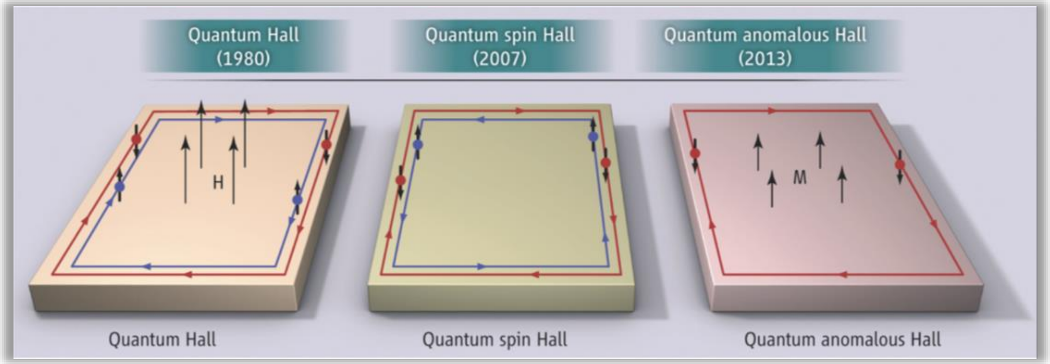
Co_2MnGa
$Co_3Sn_2S_2$
Mn_3Sn

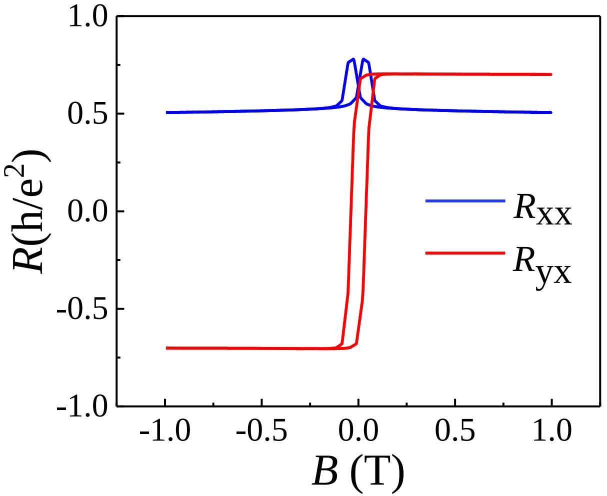




Guin, et al. Adv. Mater. 2019, 1806622, arXiv:1712.06722, arXiv:1807.07843, arXiv:1806.06753

quantum devices

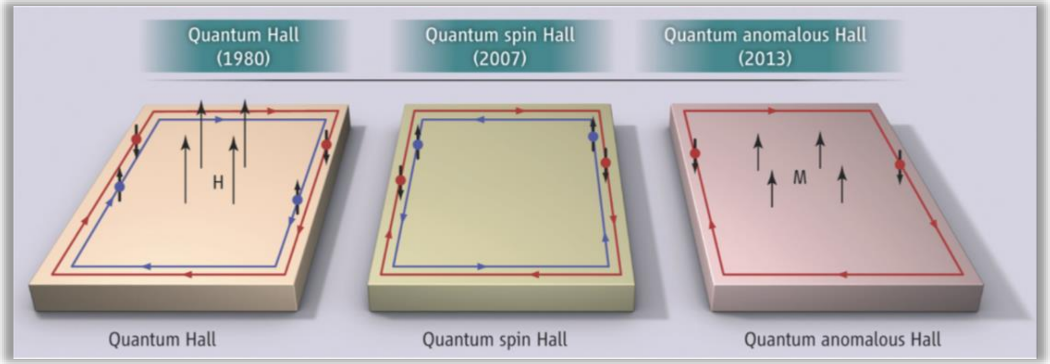


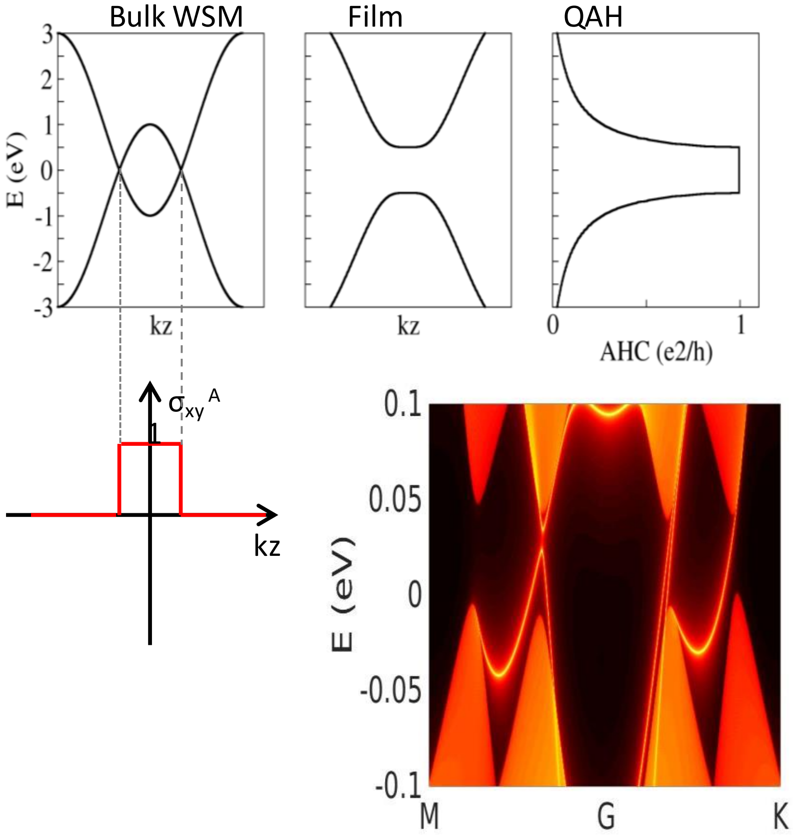


Cr-doped $(Bi,Sb)_2Te_3$

- Towards QAHE in MBE grown thin films.
- The anomalous Hall resistance is more than 0.75 h/e^2, comparable to the QAHE sample in previous reports.

quantum devices



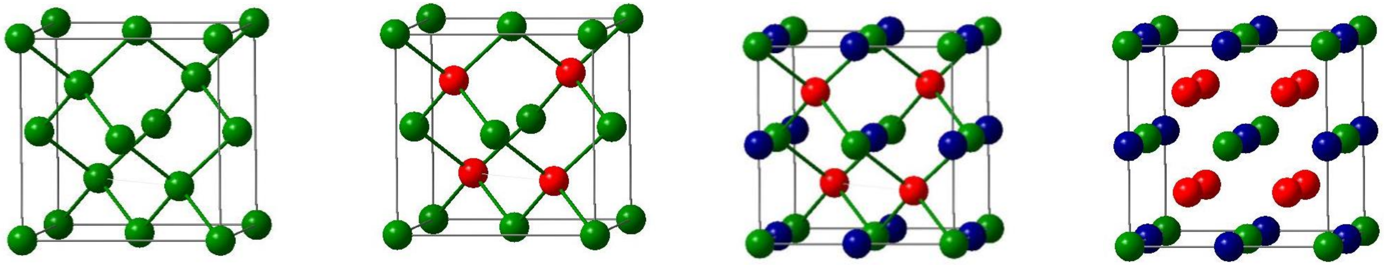


- Towards QAHE in MBE grown thin films.
- Magnetic Weyl for QAH effect in 2D

Qiunan Xu, Enke Liu, Wujun Shi, Lukas Muechler, Claudia Felser, Yan Sun, preprint arXiv:1712.08915

the Heusler Family

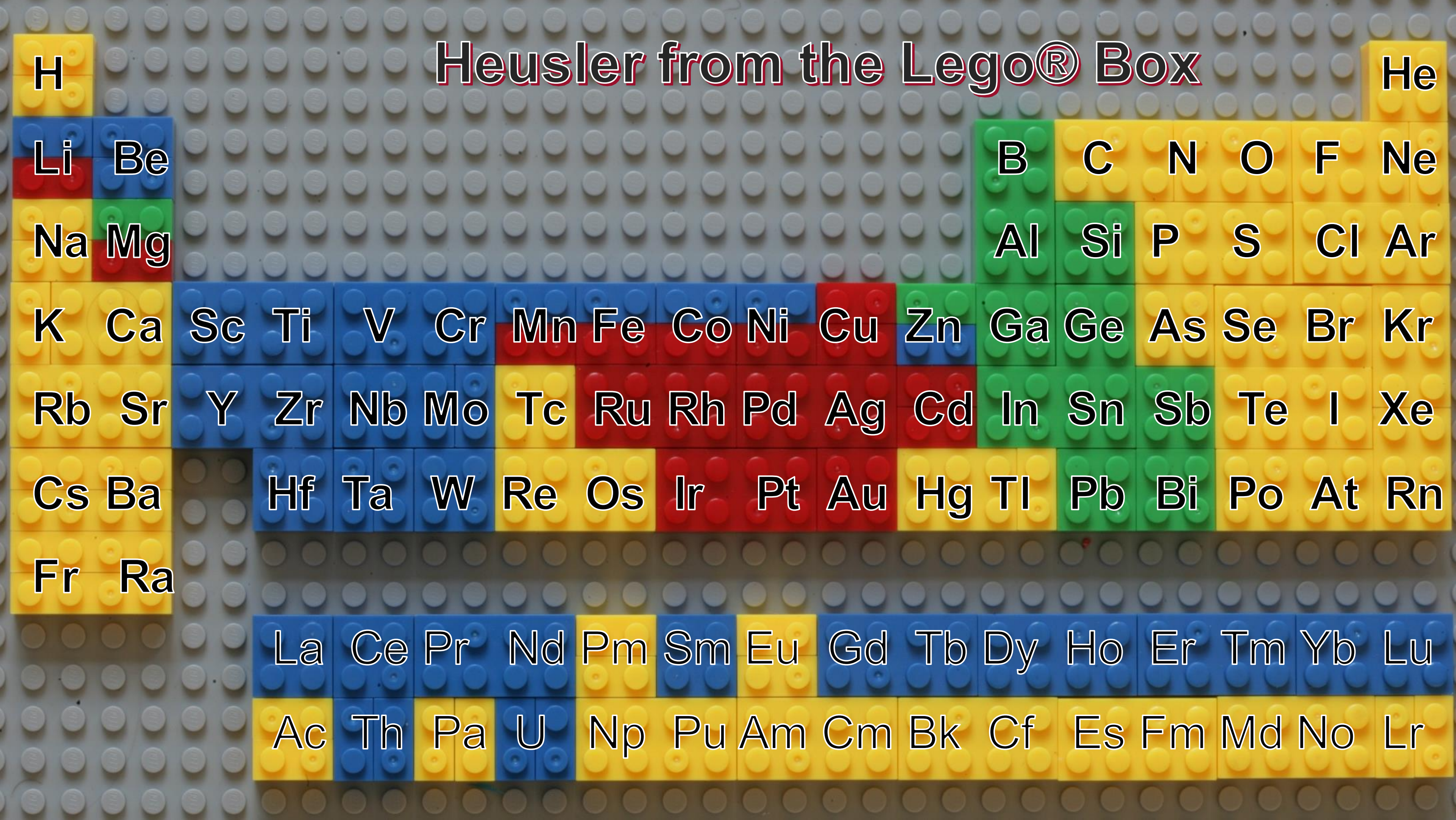
Diamond | **ZnS** | **Heusler XYZ $C1_b$** | **X_2YZ $L2_1$**



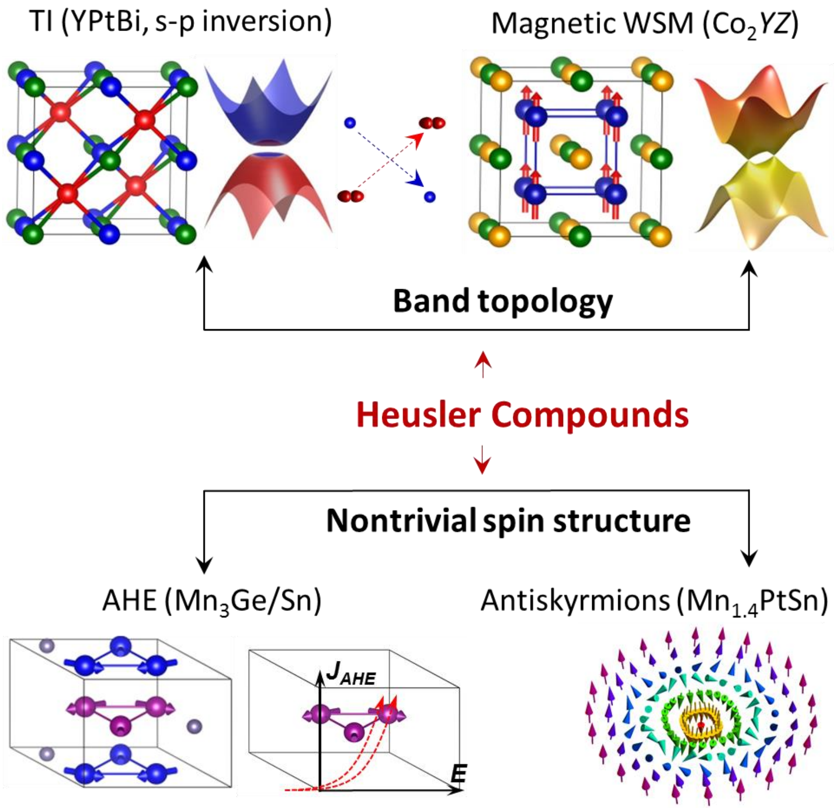
C 2.55	N 3.04
Si 1.90	P 2.19
Ge 2.01	As 2.18
Sn 1.96	Sb 2.05

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 Chemistry 39 (2011) 1


Heusler from the Lego® Box
H He
Li Be B C N O F Ne
Na Mg Al Si P S Cl Ar
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu
Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

Heusler, Weyl and Berry

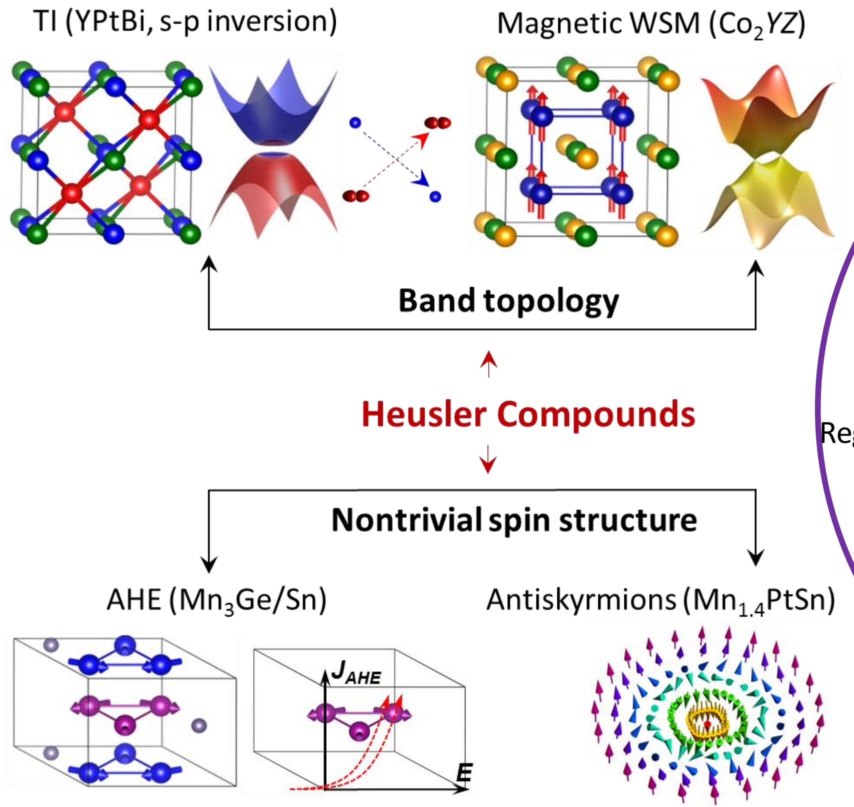


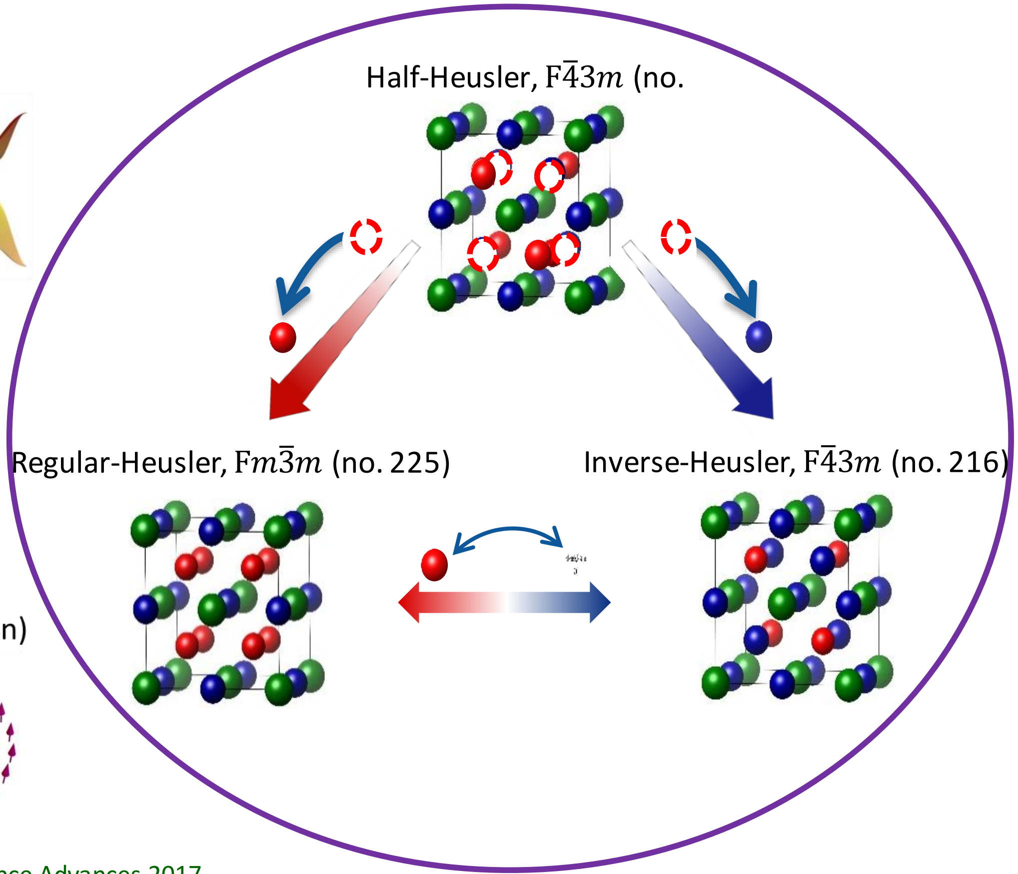
the tuning parameter

- topology is more than Σ symmetries
- insulators, semiconductors, metals, topological insulators, Weyl and Dirac, spin gapless semiconductors
- spin – ferro, ferri, antiferro, compensated ferri, non collinear
- spin – in plane, out of plane
- doping and substitution to adjust the chemical potential, rigid band model
- from isotropic to anisotropic: cubic, tetragonal and hexagonal distortion
- phase transitions

Manna et al., Nature Materials Review, 2018, Nayak, Nature 2017, Nayak, Science Advances 2017

Heusler, Weyl and Berry

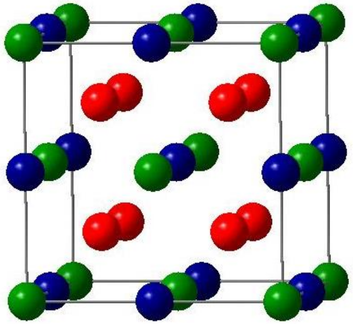




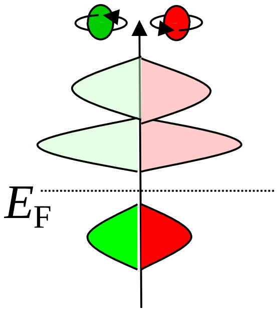
Manna et al., Nature Materials Review, 2018, Nayak, Nature 2017, Nayak, Science Advances 2017

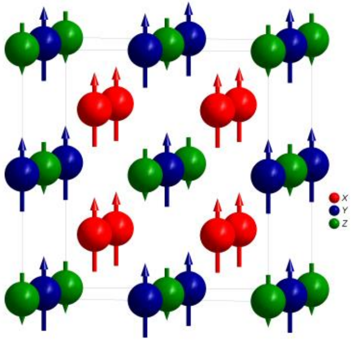
From semiconductors to half metals

X_2YZ



- magic valence electron number: 24
- valence electrons = 24 + magnetic moments

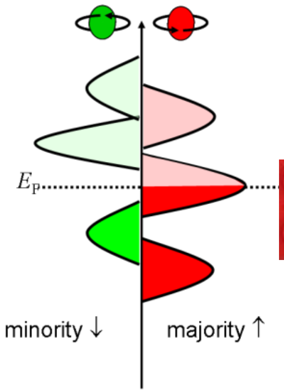




Fe_2 V Al

Co_2 Mn Ga

2 * 8 + 5 + 3 = 24



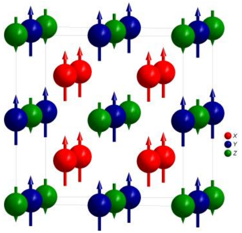
2 * 9 + 7 + 3 = 24 + 4

Kübler *et al.*, PRB **28**, 1745 (1983)
de Groot RA, et al. PRL **50** 2024 (1983)
Galanakis *et al.*, PRB **66**, 012406 (2002)

Kandpal et al., J. Phys. **D 40** (2007) 1507
Balke *et al.* Solid State Com. **150** (2010) 529
Kübler *et al.*, Phys. Rev. B **76** (2007) 024414

Tuning exchange

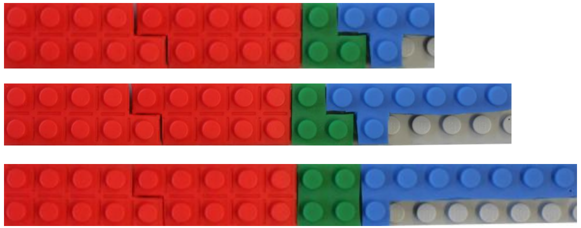
X_2YZ

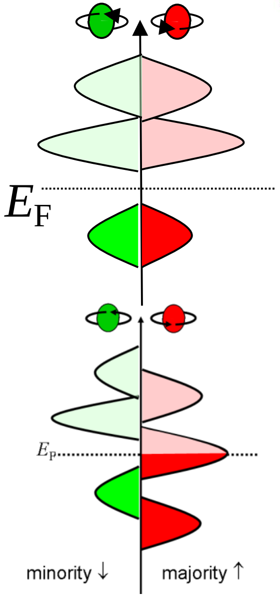


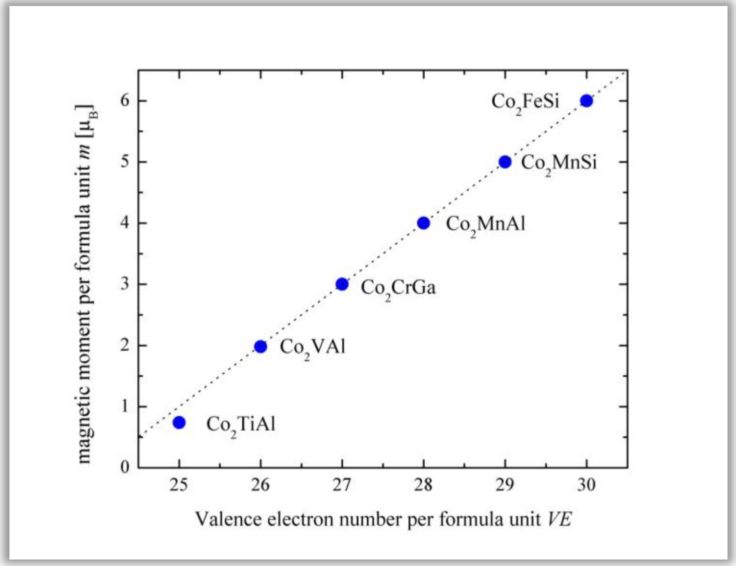
Co_2TiAl: $2\times9 + 4 + 3 = 25$ Ms = $1m_B$

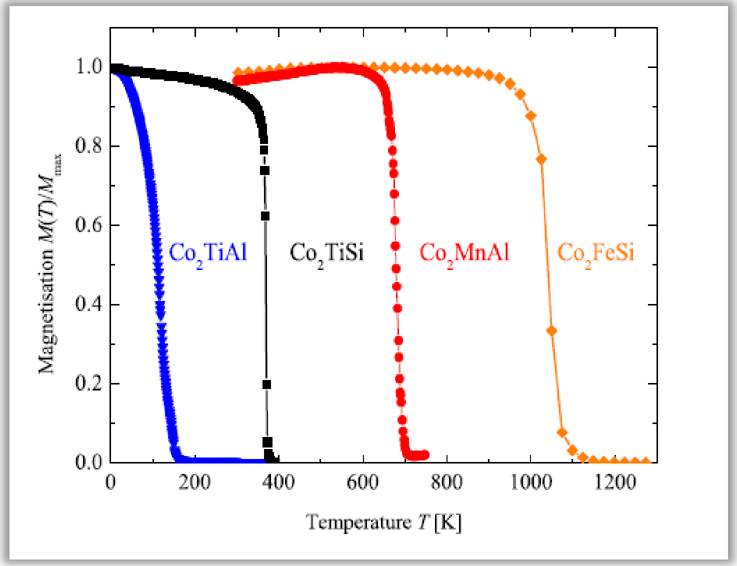
Co_2MnGa: $2\times9 + 7 + 3 = 28$ Ms = $4m_B$

Co_2FeSi: $2\times9 + 8 + 4 = 30$ Ms = $6m_B$









Kübler *et al.*, PRB **28**, 1745 (1983)
de Groot RA, et al. PRL **50** 2024 (1983)
Galanakis *et al.*, PRB **66**, 012406 (2002)

Kandpal et al., J. Phys. **D 40** (2007) 1507
Balke *et al.* Solid State Com. **150** (2010) 529
Kübler *et al.*, Phys. Rev. B **76** (2007) 024414

Heusler and Weyl

Breaking symmetry

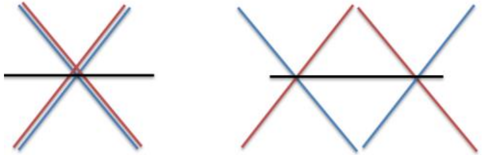
- Inversion symmetry (Strain)

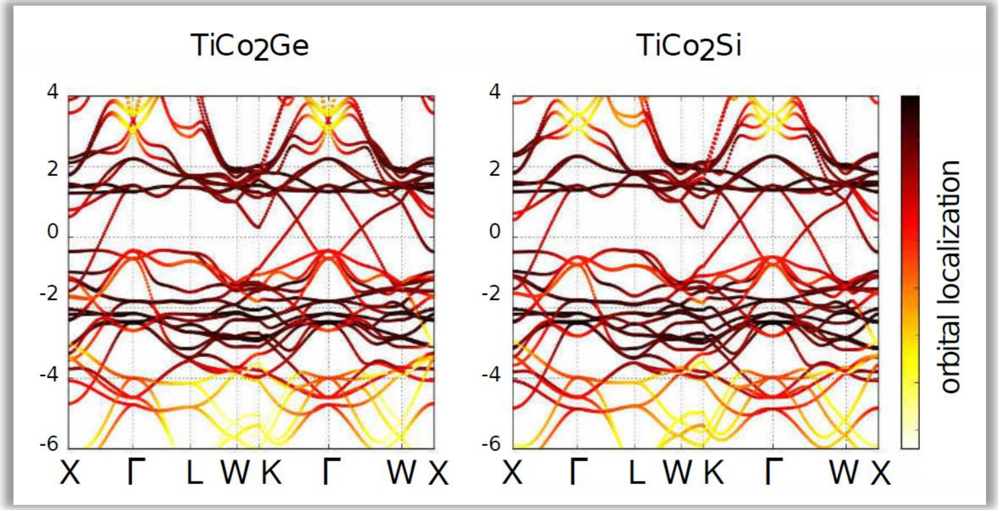
Breaking time reversal symmetry

- Magnetic field

Co$_2$TiSn

Co$_2$TiSi: $2\times9 + 4 + 4 = 26$ Ms = $2\mu_B$





- Dirac points at high symmetry
- Weyl points at low symmetry
- All crossings in ferromagnets:

Weyl points

Binghai Yan Claudia Felser,
Annual Review in Condensed Matter 8 (2017) 337

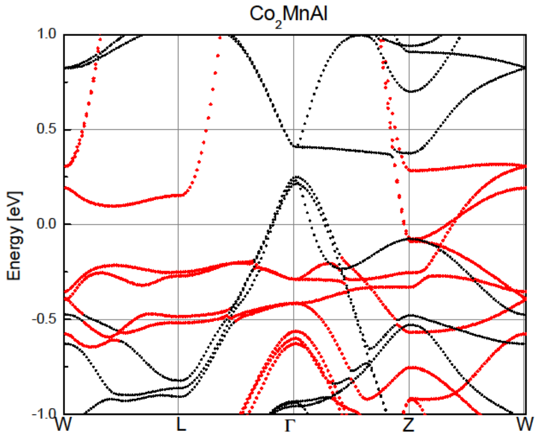
Zhijun Wang, et al., arXiv:1603.00479
Guoqing Chang et al., arXiv:1603.01255

Heusler, Weyl and Berry

Giant AHE in Co_2MnAl

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

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



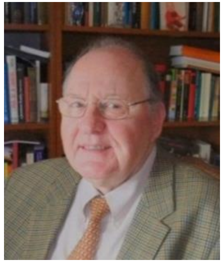
$$\sigma_{xy}^{A}(\mu) = ie^2 \left(\frac{1}{2\pi}\right)^3 \int_k dk \sum_{E(n,k)<\mu} f(n,k,\mu)\Omega_{n,xy}(k),$$

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

$$\rho_{xy}^{M} = (\alpha\rho_{xx} + \beta\rho_{xx}^2)\boldsymbol{M}.\ \mathbf{???}$$

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

Heusler, Weyl and Berry



Giant AHE in Co_2MnAl

Co_2MnGa

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

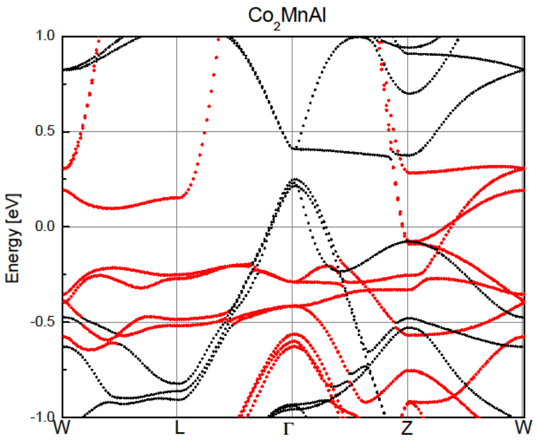
$$\sigma_{xy} \approx 2000\ \mathrm{S/cm}\ \ \text{meas.}$$

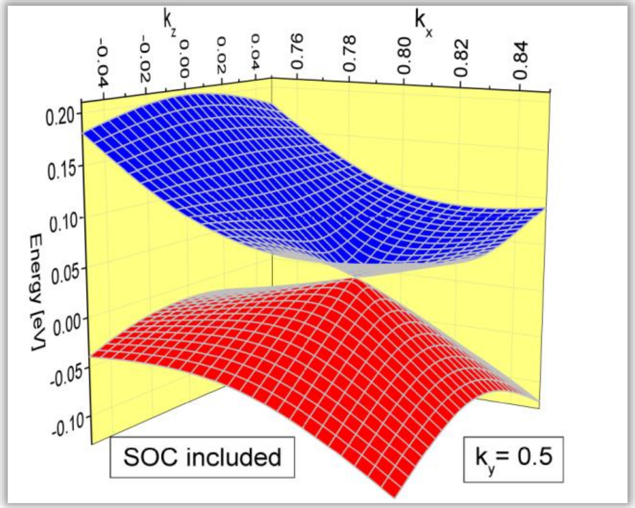
PHYSICAL REVIEW B **85**, 012405 (2012)

Berry curvature and the anomalous Hall effect in Heusler compounds

Jürgen Kübler[1,*] and Claudia Felser[2]

$$\sigma^A_{xy}(\mu) = ie^2 \left(\frac{1}{2\pi}\right)^3 \int_k dk \sum_{E(n,k)<\mu} f(n,k,\mu)\Omega_{n,xy}(k),$$





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

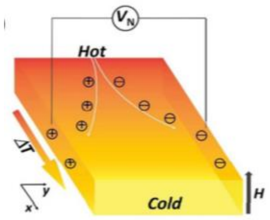
Kübler, Felser, EPL 114 (2016) 47005.

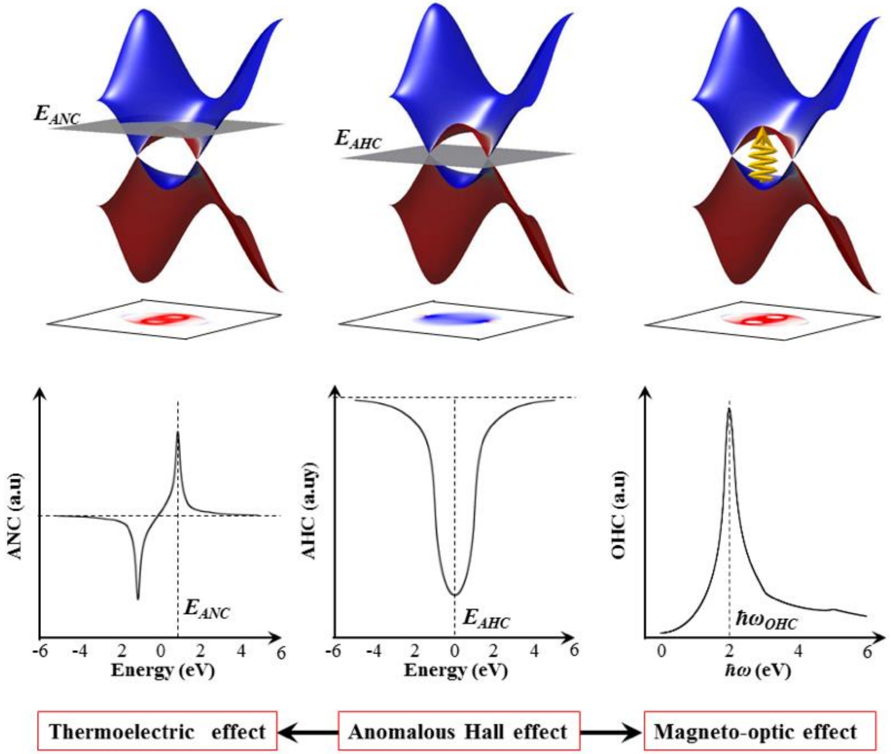
Berry curvature design

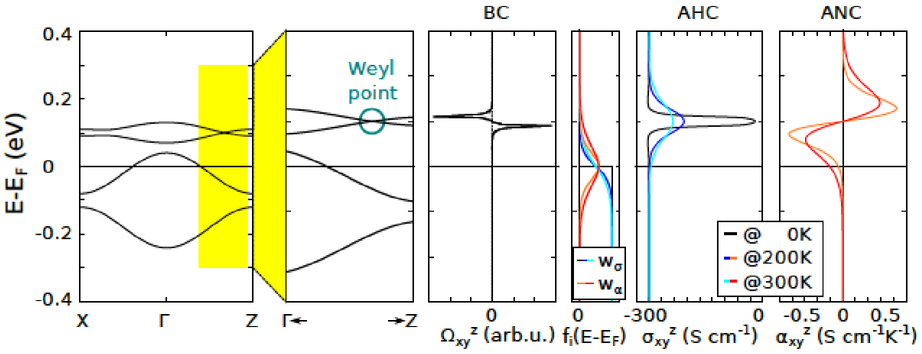
Berry curvature design

- giant spin Hall
- giant anomalous Hall
- giant topological Hall
- giant anomalous Nernst

Nernst effect



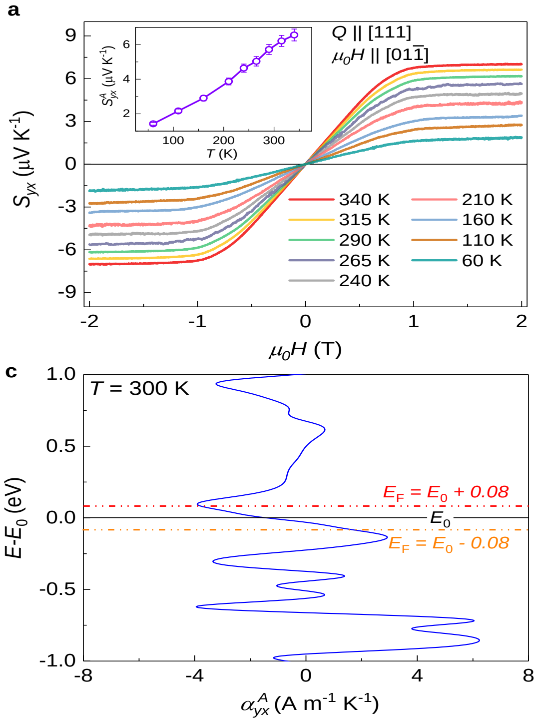




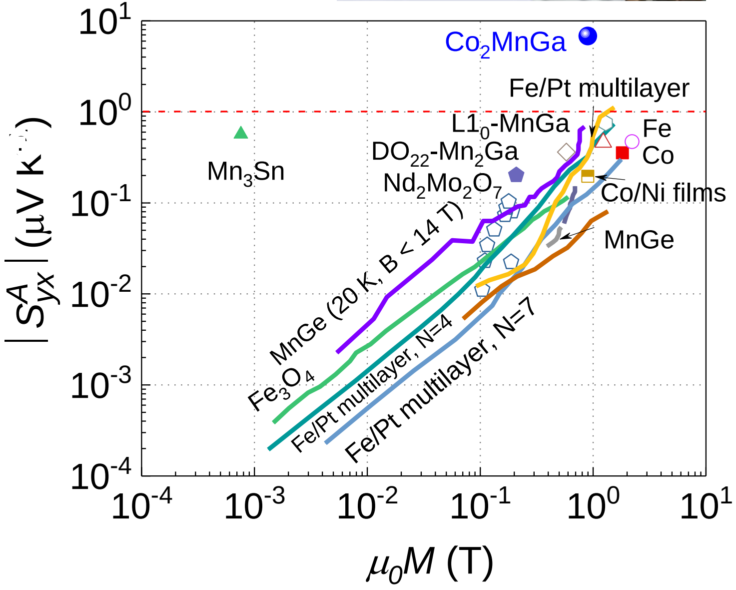
J. Noky et al., Phys. Rev. B 98, 241106(R) (2018), arXiv:1807.07843, arXiv:1806.06753

Nernst effect

Co_2MnGa



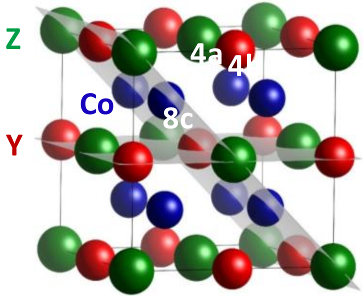
J. Noky et al., Phys. Rev. B 98, 241106(R) (2018)

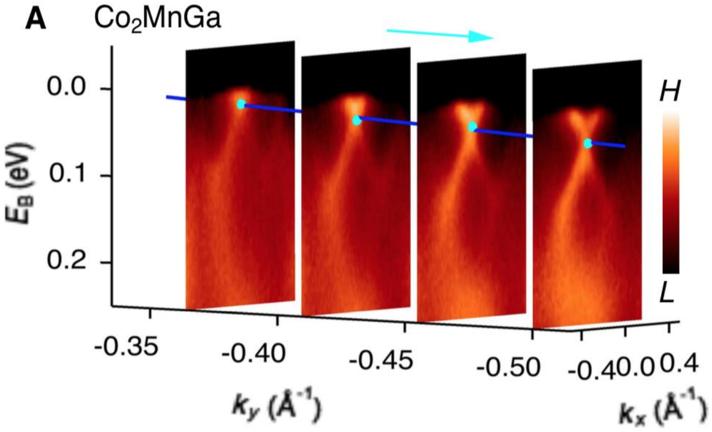


Satya N. Guin, et al., NPG Asia Mater. 11, 16 (2019), arXiv:1806.06753

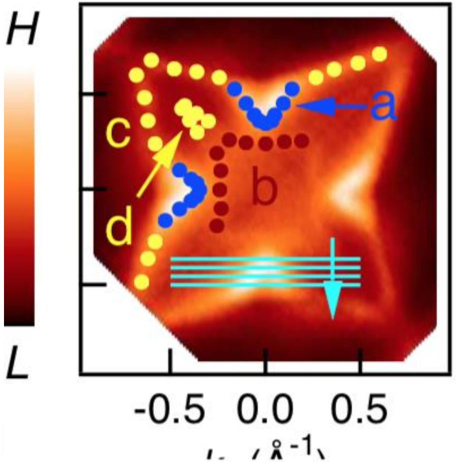
Sakain et al. Nature Physics 2018

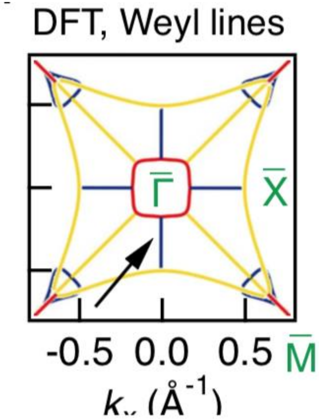
Co_2MnGa – ferromagnetic nodal line

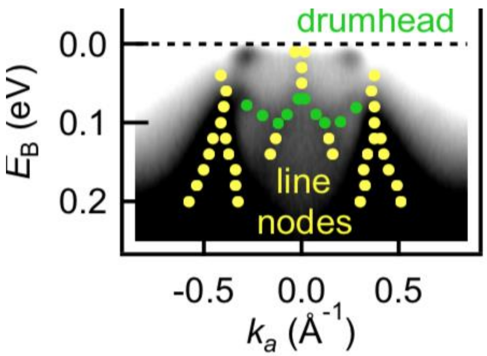


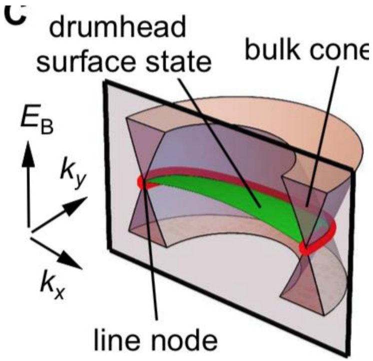


Series of ARPES cuts through the candidate line node



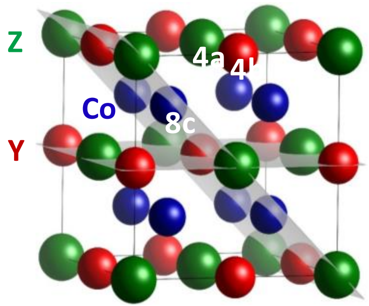






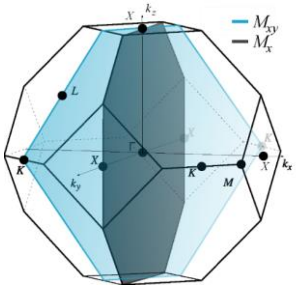
Belopolski, et al., Science accepted (2019) preprint arXiv:1712.09992

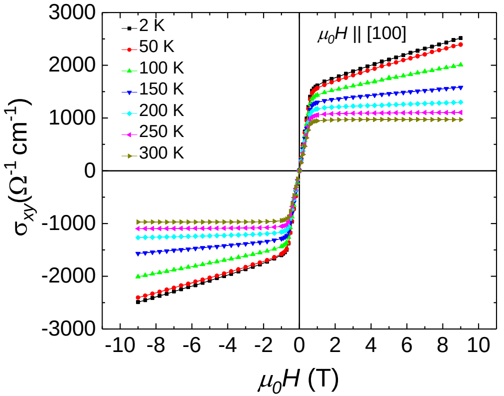
Heusler, Weyl and Berry

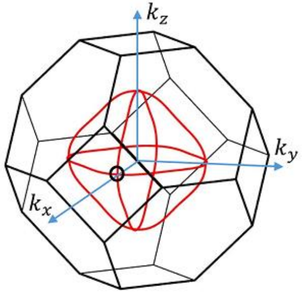


Co_2YZ (Y = IVB or VB; Z = IVA or IIIA)

$L2_1$ space group 225 ($Fm\bar{3}m$)



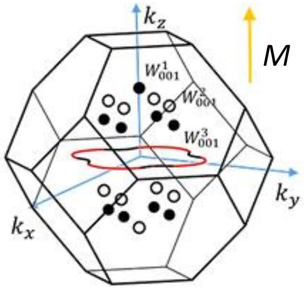




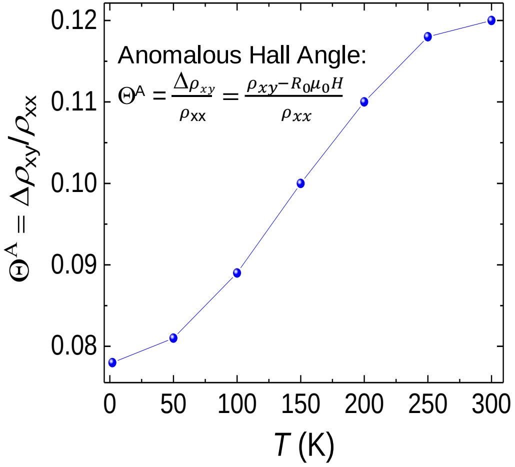
Without SOC

With SOC

Symmetry and electronic structures depend on the magnetization direction

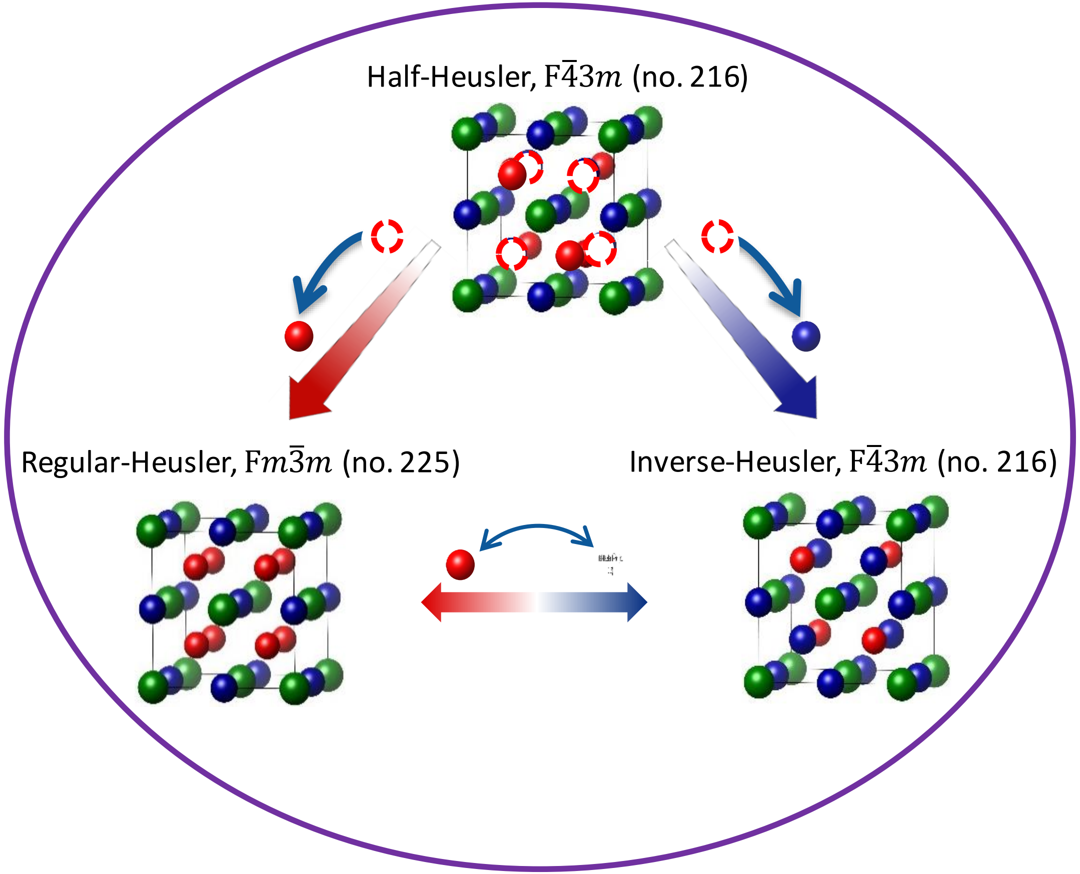


Phys. Rev. Lett. 117, 236401 (2016)
Sci. Rep. 6, 38839 (2016)



- nodal line is formed in the plane when bands of opposite mirror eigenvalues cross.
- Mirror planes are related to each other by the rotations

Manna et al., Phys. Rev. X 8 (2018) 041045, arXiv:1712.10174

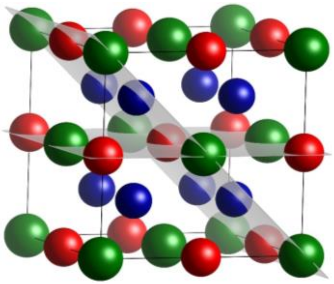


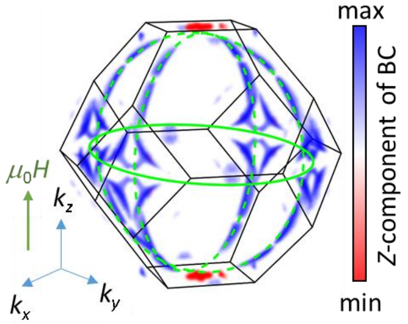
no inversion symmetry
topology !

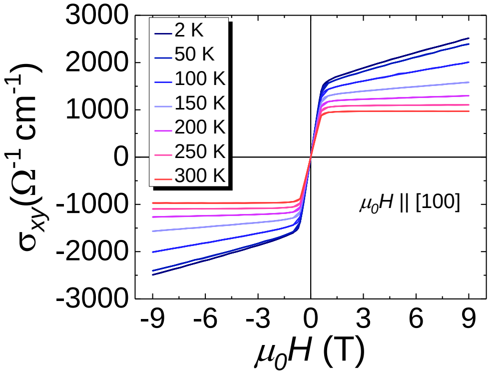
Heusler, Weyl and Berry

playing with symmetry: from Weyl to spingapless semiconductor

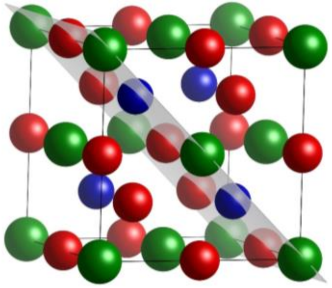
Co_2MnGa

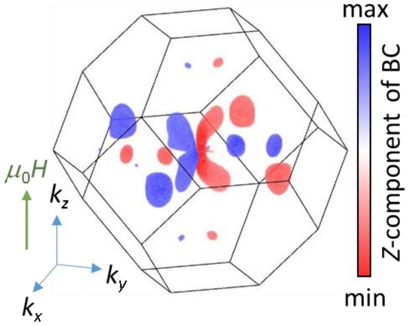


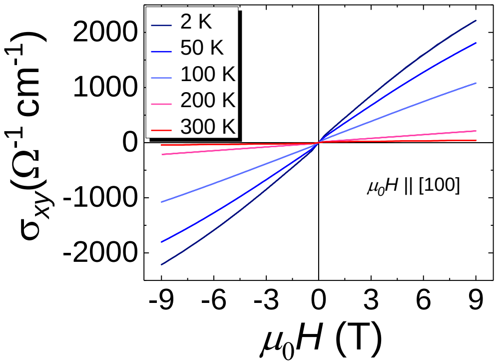




Mn_2CoGa





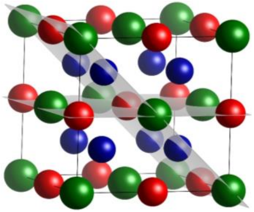


Manna et al., Phys. Rev. X 8 (2018) 041045, arXiv:1712.10174

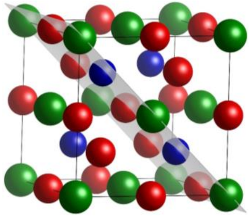
Heusler, Weyl and Berry

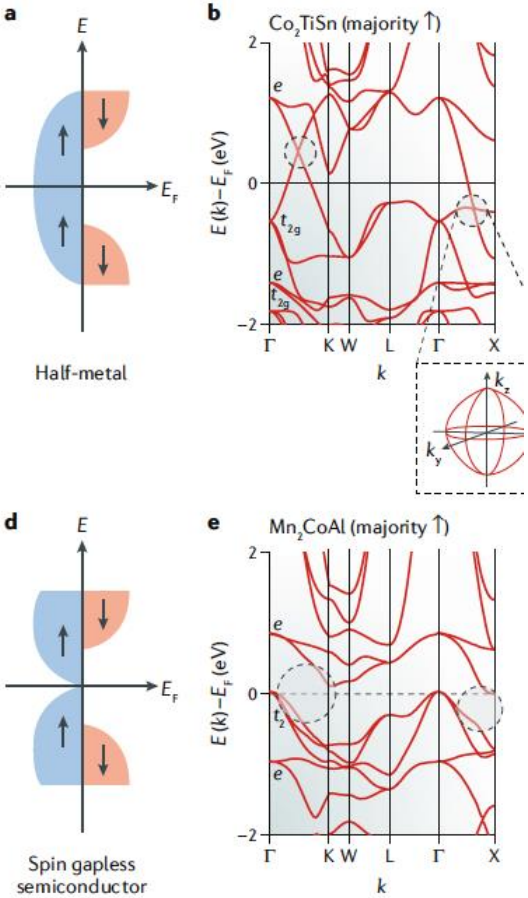
playing with symmetry: from Weyl to spingapless semiconductor

Co_2TiSn



Mn_2CoGa

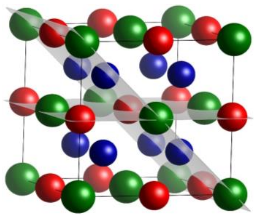


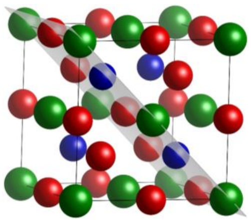


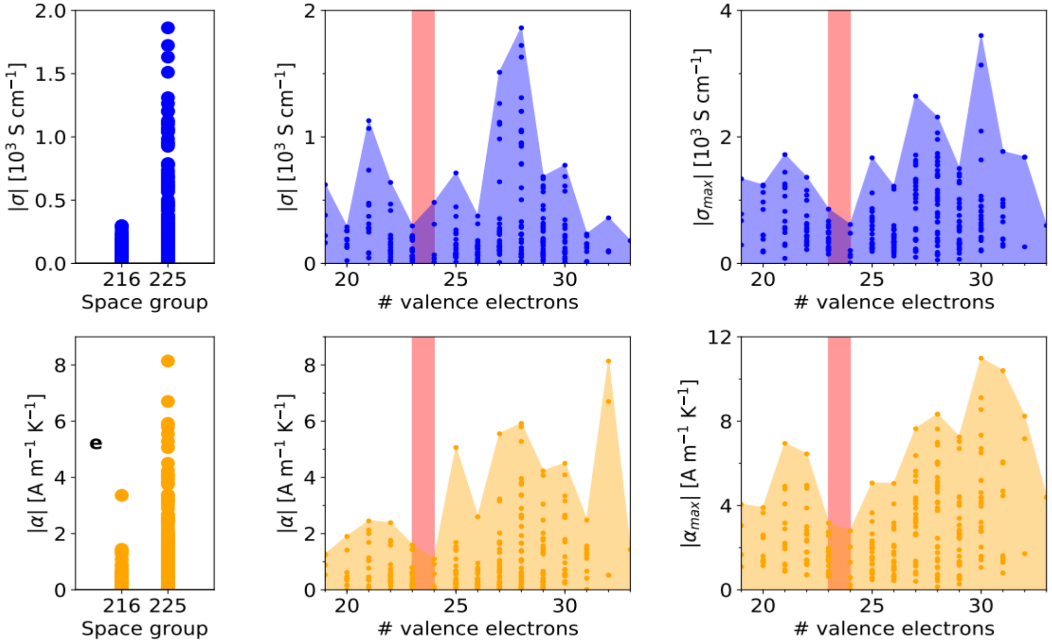
Ouardi, Fecher, Kübler, and Felser, Physical Review Letter 110 (2013) 100401
Manna et al., Phys. Rev. X 8 (2018) 041045, arXiv:1712.10174
Manna et al., Nature Review Materials, 3 (2018) 244 arXiv:1802.02838v1

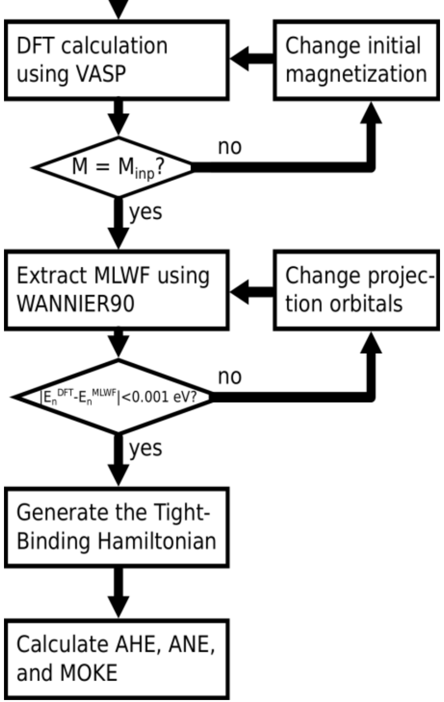
high through put

playing with symmetry:





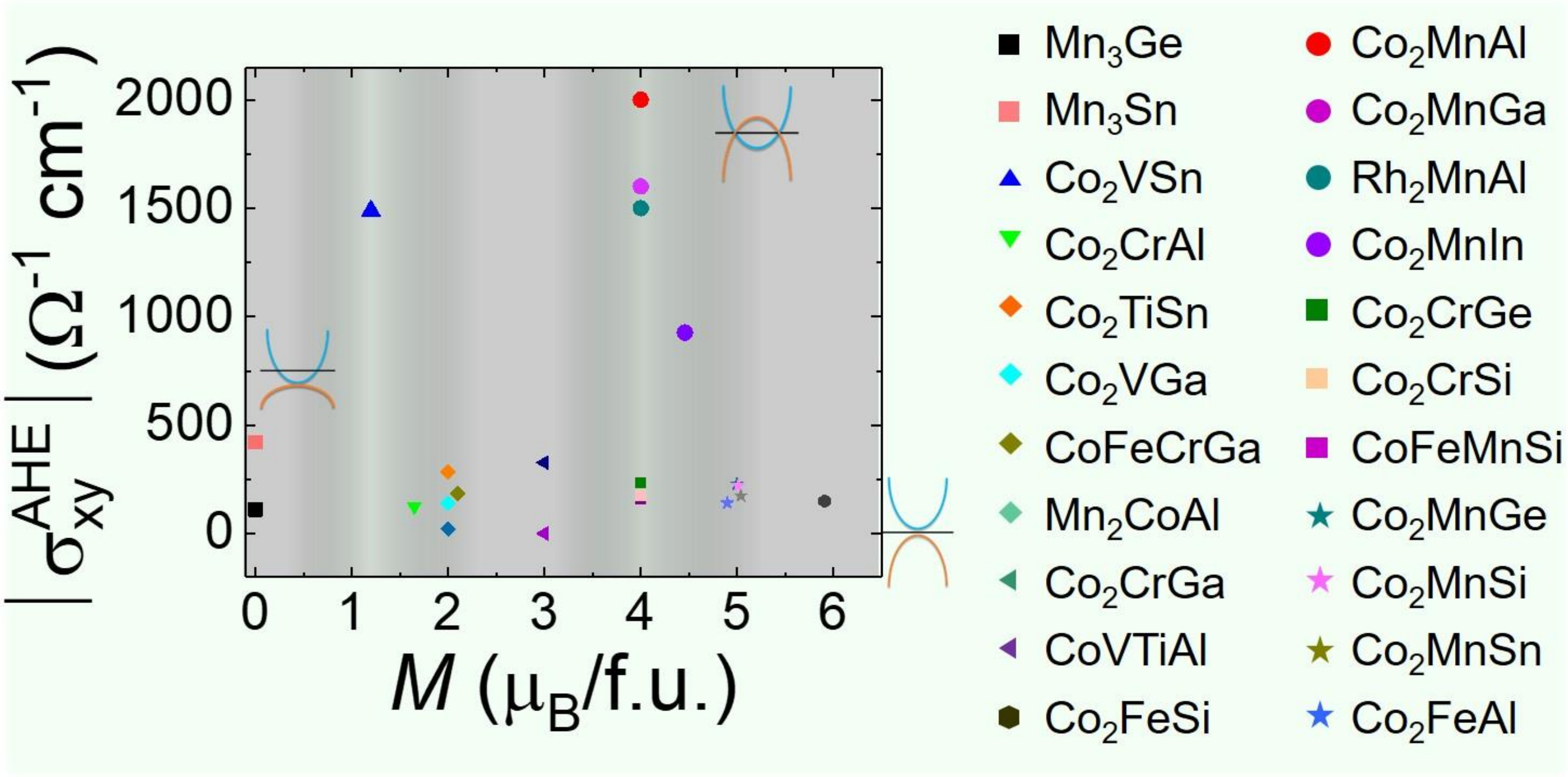




Noky et al., in submitted

Heusler and Berry

$$\rho_{xy}^{M} = (\alpha\rho_{xx} + \beta\rho_{xx}^{2})\boldsymbol{M}.\ \textbf{???}$$

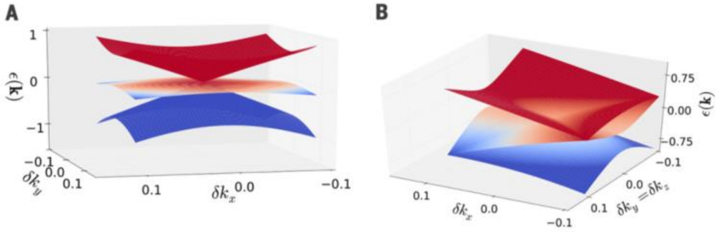


outline

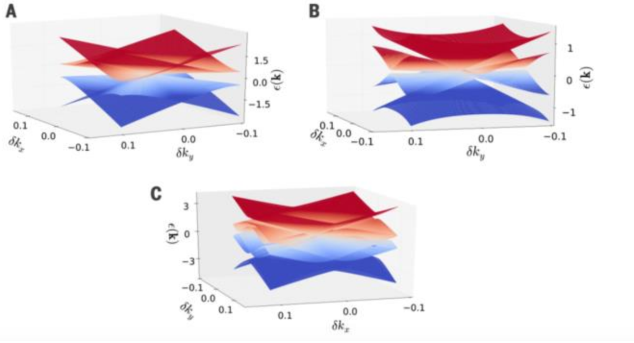
- Introduction
- Topological insulators
- Weyl semimetals – broken symmetry
- Magnetic Weyl semimetals
- New Fermions
- Outlook – axion insultors and beyond

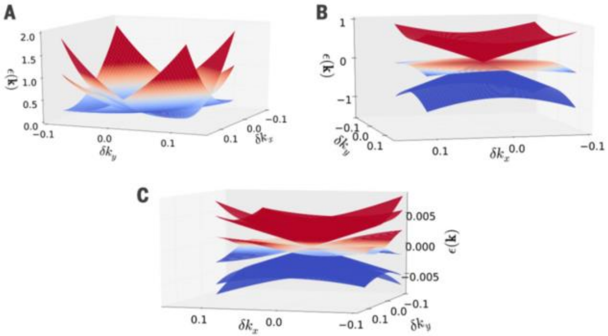
new Fermions

6-fold crossings



8-fold degenerate points





new Fermions

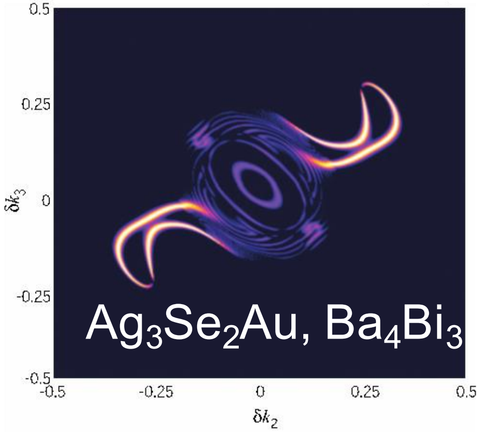
RESEARCH

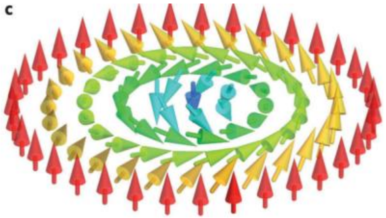
RESEARCH ARTICLE SUMMARY

TOPOLOGICAL MATTER

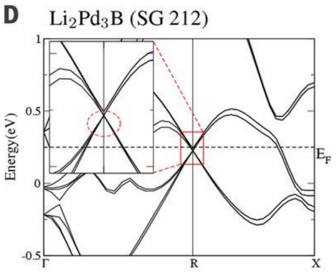
Beyond Dirac and Weyl fermions: Unconventional quasiparticles in conventional crystals

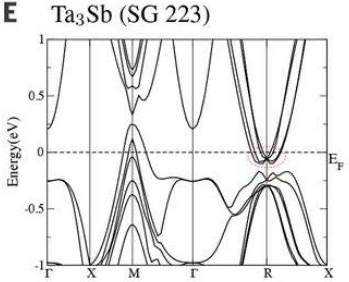
Barry Bradlyn,* Jennifer Cano,* Zhijun Wang,* M. G. Vergniory, C. Felser, R. J. Cava, B. Andrei Bernevig†





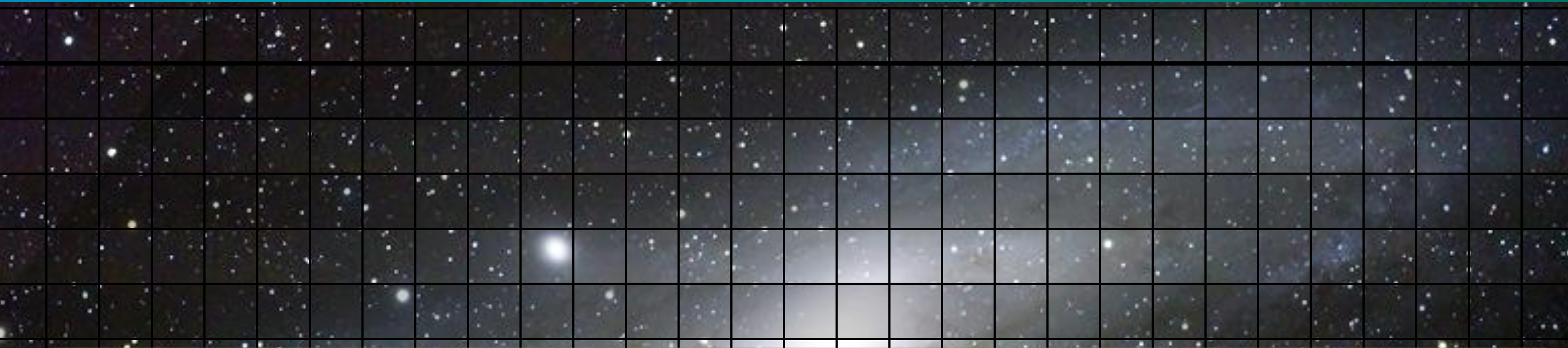
- Chiral Crystals
  - B20, Skyrmions, CoSi, MnSi, PdGa, RhSi
- Superconductors
  - A15 superconductors: Nb_3Sn, Li_2Pd_3B





Bradlyn et al., Science, 353, 6299, (2016)

universe – on a lattice



Bringing order to the expanding fermion zoo

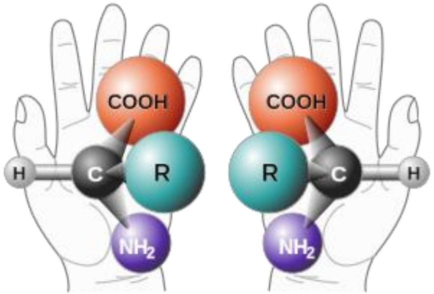
Carlo Beenakker Commentary

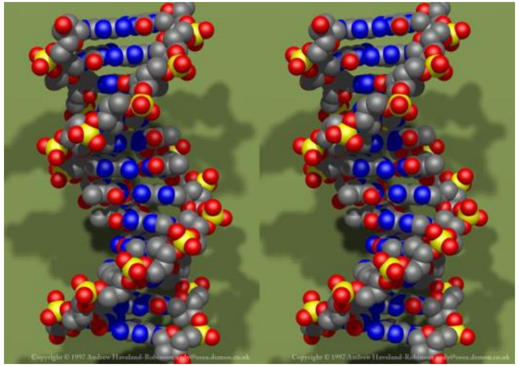
Heisenberg (1930): We observe space as a continuum, but we might entertain the thought that there is an underlying lattice and that space is actually a crystal. Which particles would inhabit such a lattice world?

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”

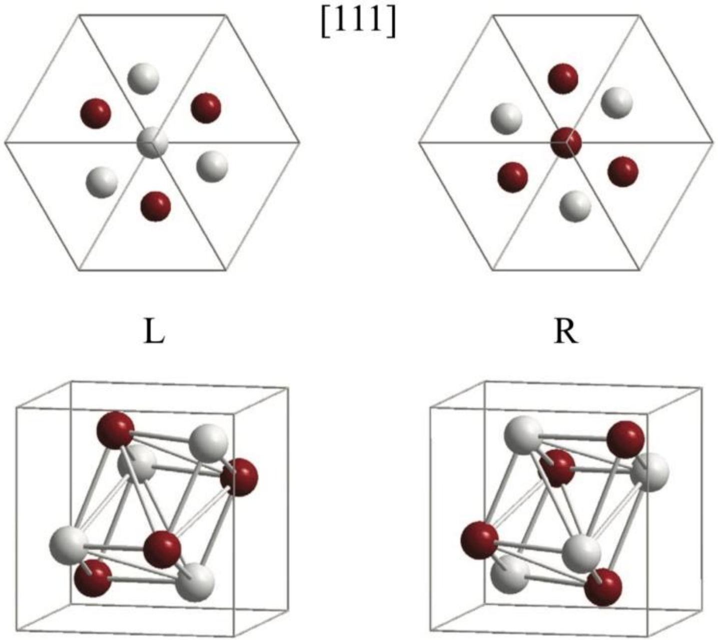
chiral topology

molecules with different chiralities have different properties





B20 type cubic noncentrosymmetric crystallographic structure described by the chiral $P2_13$ space group nr 198

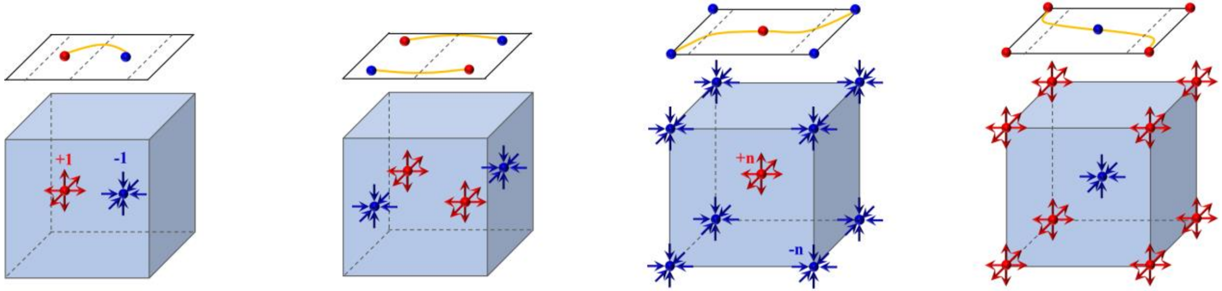


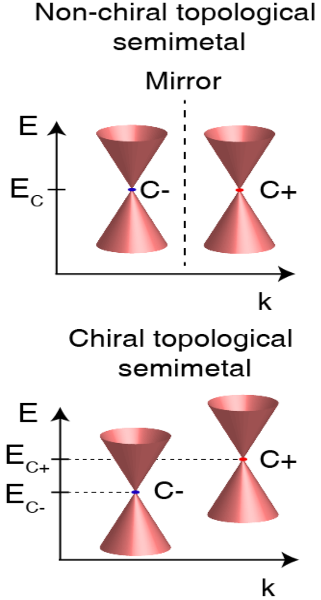
chiral topology

chiral crystals
optical activity
magnetochiral anisotropy
…

topological crystals
unusual surface states
large photogalvanic effect
…

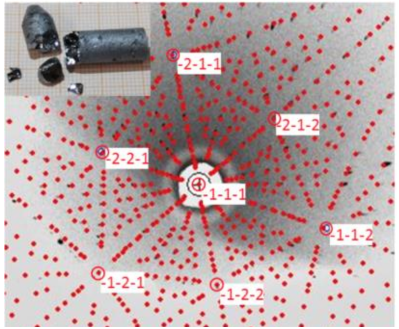
new Fermions
largest Fermi arc
unusual phonon dynamics
Gyrotropic magnetic effect
Quantized circular photogalvanic effect
…



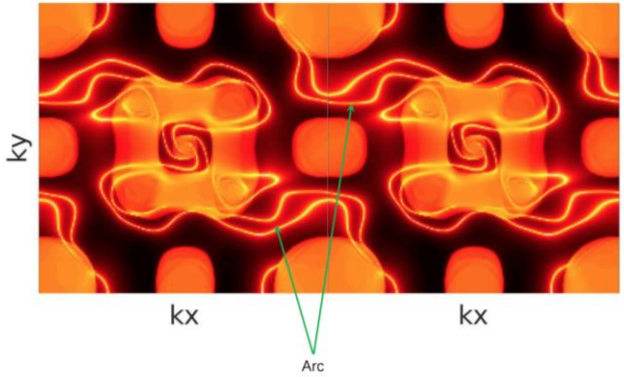


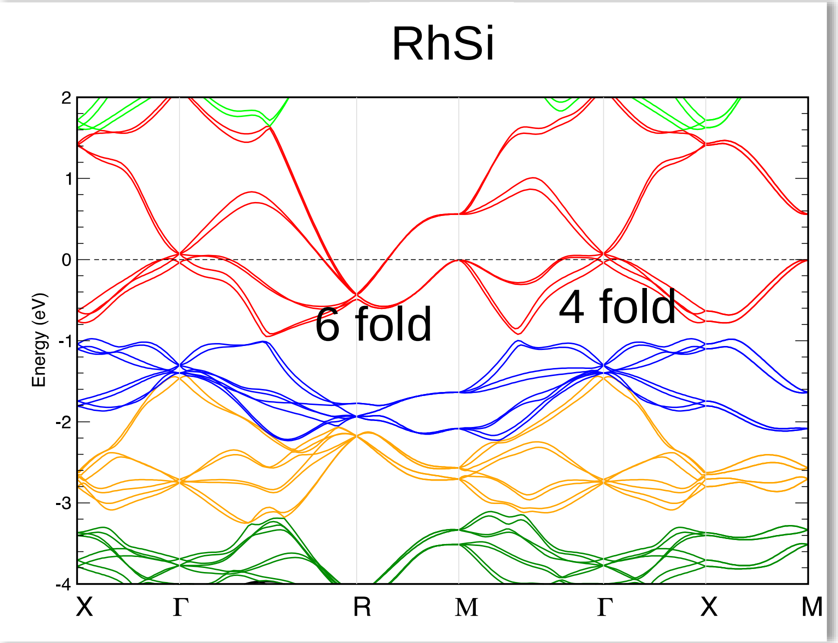
chiral topology

Polycrystal PtAl, Homochiral PdGa
Single crystals CoSi, MnSi, FeGe, RhSi, PtGa



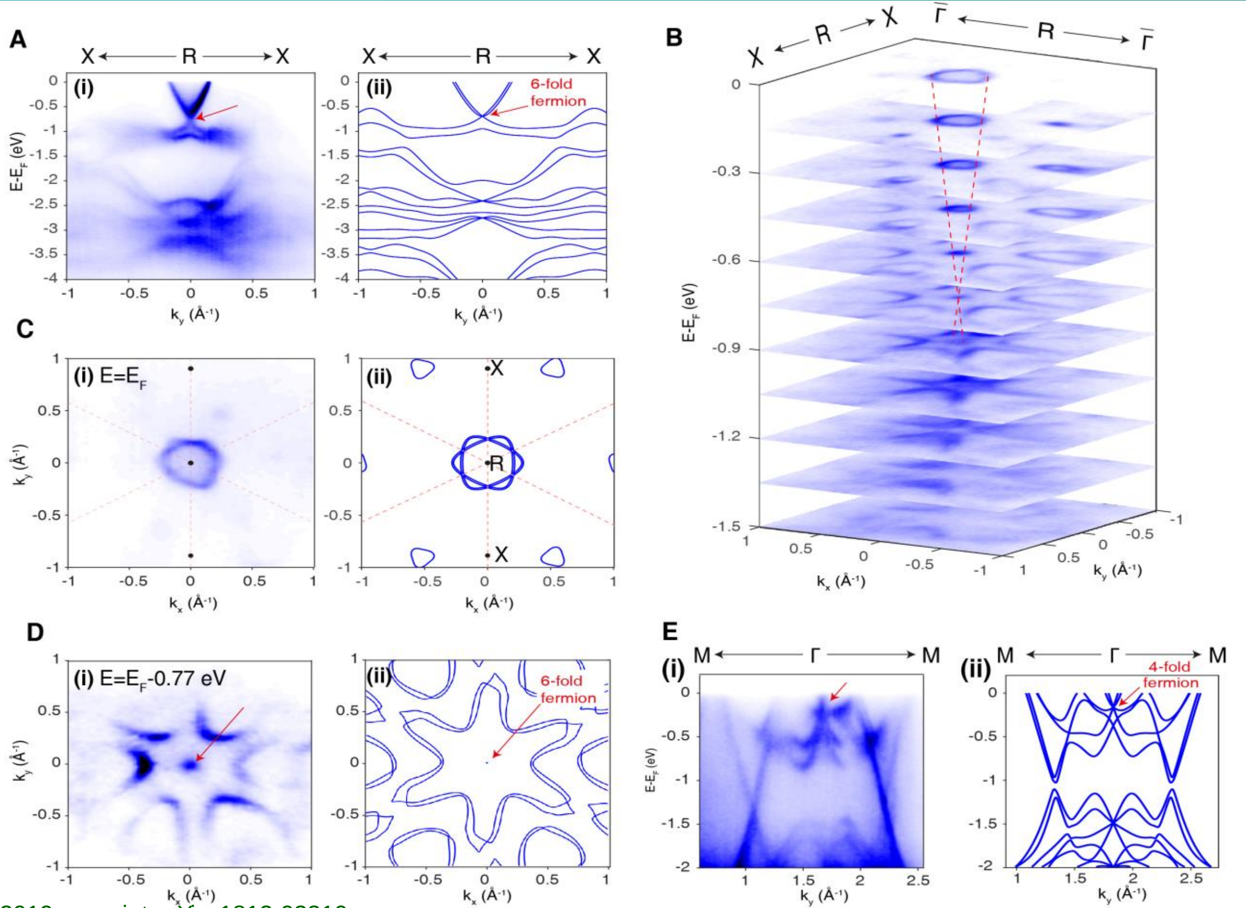
PtGa





chiral topology

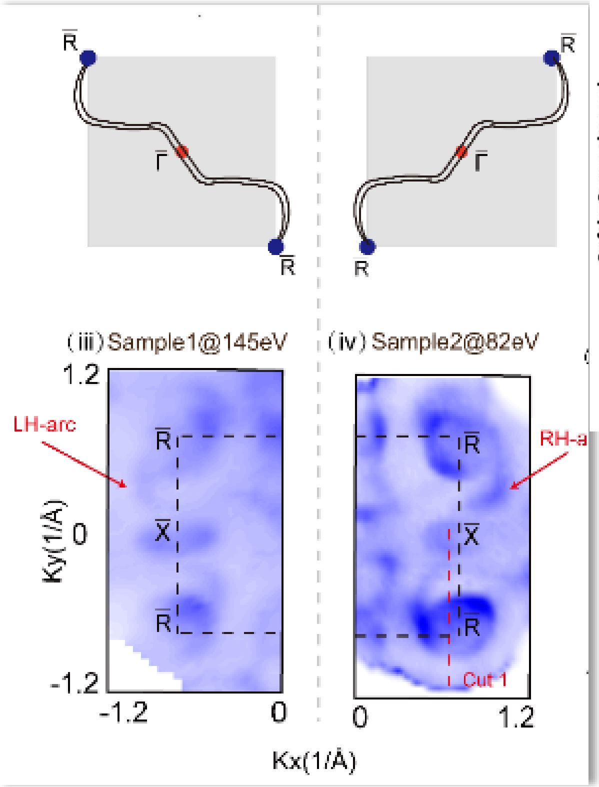
PtAl

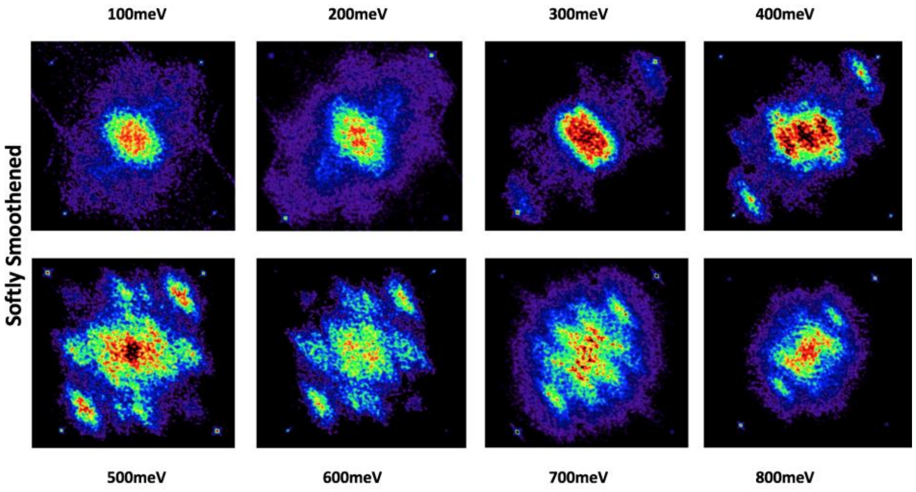


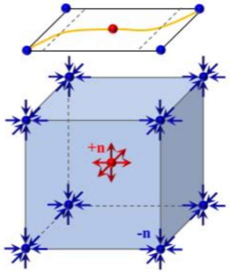
Schröter et al. Nature Physics online 2019, preprint arXiv: 1812.03310

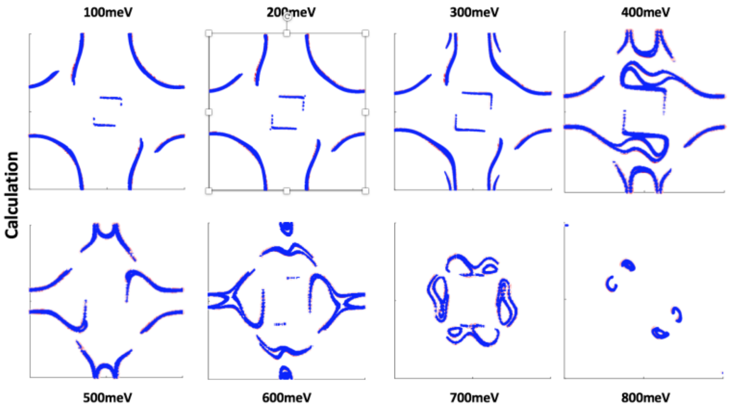
Fermi arcs

Chiral copies of the Fermi arcs



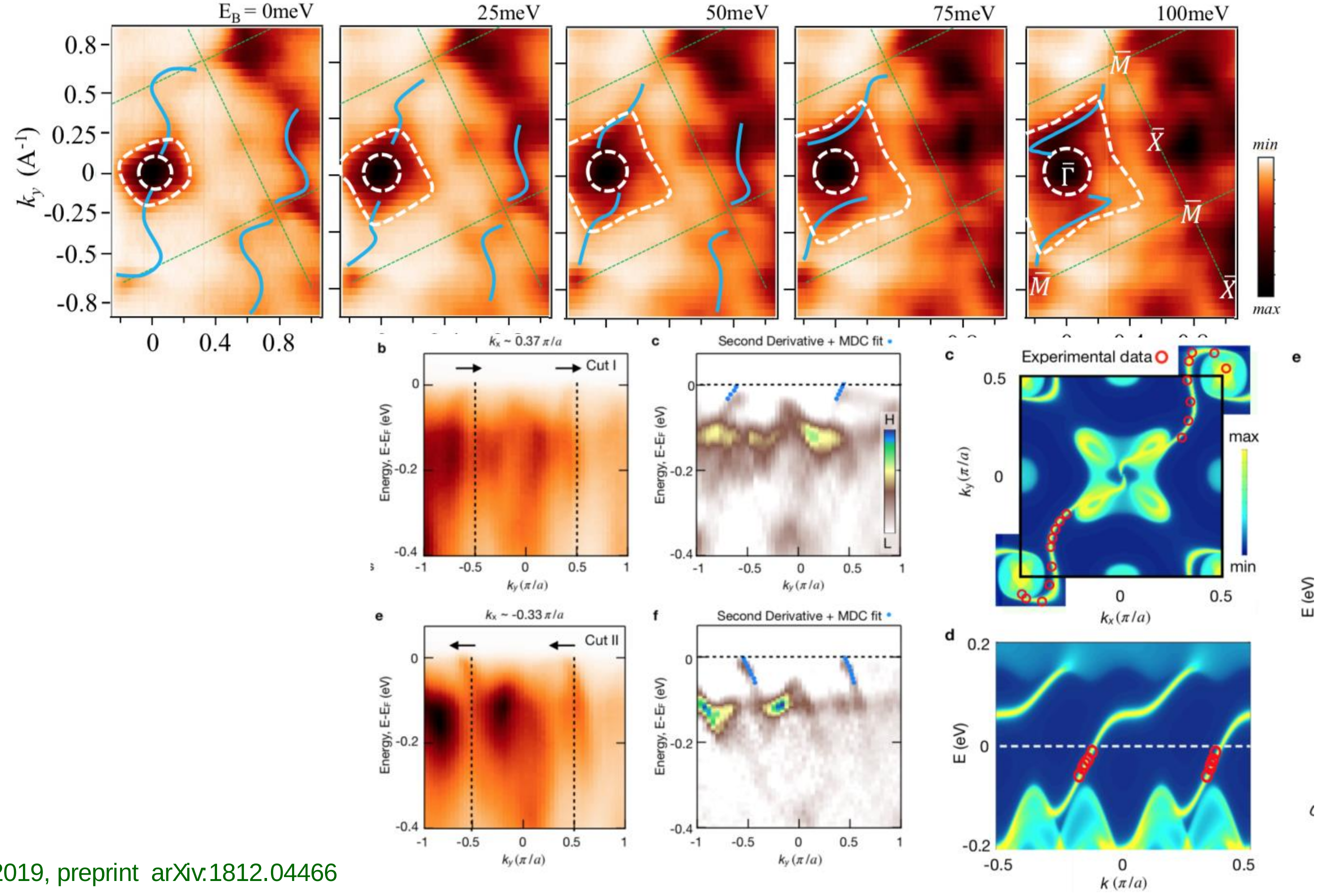






Schröter et al. Nature Physics online 2019, preprint arXiv: 1812.03310

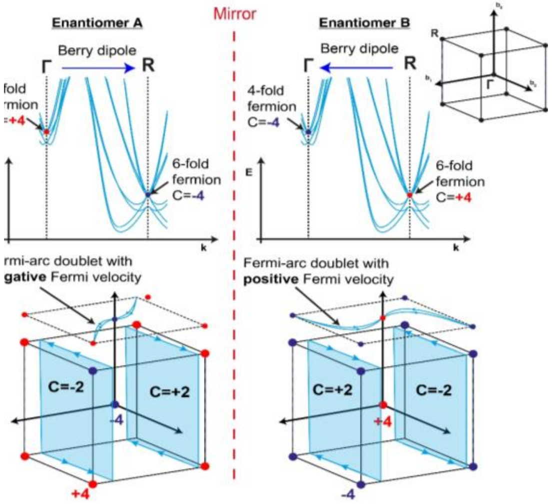
Fermi arcs

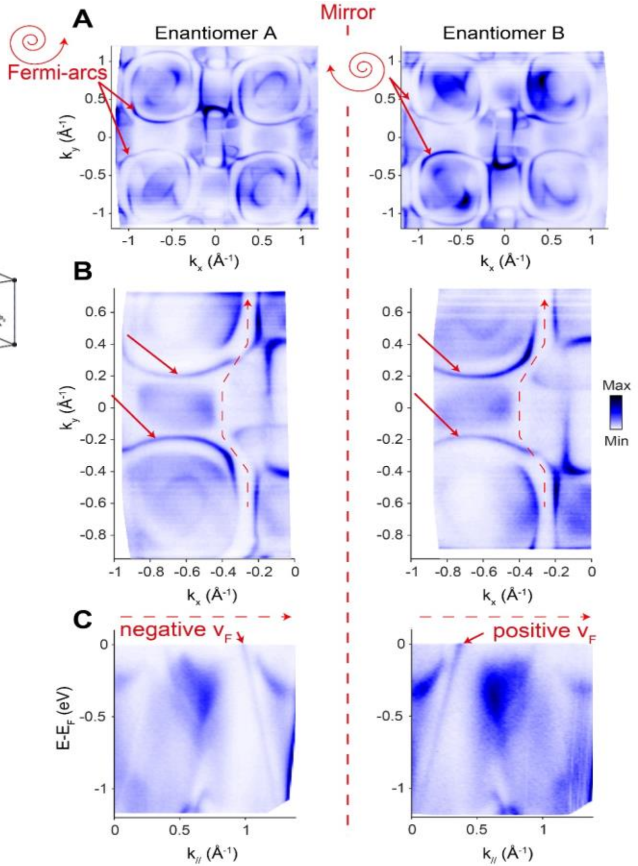


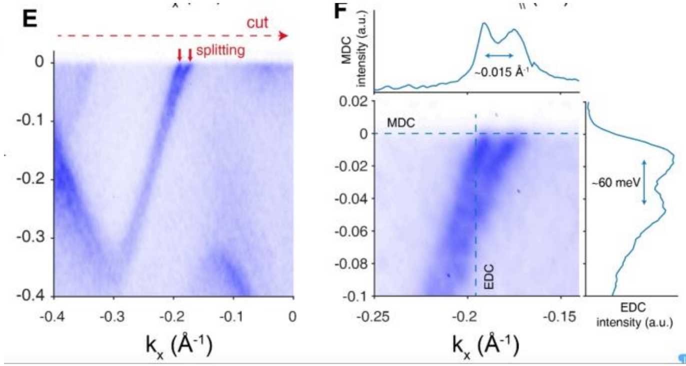
Sanchez et al. Nature online 2019, preprint arXiv:1812.04466

Fermi arcs

Chiral copies of the Fermi arcs







Schröter et al. preprint arXiv: 1907.08723

quantized circular photogalvanic effect

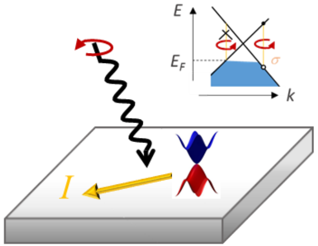
ARTICLE

Received 27 Dec 2016 | Accepted 18 May 2017 | Published 6 Jul 2017

DOI: 10.1038/ncomms15995 OPEN

Quantized circular photogalvanic effect in Weyl semimetals

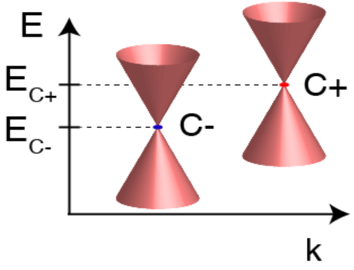
Fernando de Juan[1,2,3], Adolfo G. Grushin[1], Takahiro Morimoto[1] & Joel E. Moore[1,4]



Photogalvanic Effect

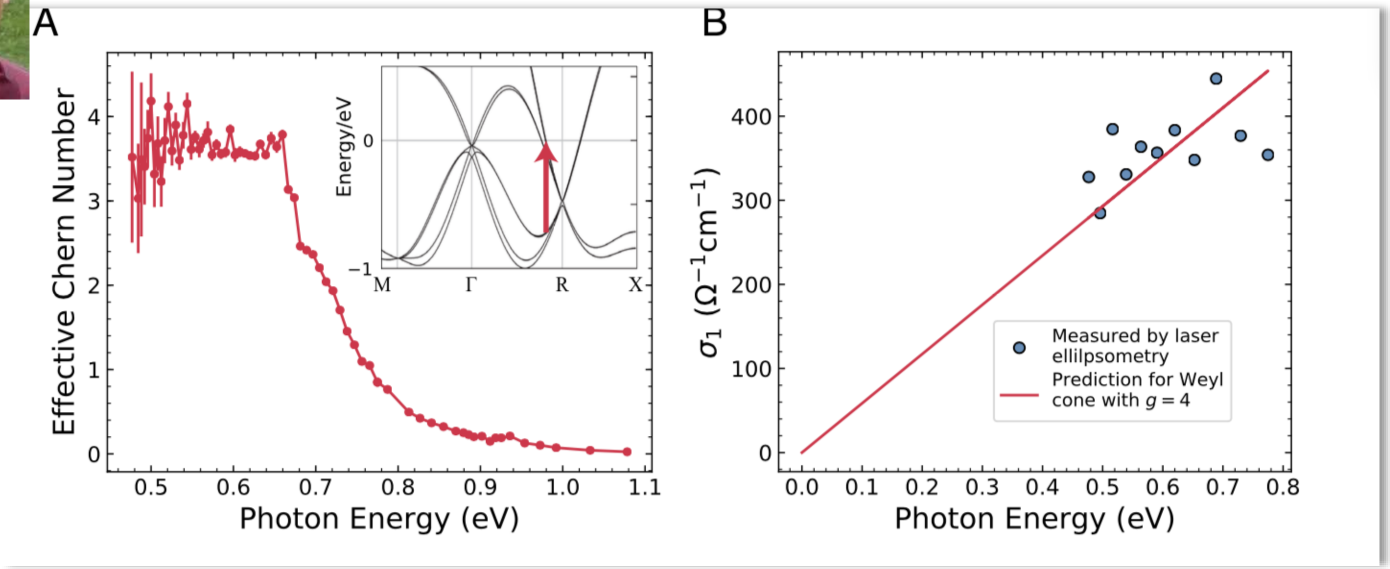
CPGE trace is **effectively quantized** in terms of the **fundamental constants** e, h, c and ε_0 with no material-dependent parameters. This is so because the CPGE directly **measures the topological charge of Weyl points**, and non-quantized corrections from disorder and additional bands can be small over a significant range of incident frequencies.

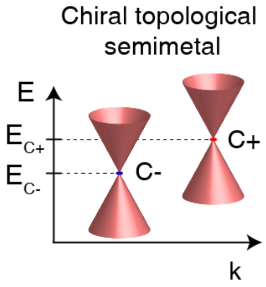
Chiral topological semimetal



quantized circular photogalvanic effect

Excitation of Weyl fermions - a current that is quantized in units of material-independent fundamental constants over a range of photon energies





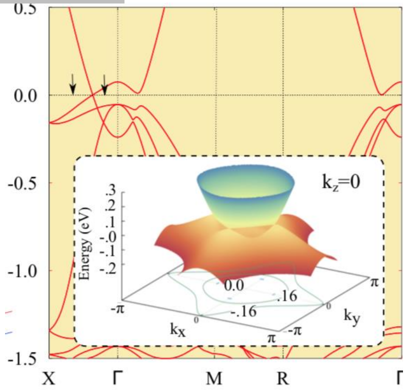
Frequency-independent plateau at low photon energy abruptly falls-off above 0.66 eV

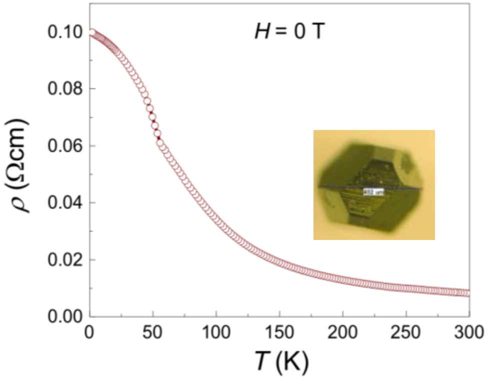
Reez et al. under review, preprint arXiv:1812.04466

What comes next?

correlated topological materials

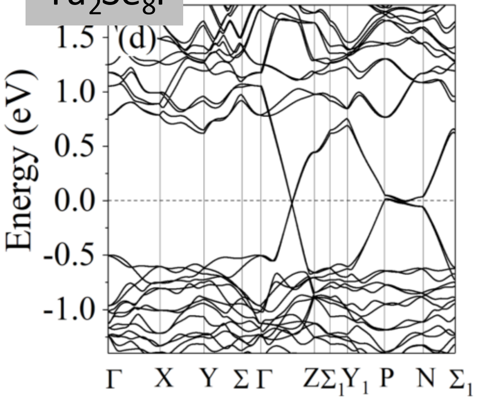
$SrPd_3O_4$

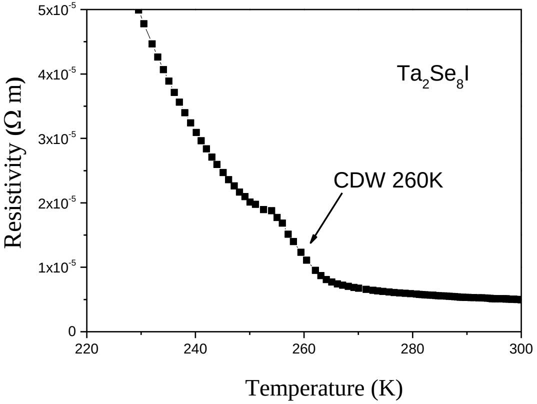


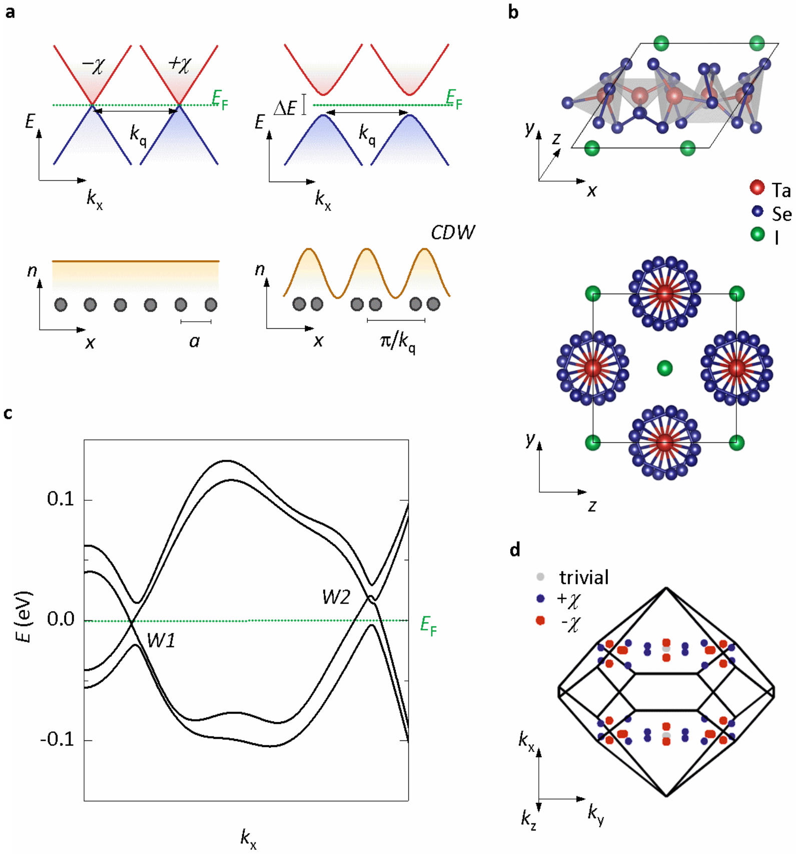


with Binghai Yan, Jansen

Ta_2Se_8I







with Bernevig, Sun, Gooth

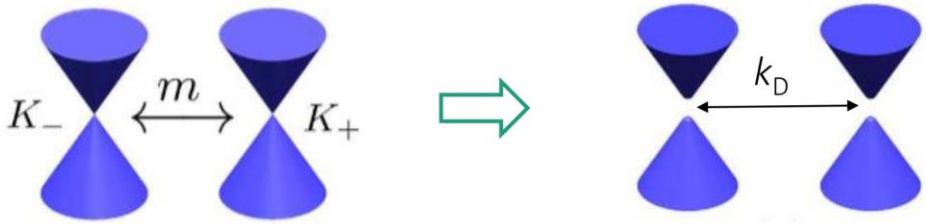
axion insulator

- The **axion** is a hypothetical elementary particle postulated by the Peccei–Quinn theory in 1977 to resolve the strong CP (combined symmetries of charge conjugation and parity) problem in quantum chromodynamics (QCD). If axions exist and have low mass within a specific range, they are of interest as a possible component of cold **dark matter.**

Wikipedia

Start with a Weyl semimetal

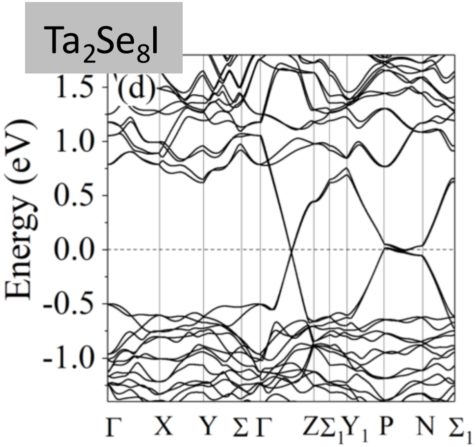
add Dirac mass

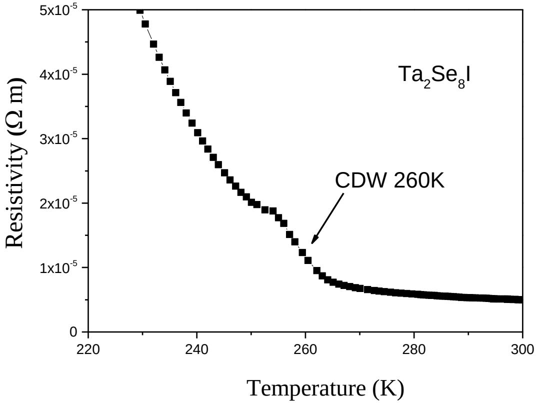


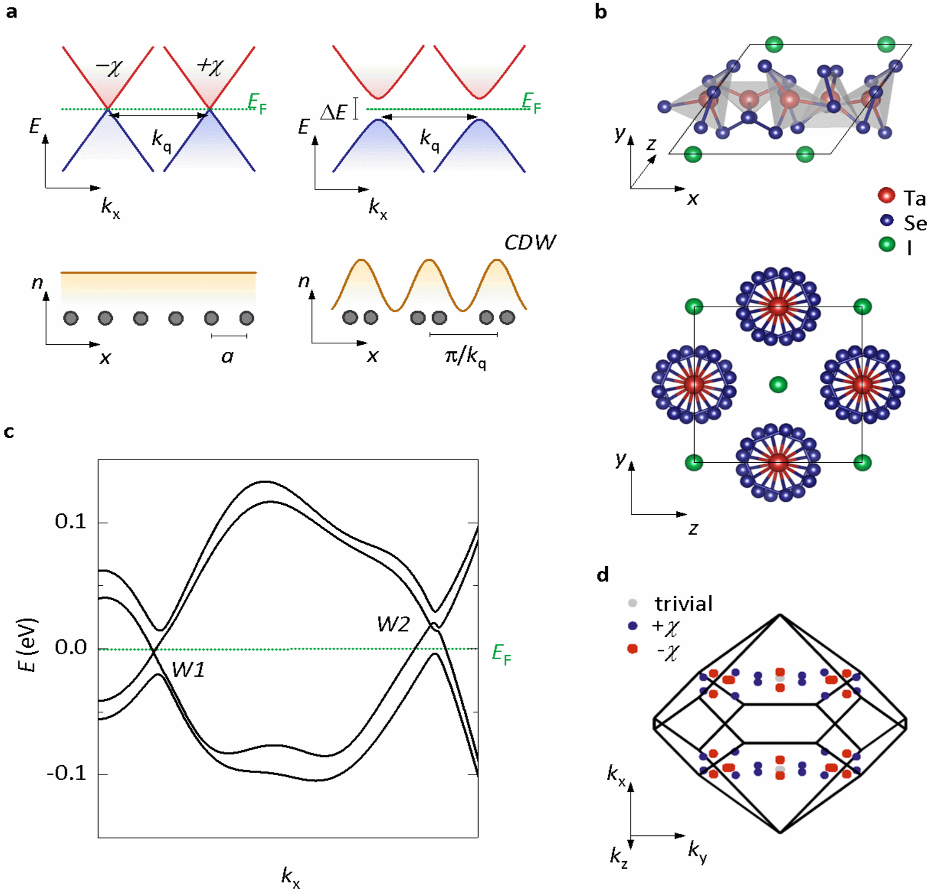
Z. Wang *et al.*, Phys. Rev. B (2013)
R. Bi *et al.*, Phys. Rev. B (2015)

nesting vector of the DW
=
distance of the Weyl points

correlated topological materials

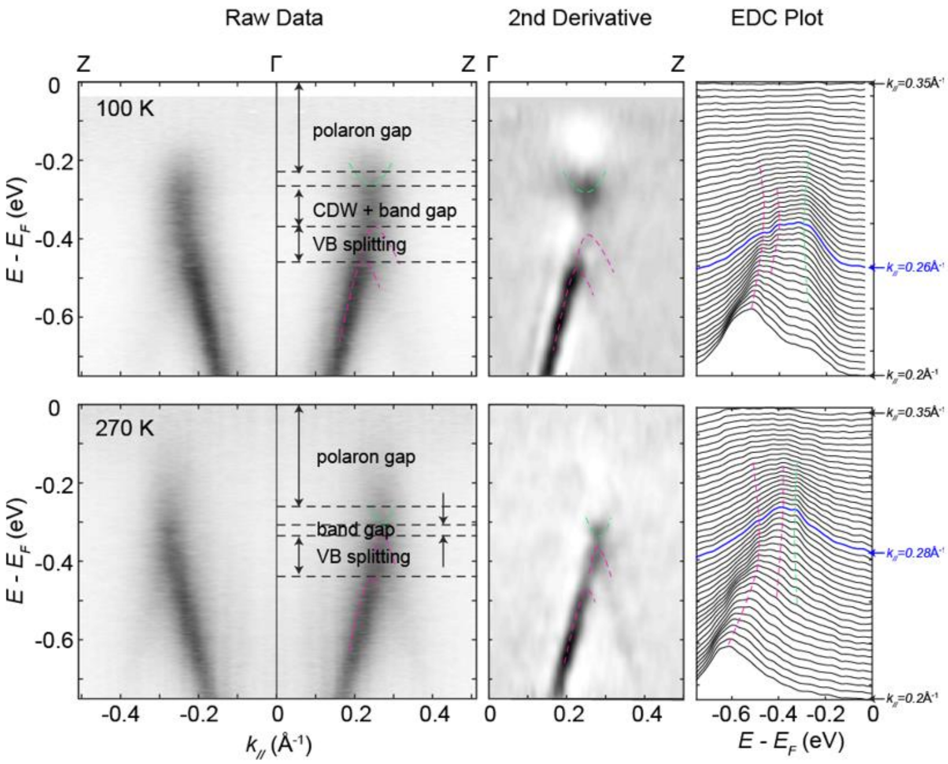


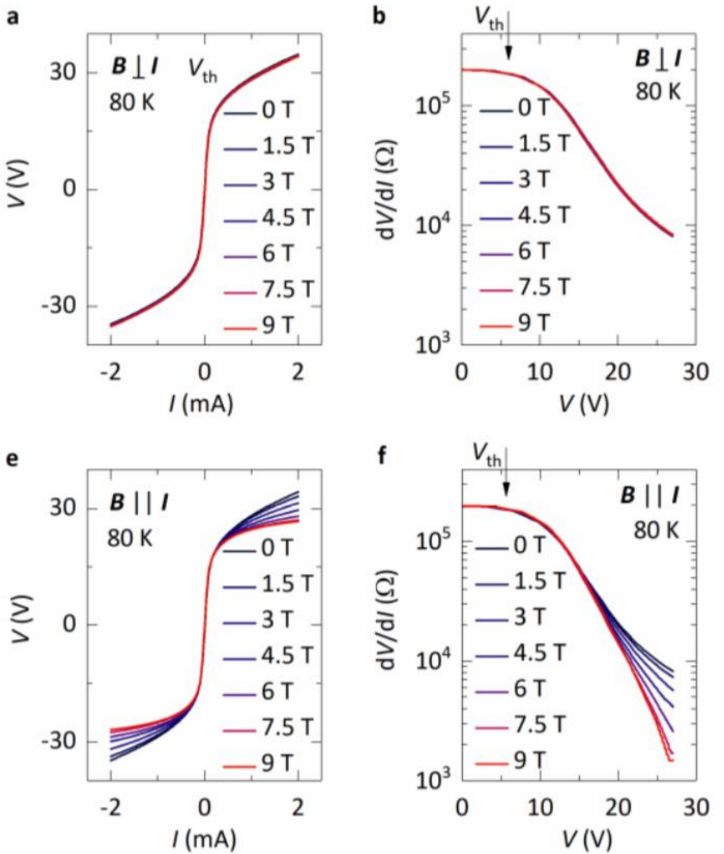




Gooth et al. Nature accepted, preprint arXiv:1906.04510

axion insulator





Gooth et al. Nature accepted, preprint arXiv:1906.04510

axion insulator

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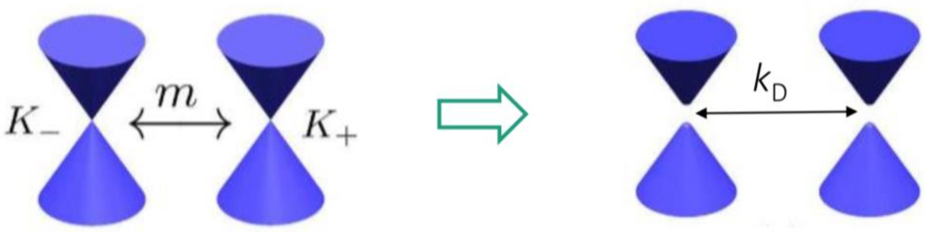
Wikipedia

add a magnetic moment



more axion …

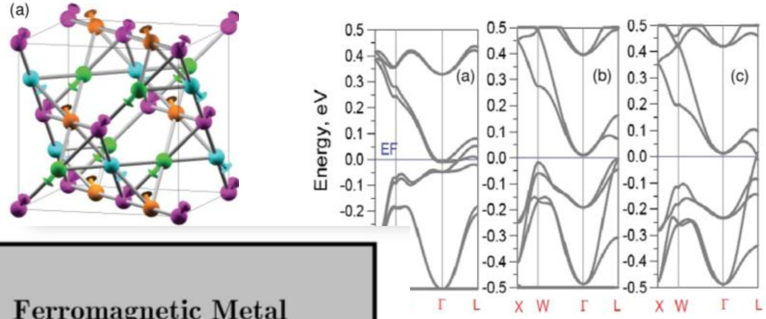
Selected for a Viewpoint in *Physics*

PHYSICAL REVIEW B **83**, 205101 (2011)

Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates

Xiangang Wan,[1] Ari M. Turner,[2] Ashvin Vishwanath,[2,3] and Sergey Y. Savrasov[1,4]

[1]*National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China*



…lor online) Evolution of electronic band structure of … along high-symmetry directions, calculated using the …SO method with three different values of U equal …), (b) 1.5 eV, and (c) 2 eV (insulator with small …l point that is present in case (b), is not visible along … lines.

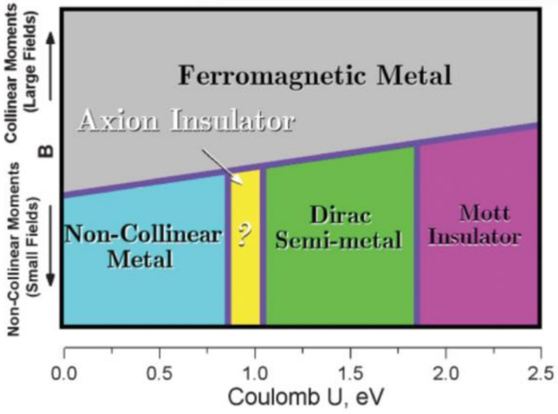
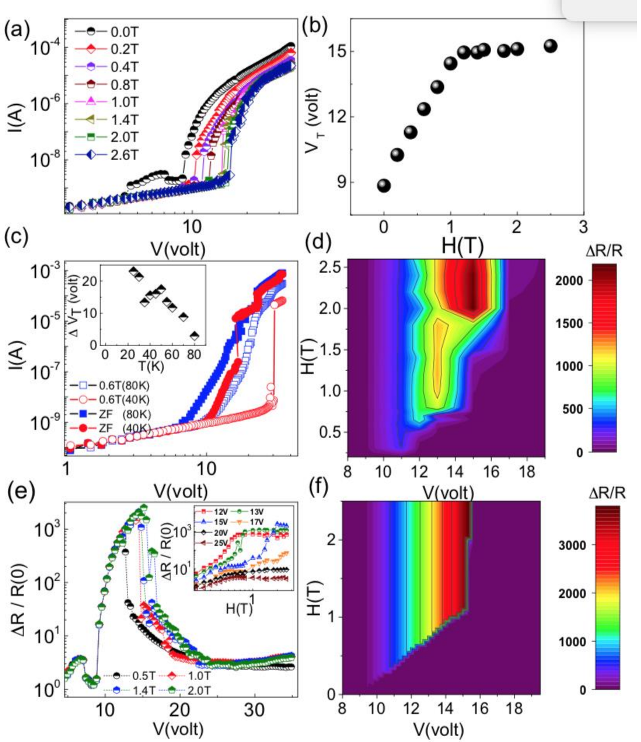


FIG. 1. (Color online) Sketch of the predicted phase diagram

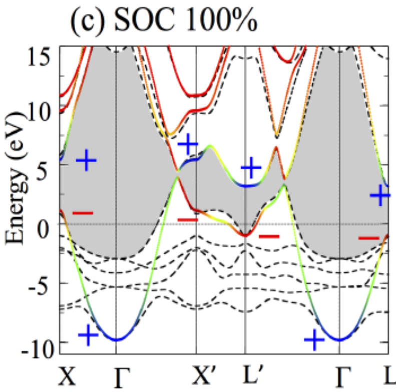
Negative longitudinal magnetoresistance in the density wave phase of $Y_2Ir_2O_7$

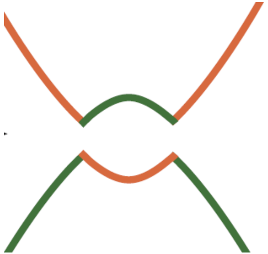
Abhishek Juyal,* Amit Agarwal,† and Soumik Mukhopadhyay‡

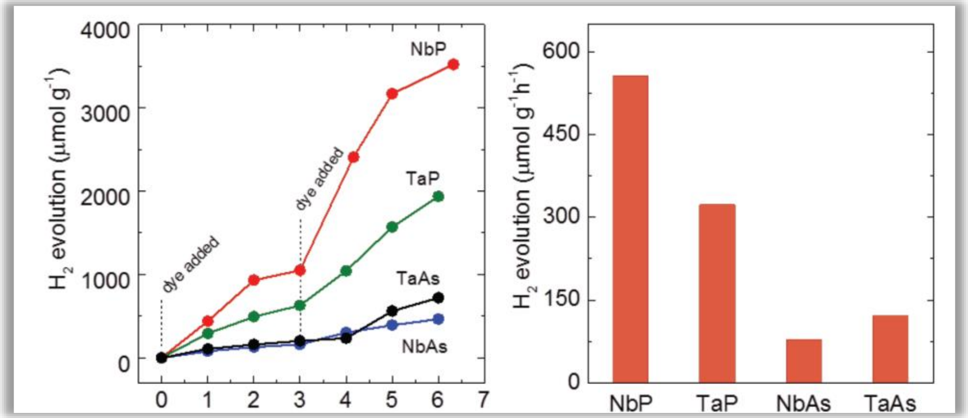
Department of Physics, Indian Institute of Technology Kanpur, Kanpur 208016, India



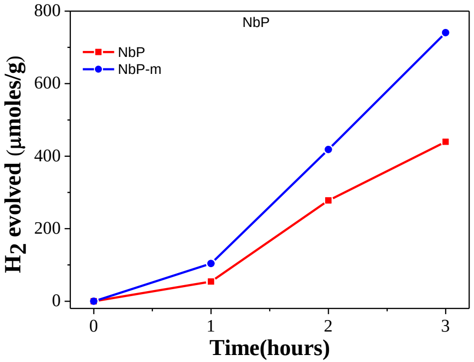
catalysis

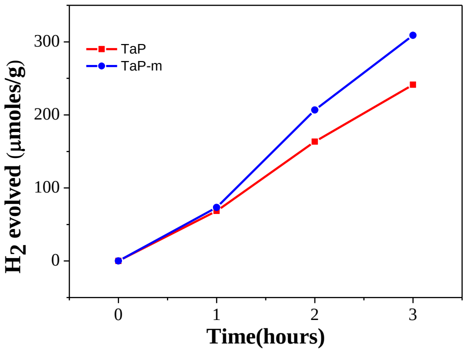






Hydrogen evolution





Hydrogen evolution in magnetic field (m=3000 Gauss)

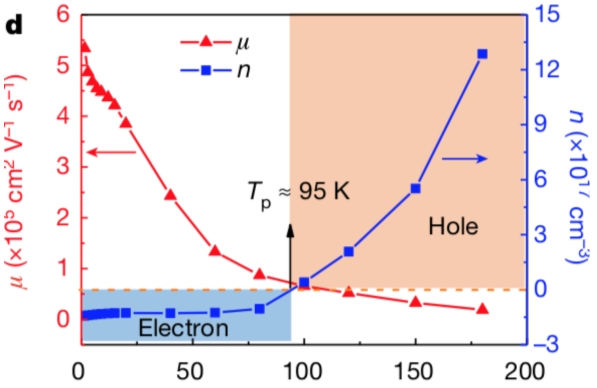
C. R. Rajamathi, et la., Advanced Materials 29 (2017) 1606202

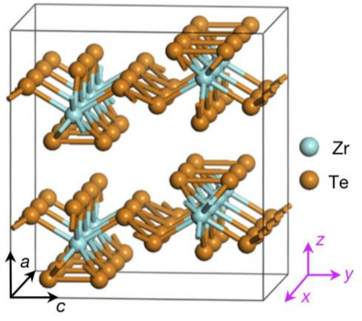
CATALYSIS

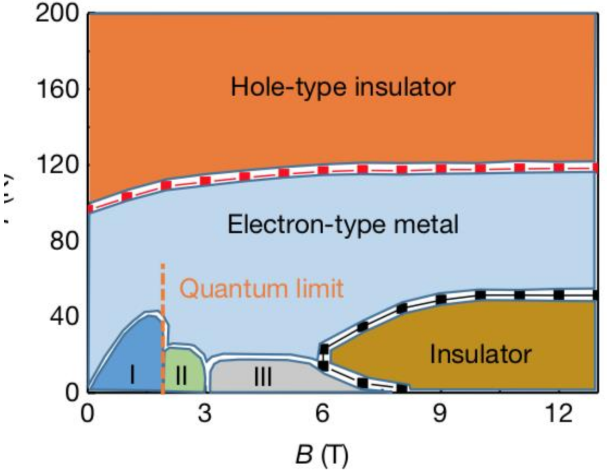
Topology does the water splits

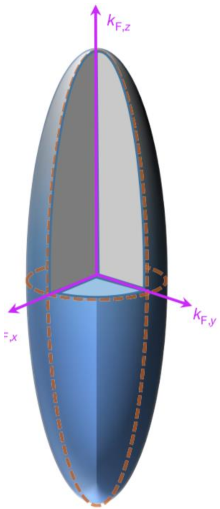
Meiser *Nature Reviews Materials* 2017, doi:10.1038/natrevmats.2017.21

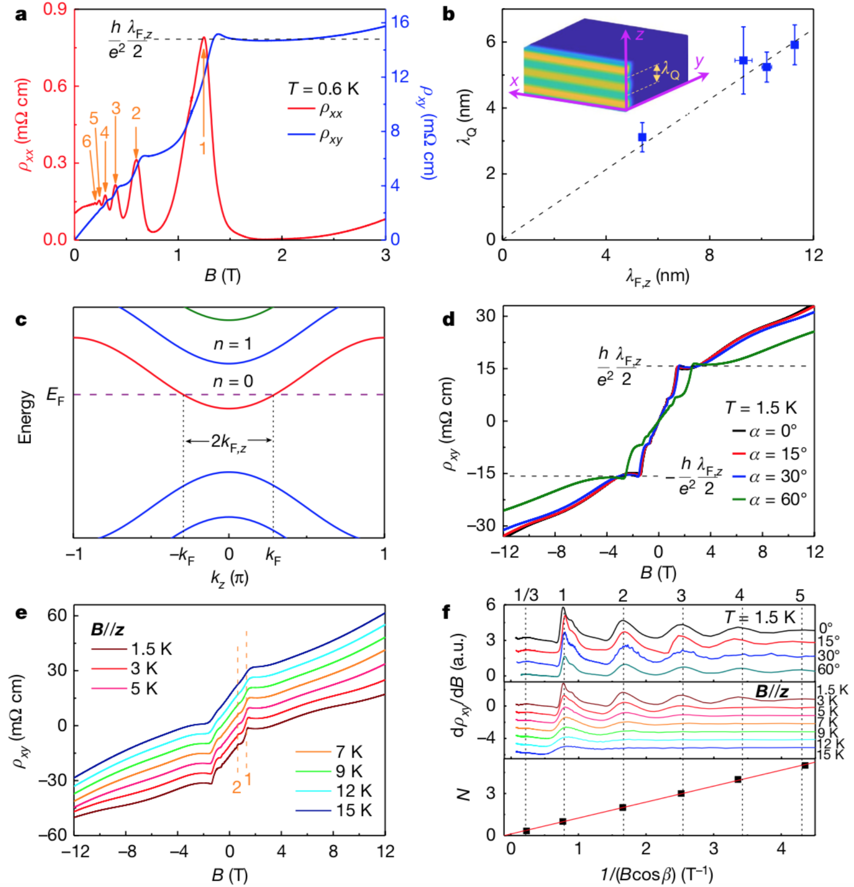
semimetals and 3D QHE







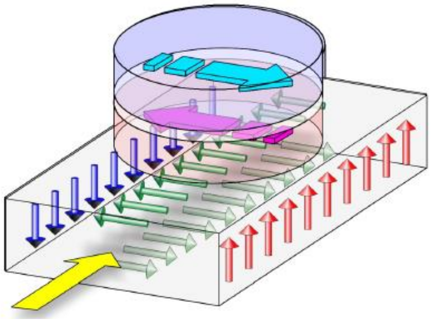




vision

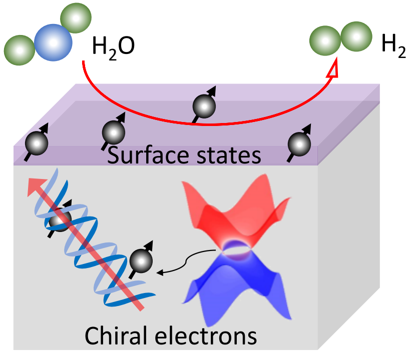
new chemistry and physics

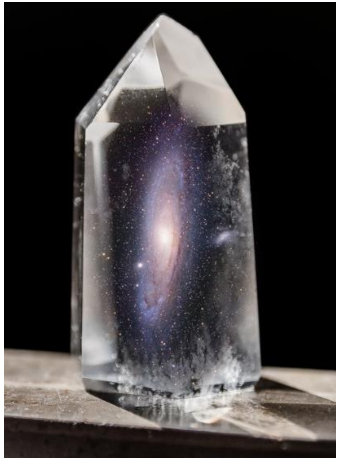
- New topological materials beyond the single particle picture
- high mobility, topological surface states for catalysis
- new emergent properties beyond condensed matter physics - inspired by astrophysics and high energy physics



potential applications

- spintronics
- quantum computing
- energy conversion
- catalysis ...





thank you for your attention

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Stuart Parkin
and teams

Andrei
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