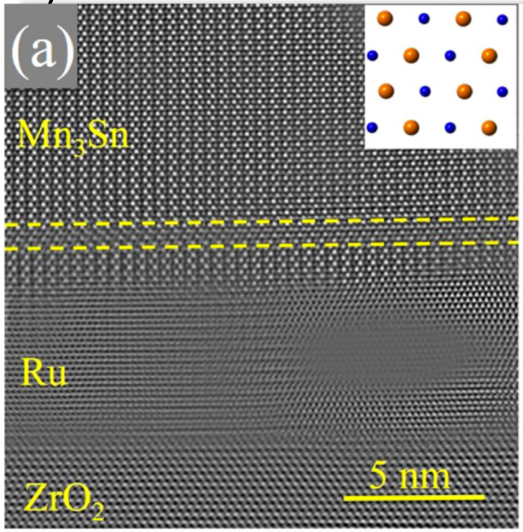
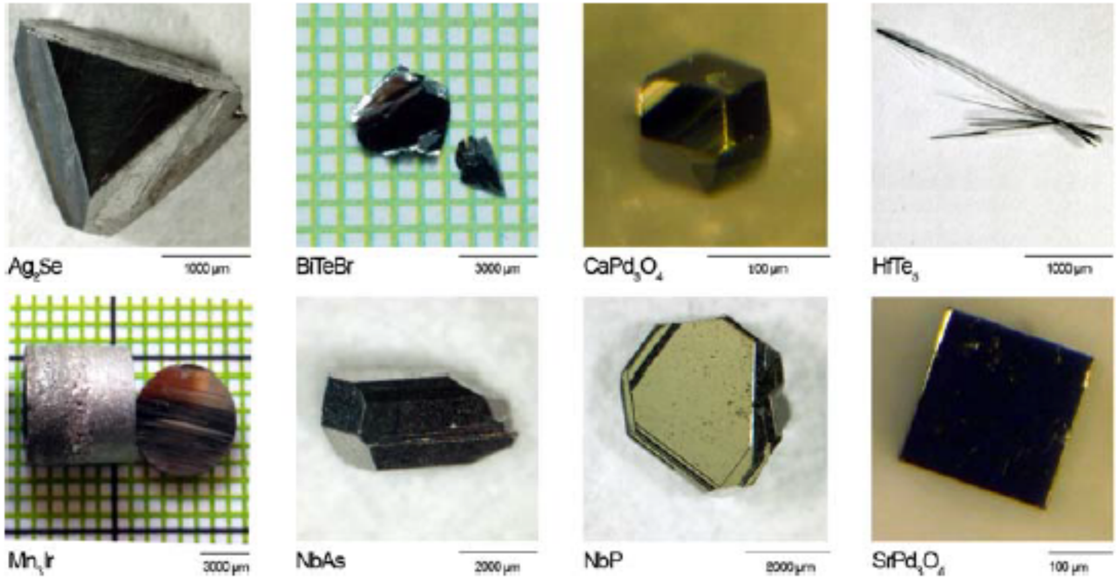
Topology: Magnetic Weyl semimetals

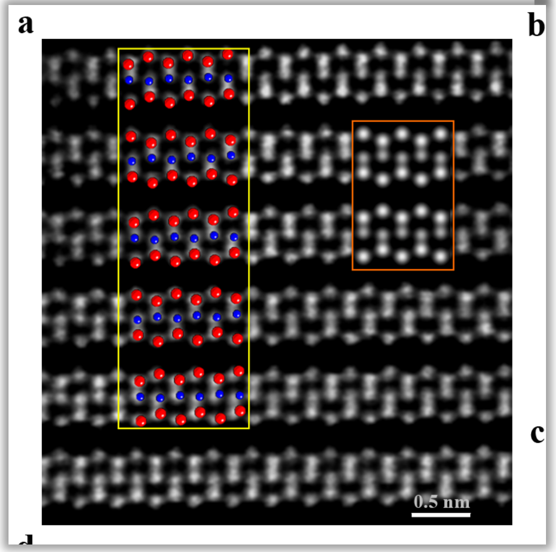
Claudia Felser

Novel topological materials

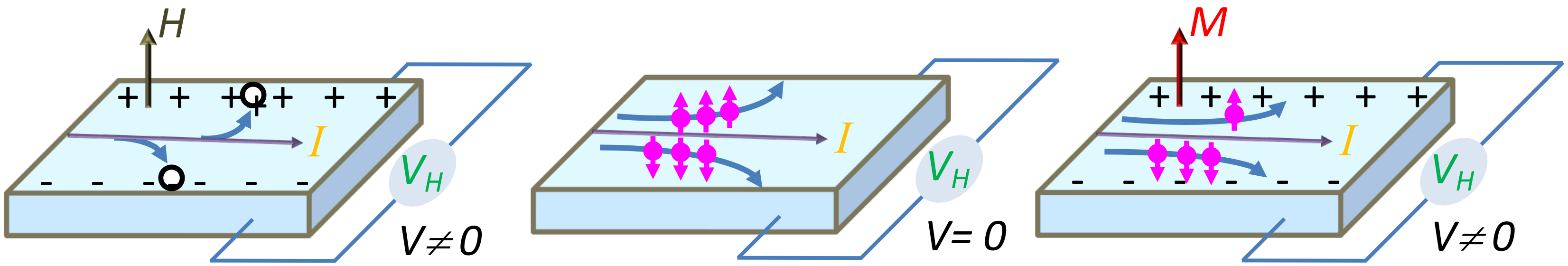
- **Explorative search for new materials** & **predictive design** (Yan Sun)
- 200 high quality **single crystal growth** (Shekhar Chandra)
- **Epitaxial growth** of thin films (Anastasious Markou)
- **2D materials – Nanowires** (Johannes Gooth)







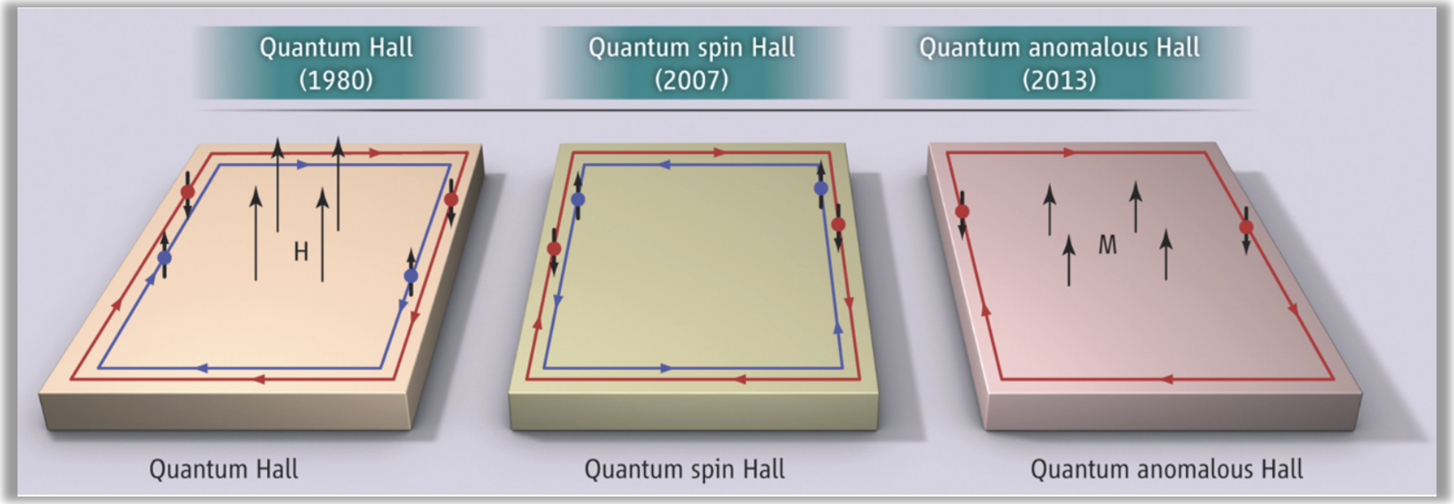
Family of Quantum Hall Effects



Hall Effect

Spin Hall Effect

Anomalous Hall Effect

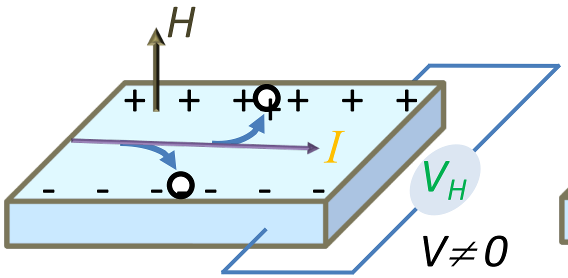


S Oh Science 340 (2013) 153

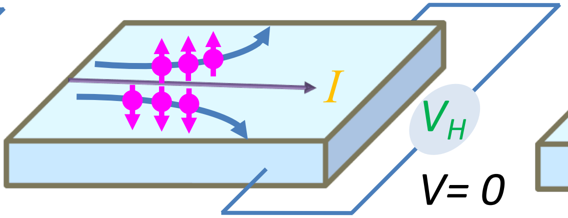
1985
Klaus von Klitzing
1998
Horst Ludwig Störmer and Daniel Tsui
2010
Andre Geim and Konstantin Novoselov

2016
David Thouless, Duncan Haldane und Michael Kosterlitz

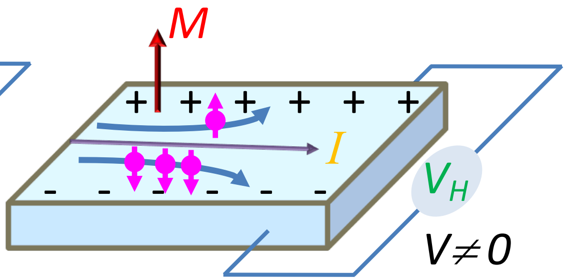
Family of Quantum Hall Effects



Hall Effect

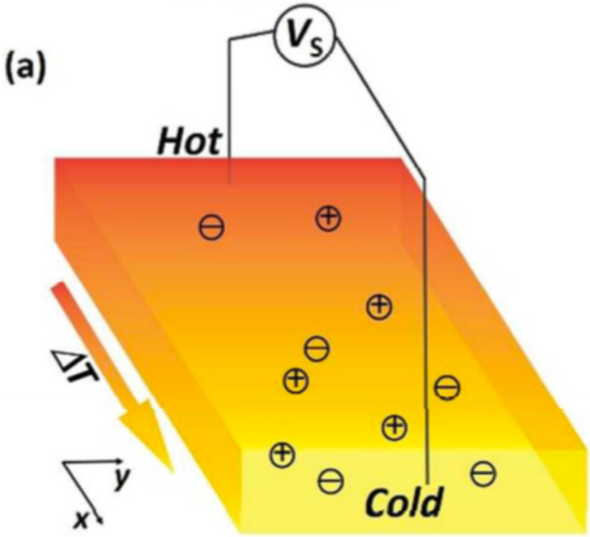


Spin Hall Effect

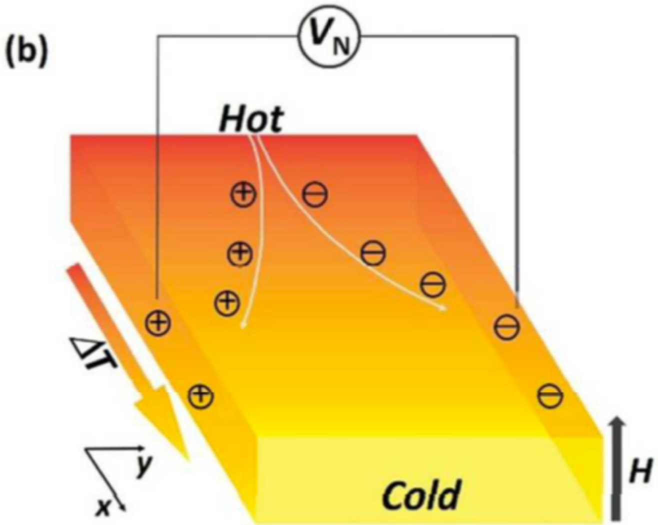


Anomalous Hall Effect

Seebeck effect



Nernst effect



Anomalous Hall effect

REVIEWS OF MODERN PHYSICS, VOLUME 82, APRIL–JUNE 2010

Anomalous Hall effect

Naoto Nagaosa

Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan and Cross-Correlated Materials Research Group (CMRG), and Correlated Electron Research Group (CERG), ASI, RIKEN, Wako, 351-0198 Saitama, Japan

Jairo Sinova

Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA and Institute of Physics ASCR, Cukrovarnická 10, 162 53 Praha 6, Czech Republic

Shigeki Onoda

Condensed Matter Theory Laboratory, ASI, RIKEN, Wako, 351-0198 Saitama, Japan

A. H. MacDonald

Department of Physics, University of Texas at Austin, Austin, Texas 78712-1081, USA

N. P. Ong

Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

(Published 13 May 2010)

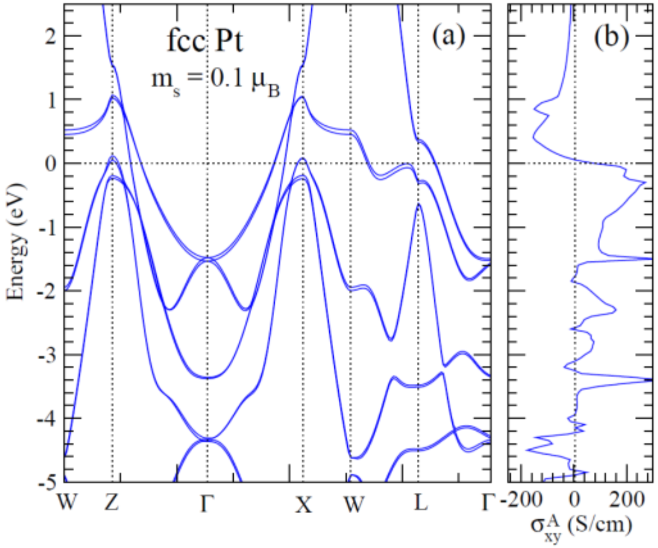
The anomalous Hall effect (AHE) occurs in solids with broken time-reversal symmetry, typically in a ferromagnetic phase, as a consequence of spin-orbit coupling. Experimental and theoretical studies of the AHE are reviewed, focusing on recent developments that have provided a more complete framework for understanding this subtle phenomenon and have, in many instances, replaced controversy by clarity. Synergy between experimental and theoretical works, both playing a crucial role, has been at the heart of these advances. On the theoretical front, the adoption of the Berry-phase concepts has established a link between the AHE and the topological nature of the Hall currents. On the experimental front, new experimental studies of the AHE in transition metals, transition-metal oxides, spinels, pyrochlores, and metallic dilute magnetic semiconductors have established systematic trends. These two developments, in concert with first-principles electronic structure calculations, strongly favor the dominance of an intrinsic Berry-phase-related AHE mechanism in metallic ferromagnets with moderate conductivity. The intrinsic AHE can be expressed in terms of the Berry-phase curvatures and it is therefore an intrinsic quantum-mechanical property of a perfect crystal. An extrinsic mechanism, skew scattering from disorder, tends to dominate the AHE in highly conductive ferromagnets. The full modern semiclassical treatment of the AHE is reviewed which incorporates an anomalous contribution to wave-packet group velocity due to momentum-space Berry curvatures and correctly combines the roles of intrinsic and extrinsic (skew-scattering and side-jump) scattering-related mechanisms. In addition, more rigorous quantum-mechanical treatments based on the Kubo and Keldysh formalisms are reviewed, taking into account multiband effects, and demonstrate the equivalence of all three linear response theories in the metallic regime. Building on results from recent experiment and theory, a tentative global view of the AHE is proposed which summarizes the roles played by intrinsic and extrinsic contributions in the disorder strength versus temperature plane. Finally outstanding issues and avenues for future investigation are discussed.

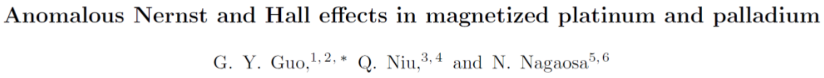
Intrinisic Hall

- Berry curvature
- Magnetisation?

Extrinsic Hall

- Skew scattering
- Side jumps

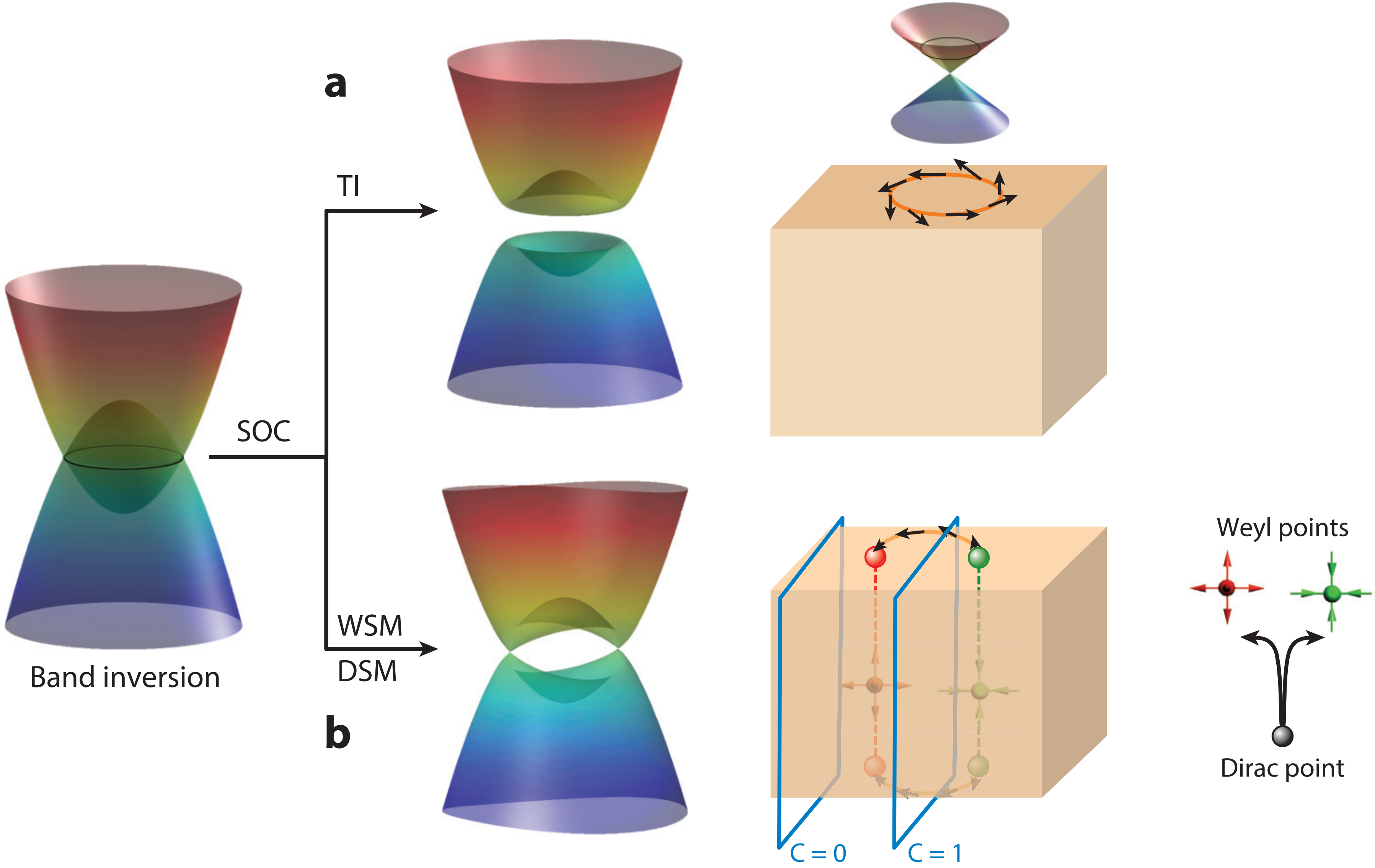




Anomalous Nernst and Hall effects in magnetized platinum and palladium

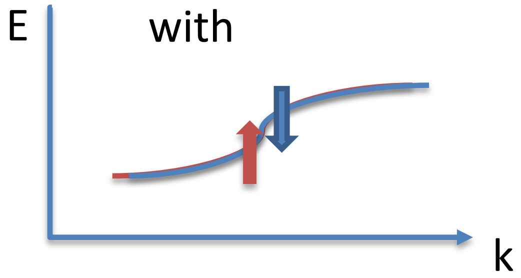
G. Y. Guo,[1,2,*] Q. Niu,[3,4] and N. Nagaosa[5,6]

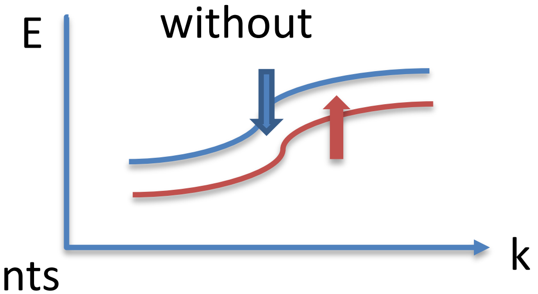
Weyl semimetals



Weyl Semimetal

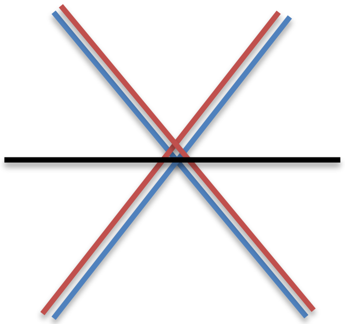
- Breaking symmetry
  - Inversion symmetry (Structural distortion)
- Breaking time reversal symmetry
  - Magnetic field

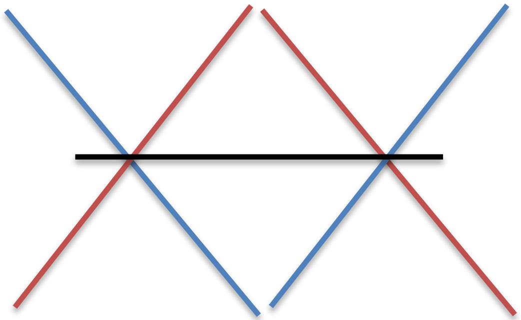


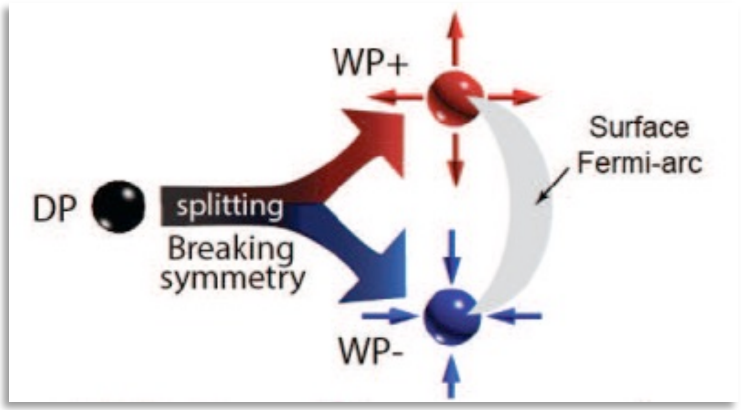


Dirac points are at high symmetry points

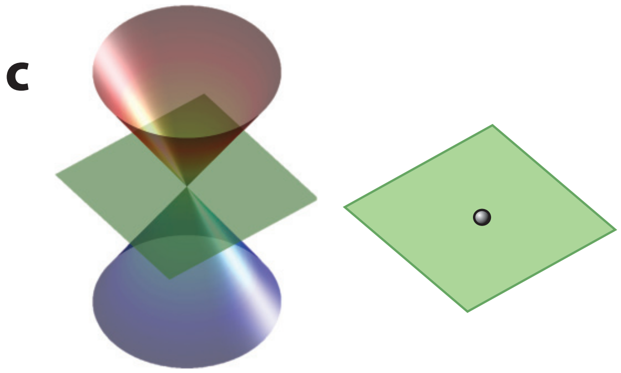
Weyl points are not at high symmetry points



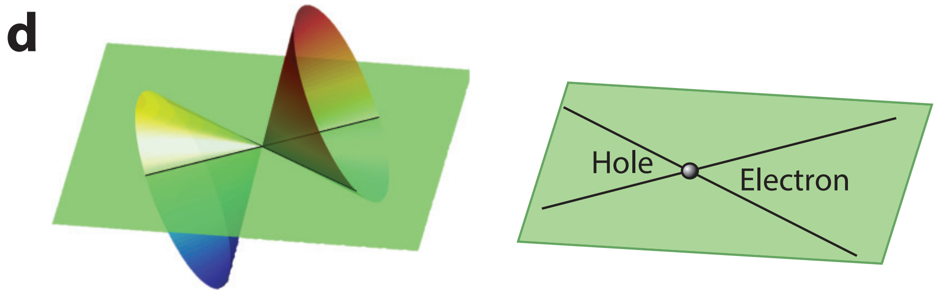




Type I or II

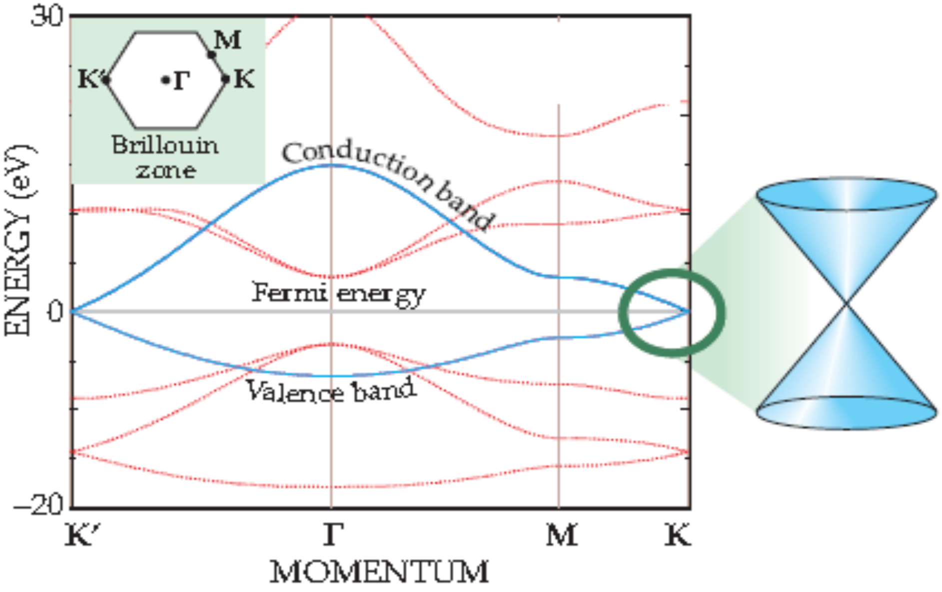


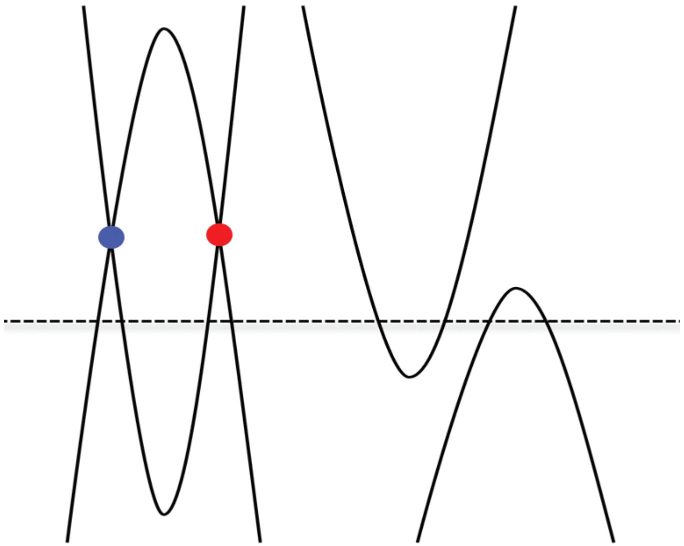
Type-I WSM



Type-II WSM

Graphene





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

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

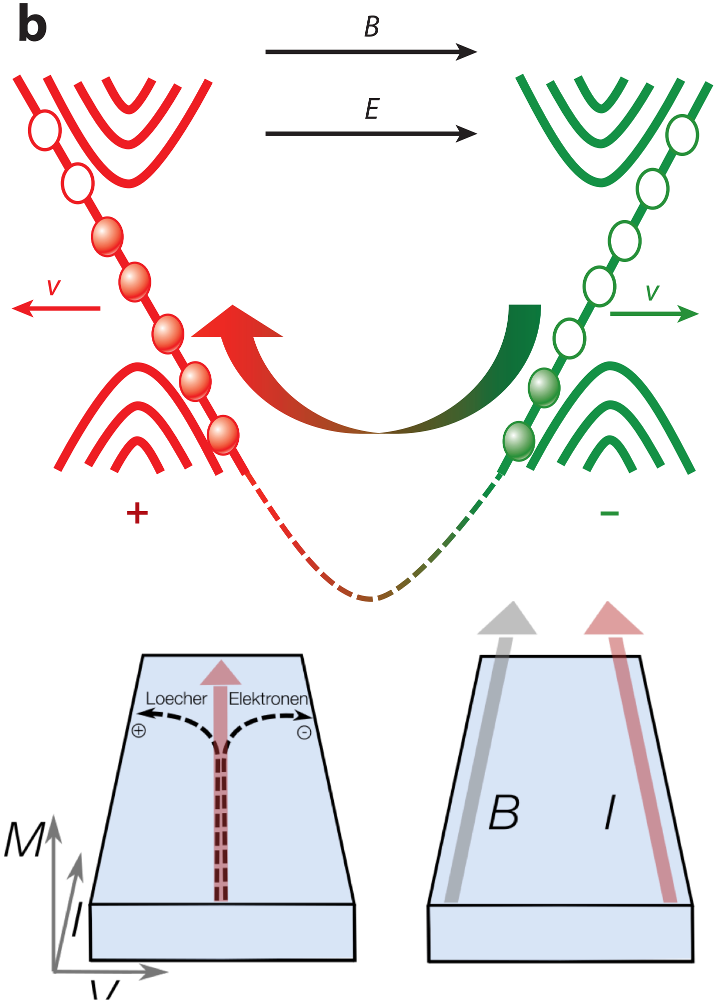
Weyl semimetals

3D topological Weyl semimetals - breaking time reversal symmetry – in transport measurement we should see:

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

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

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



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

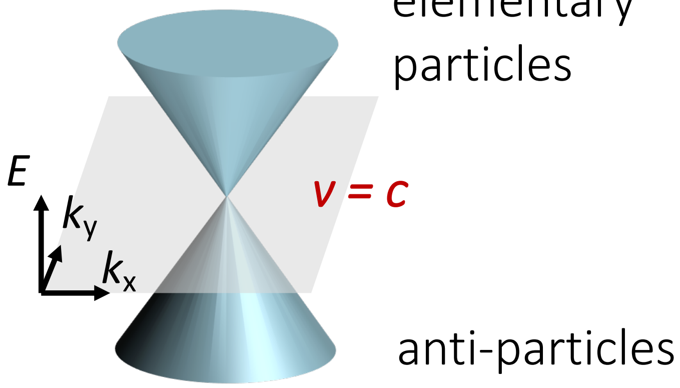
Chiral Anomaly

- 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.

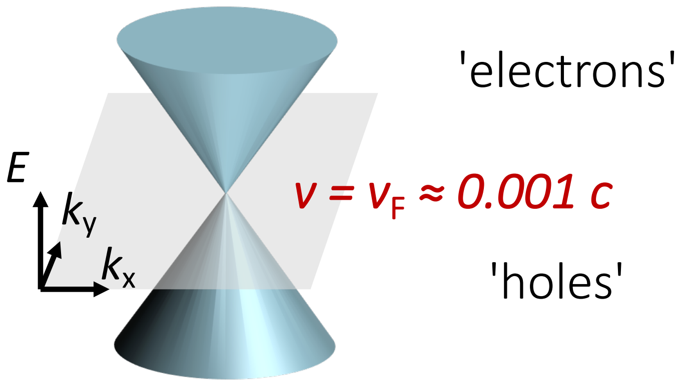
- Events are expected to be prohibited according to classical conservation laws, must be ways they can be broken, because the observable **universe contains more matter than antimatter** Wikipedia

Vacuum state



vacuum dispersion

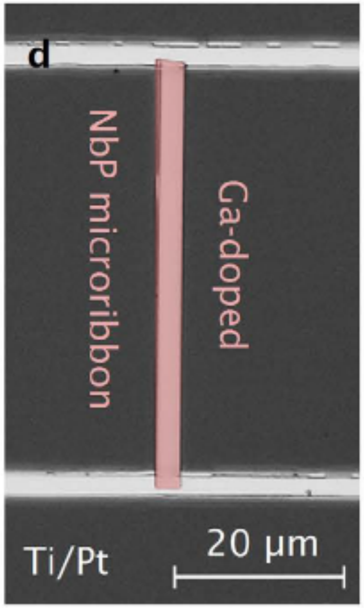
Dirac semimetal

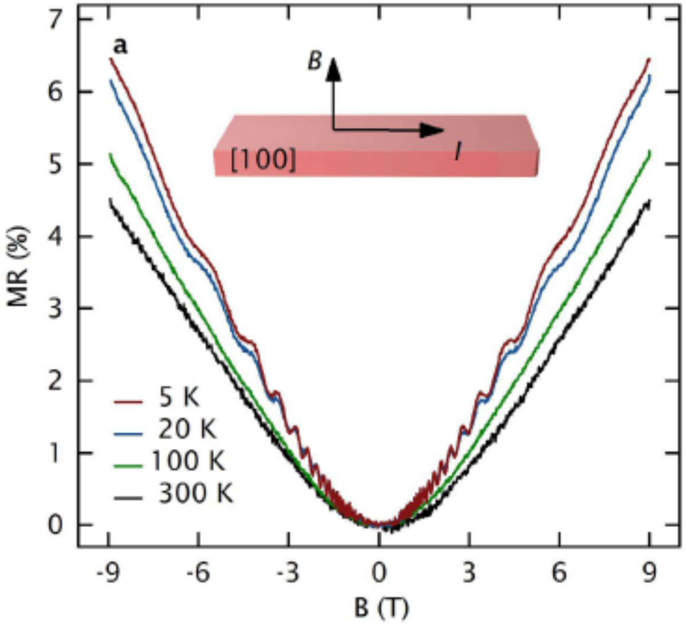


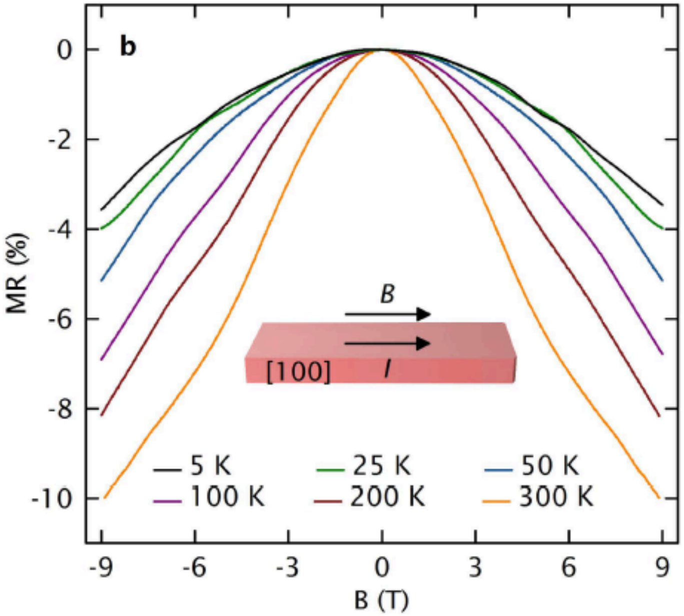
band structure

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







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

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

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

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

Chiral Anomaly

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

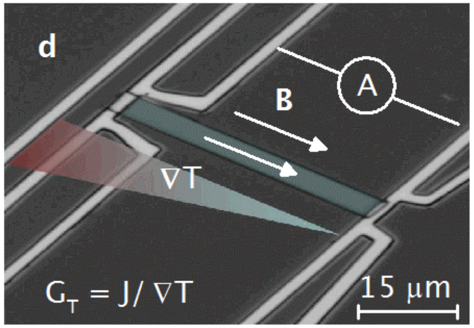
- In solid state physics, mixed axial-gravitational anomaly can be identified by a positive magneto-thermoelectric conductance (PMTG) for $\Delta T \parallel B$.

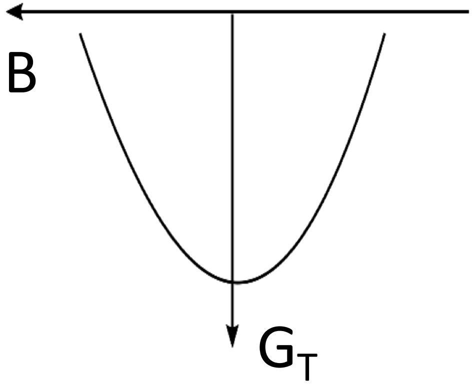
- Low fields: quadratic

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

- High fields: deminishes

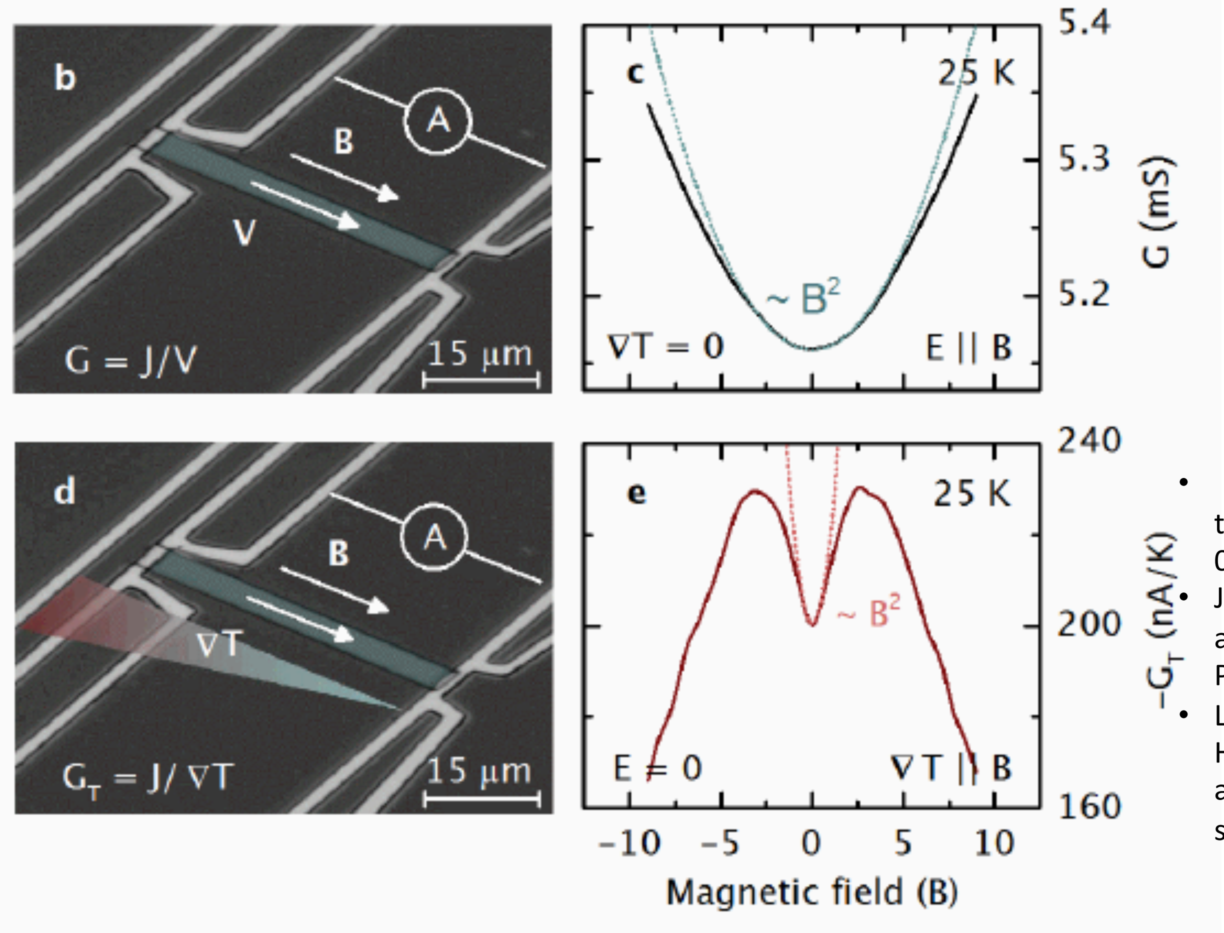
- $\Delta T \parallel B$ dictates sensitivity on alignement of B and ΔT.





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

Gravitational Anomaly



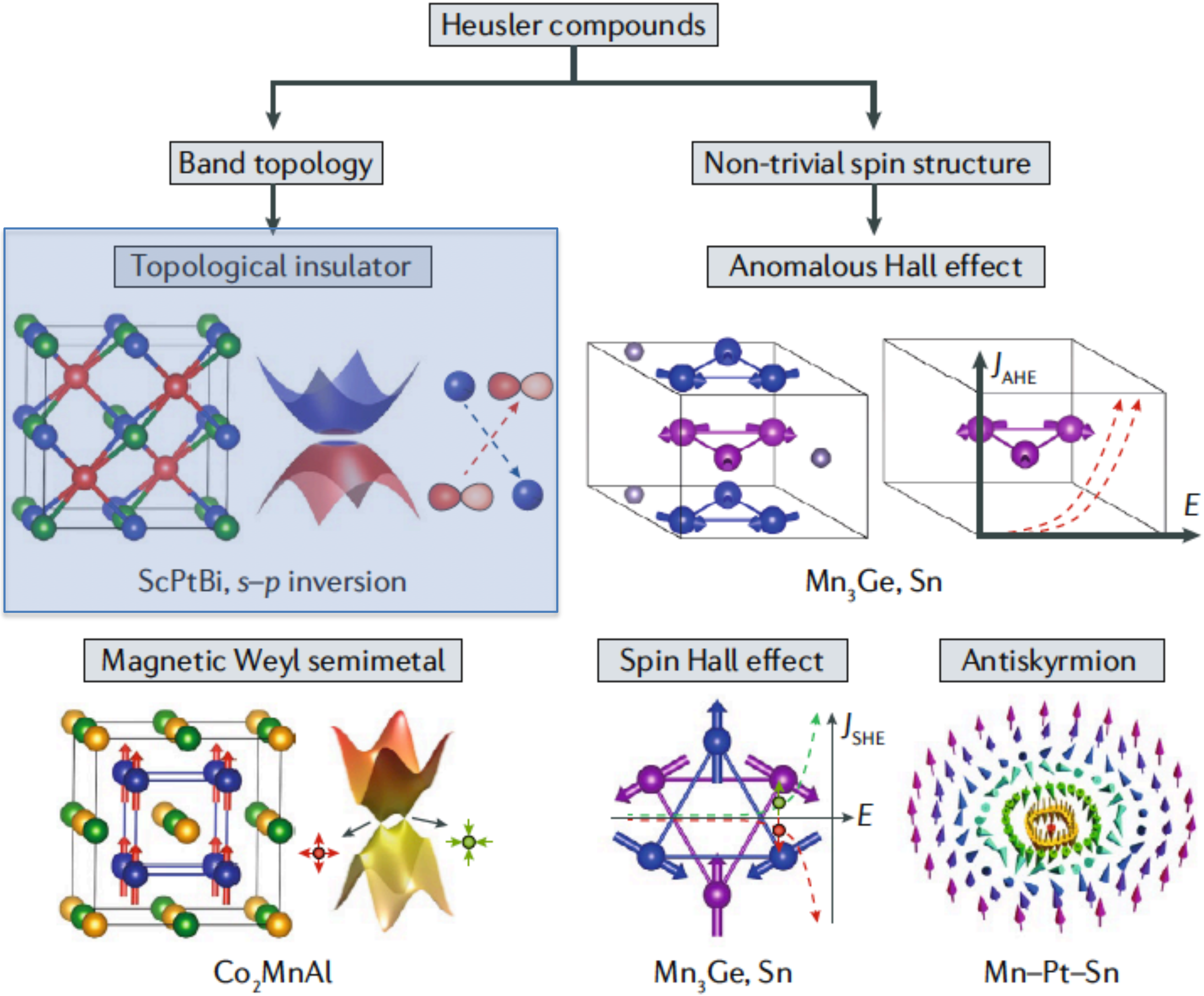
- Landsteiner, et al. Gravitational anomaly and transport phenomena. Phys. Rev. Lett. 107, 021601 (2011). URL
- Jensen, et al. Thermodynamics, gravitational anomalies and cones. Journal of High Energy Physics 2013, 88 (2013).
- Lucas, A., Davison, R. A. & Sachdev, S. Hydrodynamic theory of thermoelectric 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.

Johannes Gooth et al., Nature 547 (2017) 324

Topology and Magnetism

Magnetism and Topology



Heusler compounds

Band topology

Non-trivial spin structure

Topological insulator

ScPtBi, *s*–*p* inversion

Anomalous Hall effect

Mn_3Ge, Sn

Magnetic Weyl semimetal

Co_2MnAl

Spin Hall effect

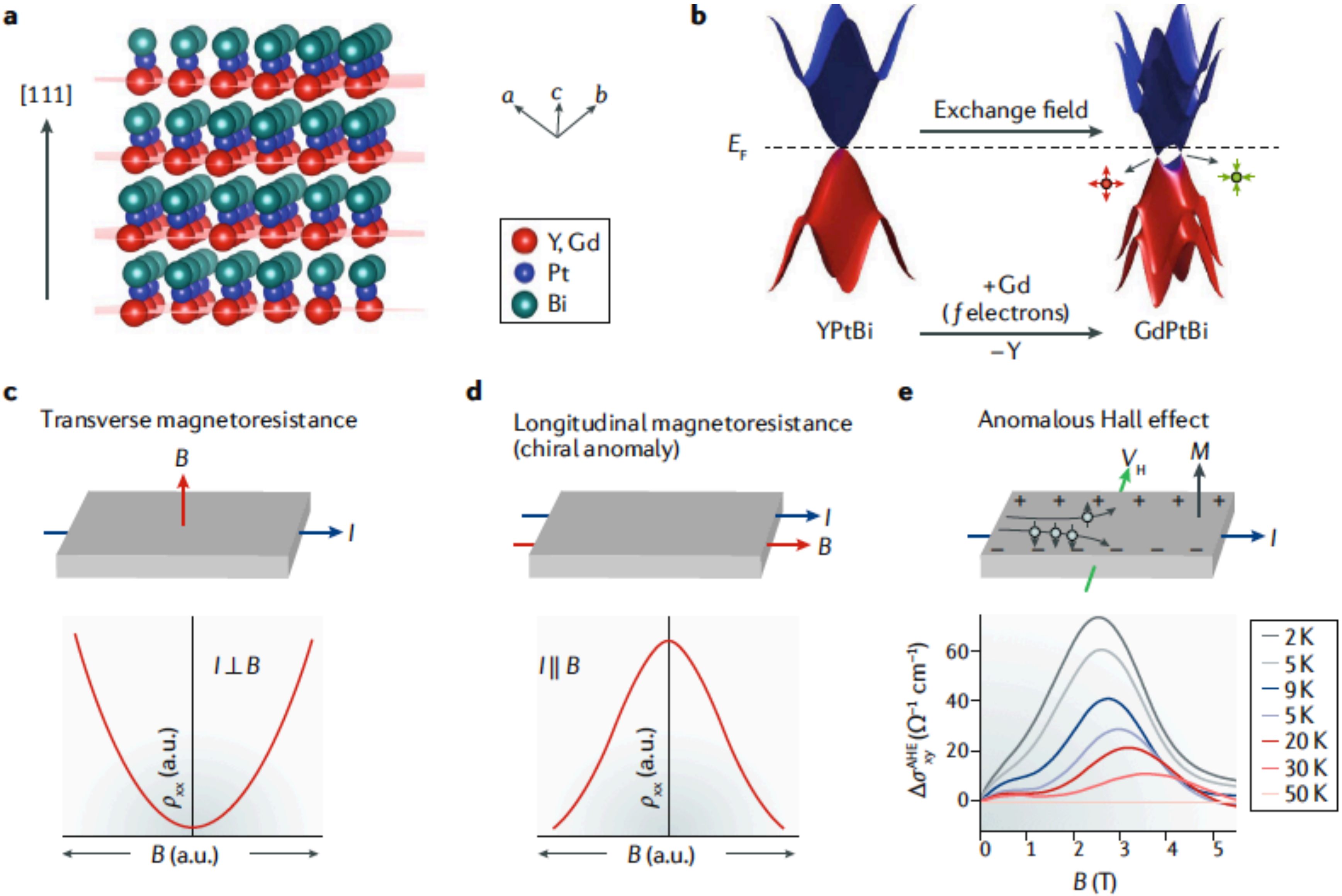
Mn_3Ge, Sn

Antiskyrmion

Mn–Pt–Sn

Kaustuv Manna et al., Nature Materials Review, in press, arXiv:1802.02838v1

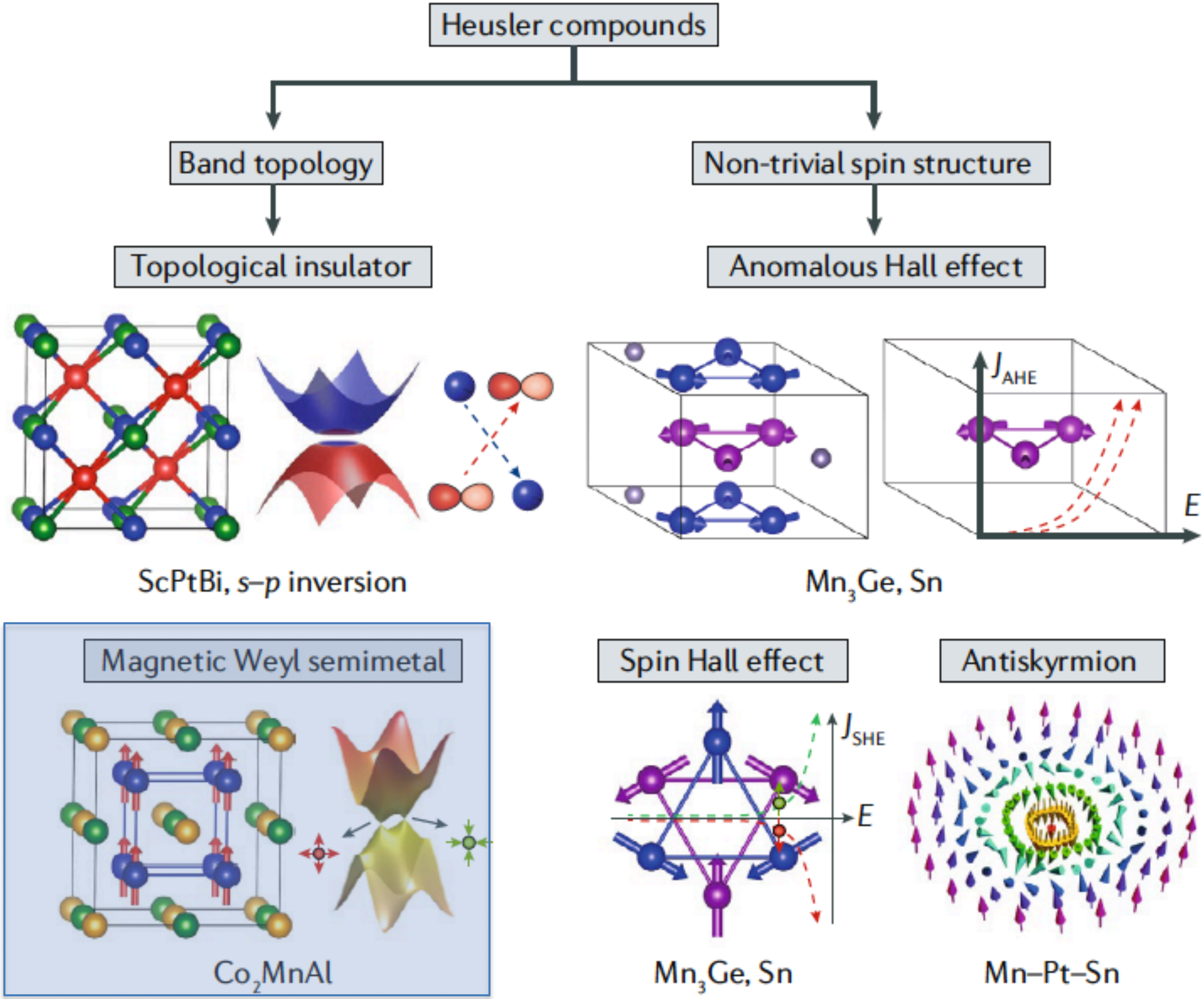
GdPtBi – an ideal Weyl



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

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

Magnetism and Topology



Heusler compounds

Band topology

Non-trivial spin structure

Topological insulator

Anomalous Hall effect

ScPtBi, *s*–*p* inversion

Mn_3Ge, Sn

Magnetic Weyl semimetal

Spin Hall effect

Antiskyrmion

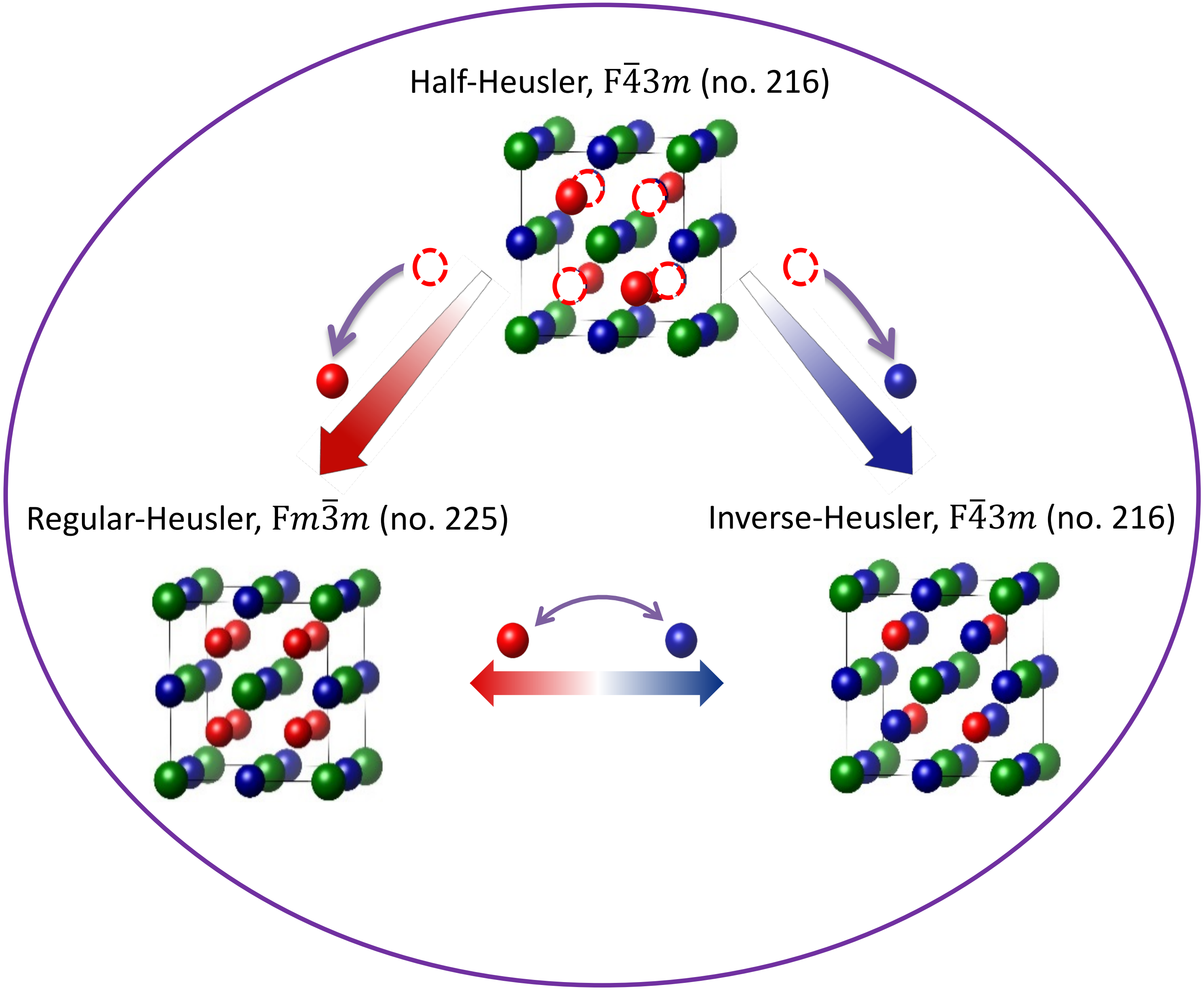
Co_2MnAl

Mn_3Ge, Sn

Mn–Pt–Sn

Kaustuv Manna et al., Nature Materials Review, in press, arXiv:1802.02838v1

Tuning the symmetry

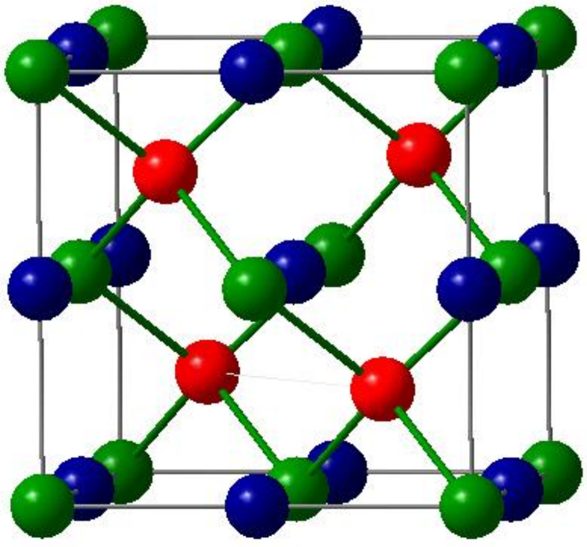


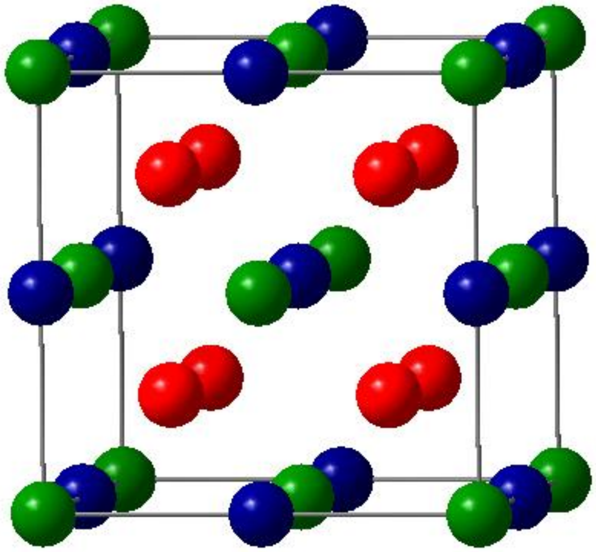
Half-Heusler, $\mathrm{F}\bar{4}3m$ (no. 216)

Regular-Heusler, $\mathrm{F}m\bar{3}m$ (no. 225)

Inverse-Heusler, $\mathrm{F}\bar{4}3m$ (no. 216)

Ternary Semiconductors ...





Ga **As**

$13 + 5 = 18$

La **Pt** **Bi**

$3 + 10 + 5 = 18$

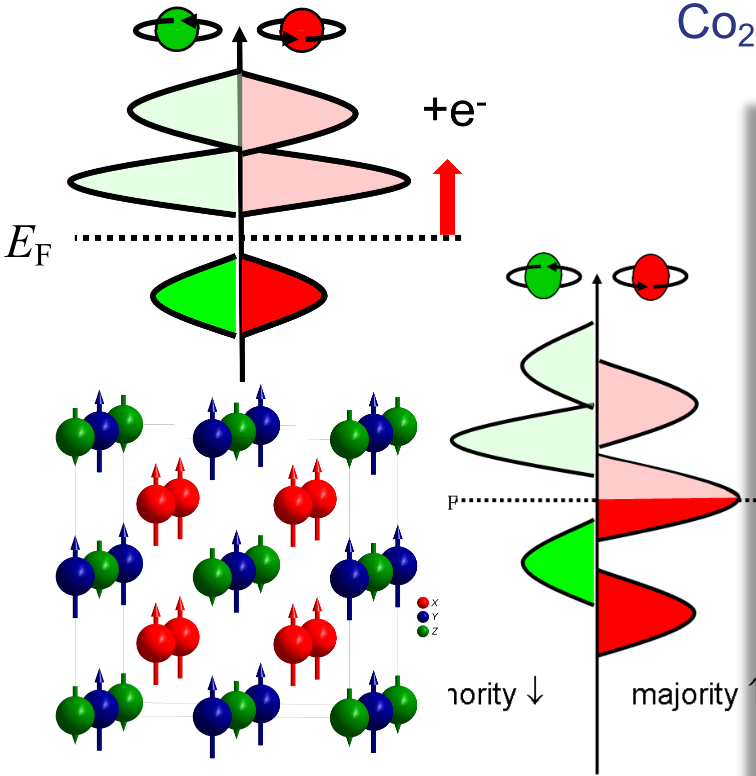
Fe_2 **V** **Al**

$2*8 + 5 + 3 = 24$

additional t_2-levels

Materials: … to half metallic ferromagnets

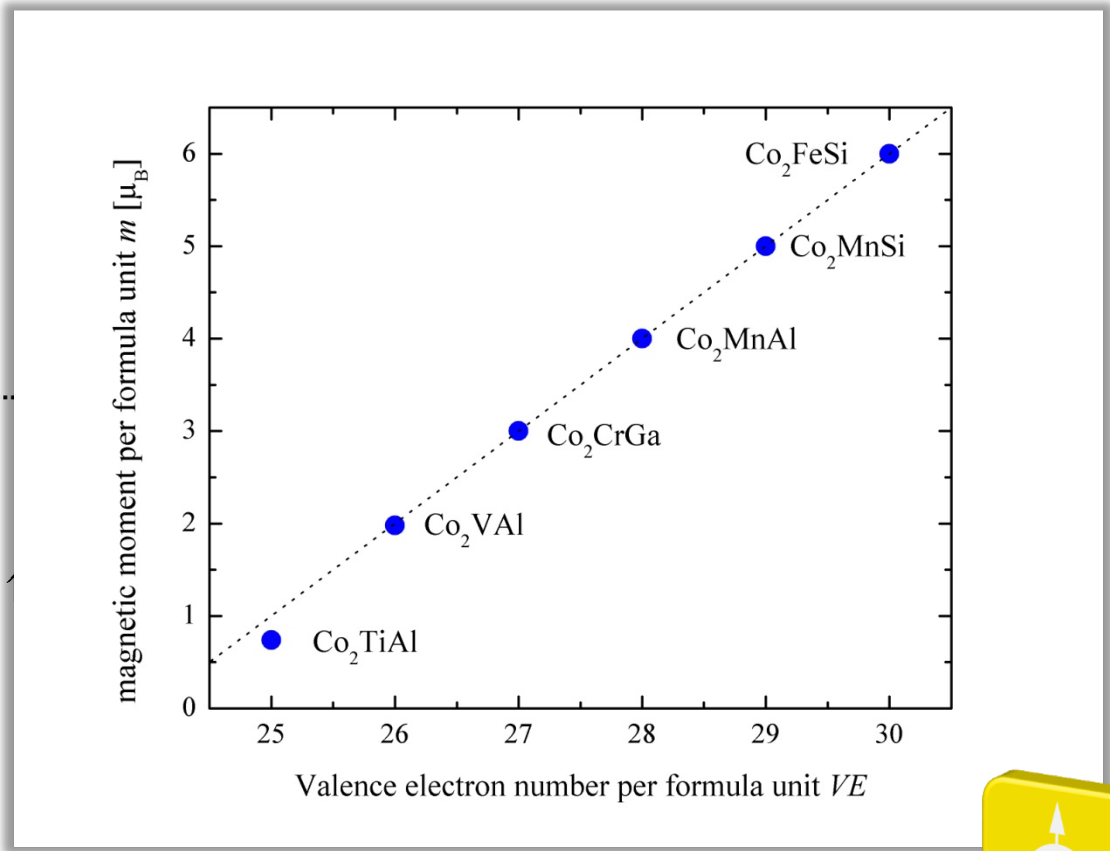
X_2YZ



Example: Co_2MnSi

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

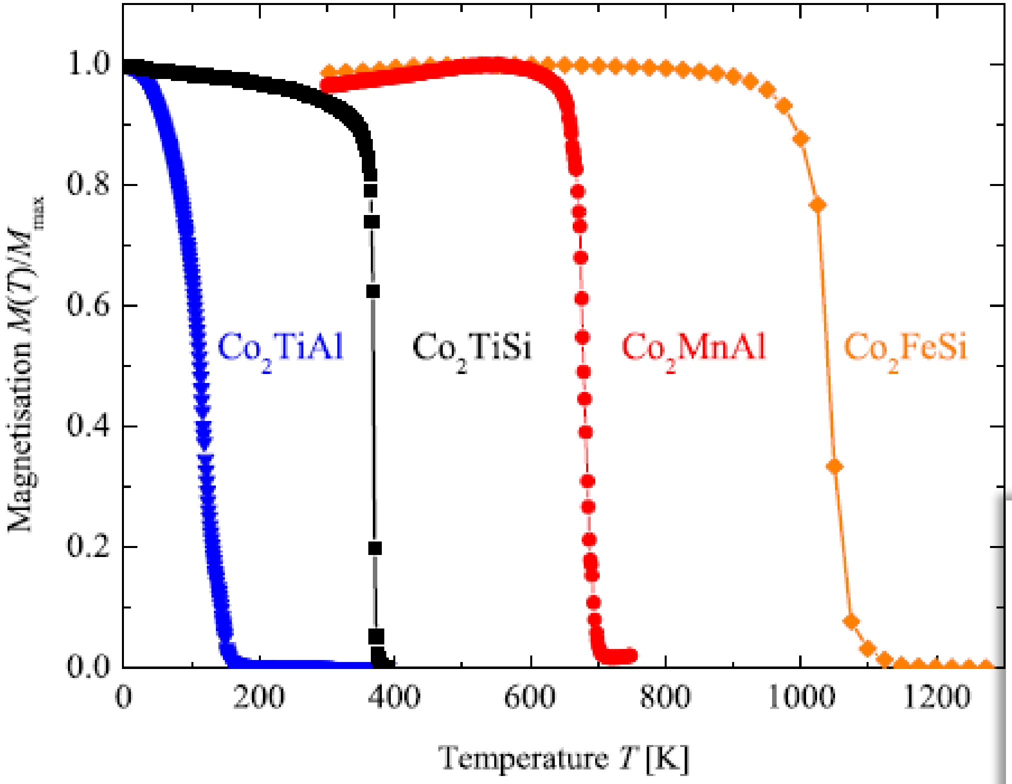
Co_2MnSi: 2×9 + 7 + 4 = 29 Ms = 5μ_B

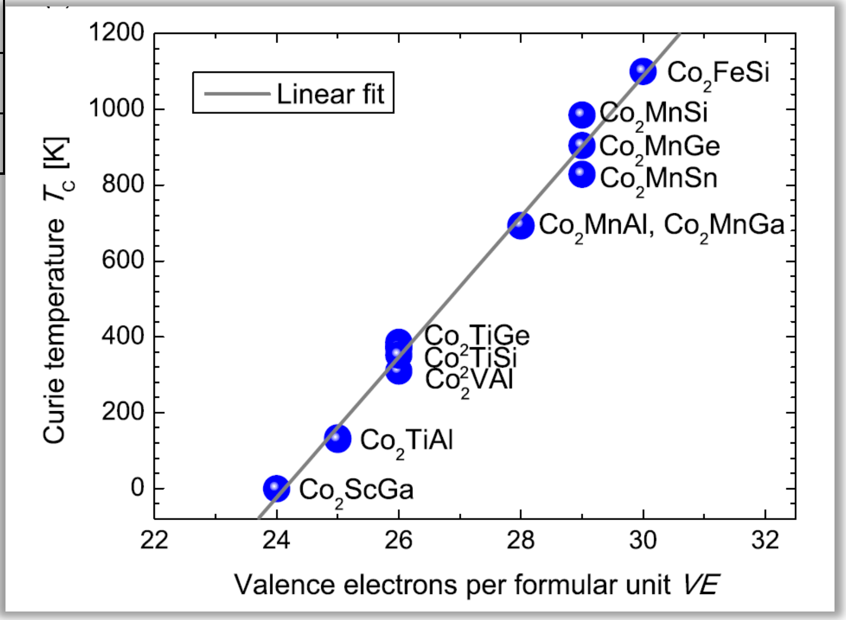


Kübler *et al.*, PRB **28**, 1745 (1983)
de Groot RA, et al. PRL **50** 2024 (1983)
Galanakis *et al.*, PRB **66**, 012406 (2002)

Tunability Co_2YZ

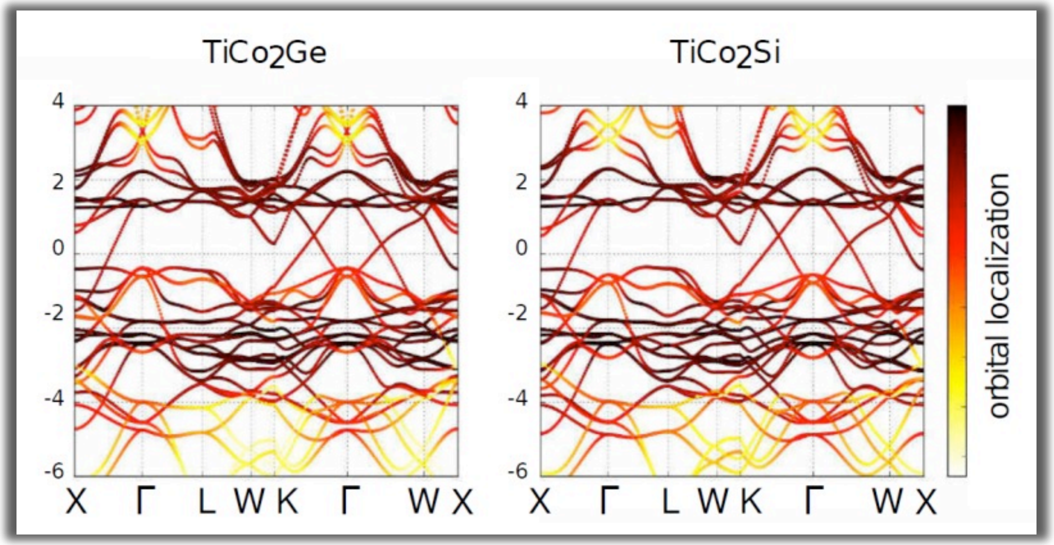
VE	m_B/formula		T_C [K]
24	0		0
25	1		~175
26	2		~350
27	3		~520
28	4		~700
29	5		~970
30	6		~1120

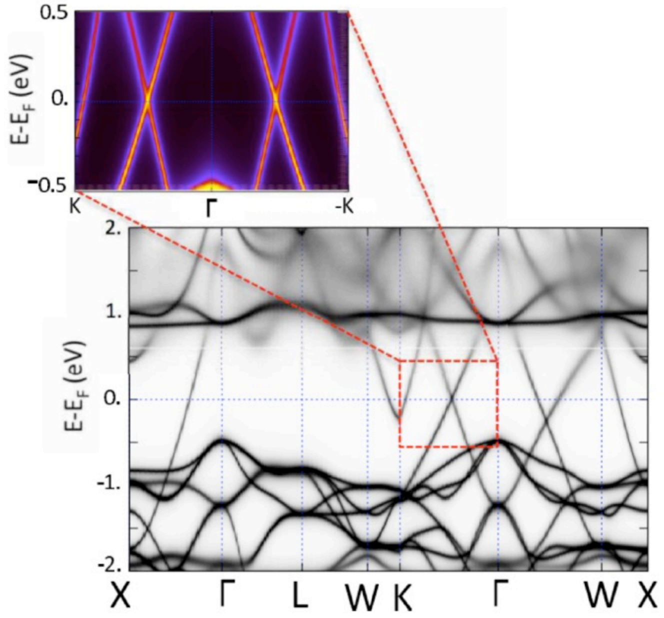




Kandpal et al., J. Phys. **D 40** (2007) 1507.
Balke *et al.* Solid State Com. **150** (2010) 529
Kübler *et al.*, Phys. Rev. B **76** (2007) 024414

Weyl semimetals in Heusler compounds



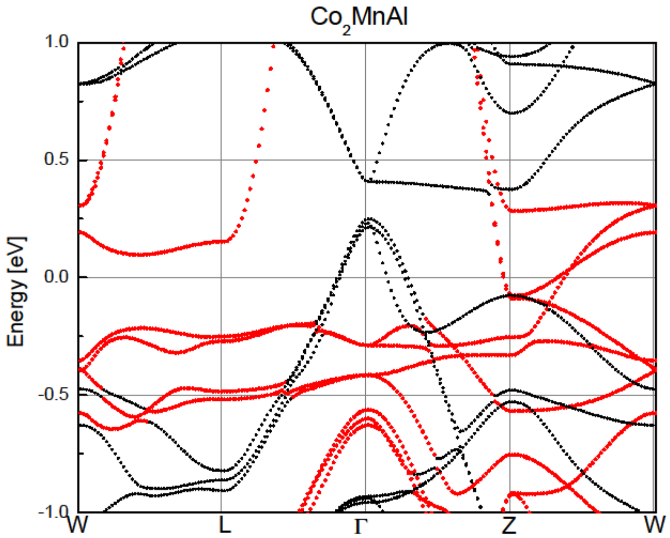


Zhijun Wang, et al., arXiv:1603.00479
Guoqing Chang et al., arXiv:1603.01255

Giant AHE in Co_2MnAl

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

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



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

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 Felser[2]

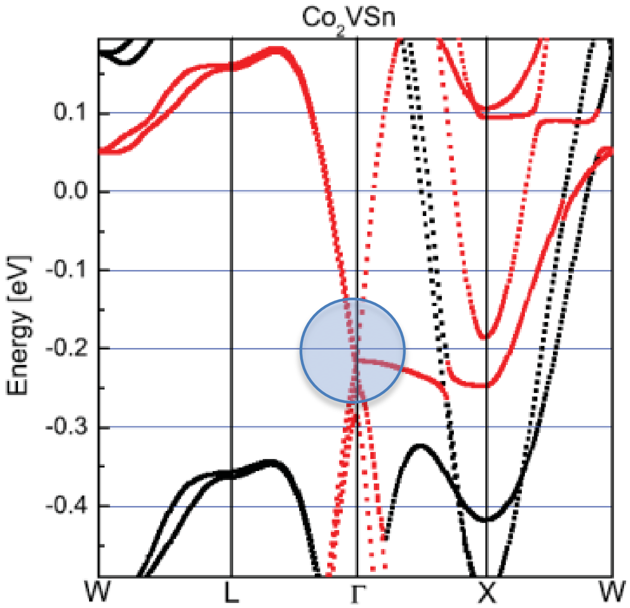
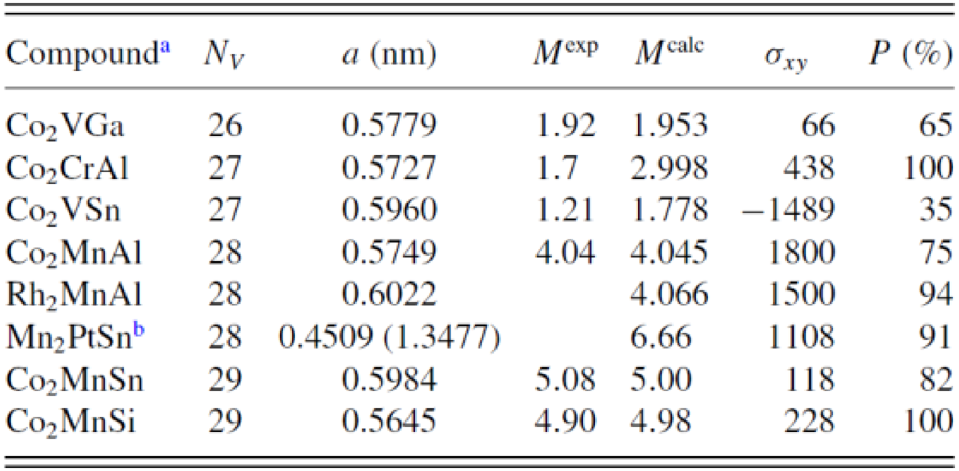


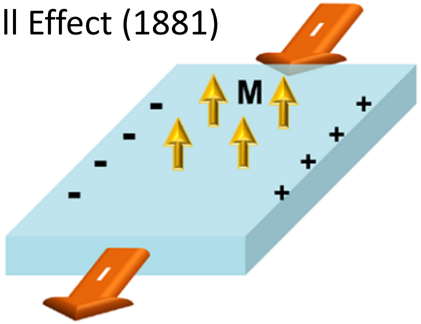
FIG. 4. (Color online) Band structure near the Fermi edge of Co_2VSn. Majority-spin electron states appear in red, minority-spin states in black. Note the Dirac cone at the Γ point at about −0.22 eV.



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

Anomalous Hall Effect (1881)



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

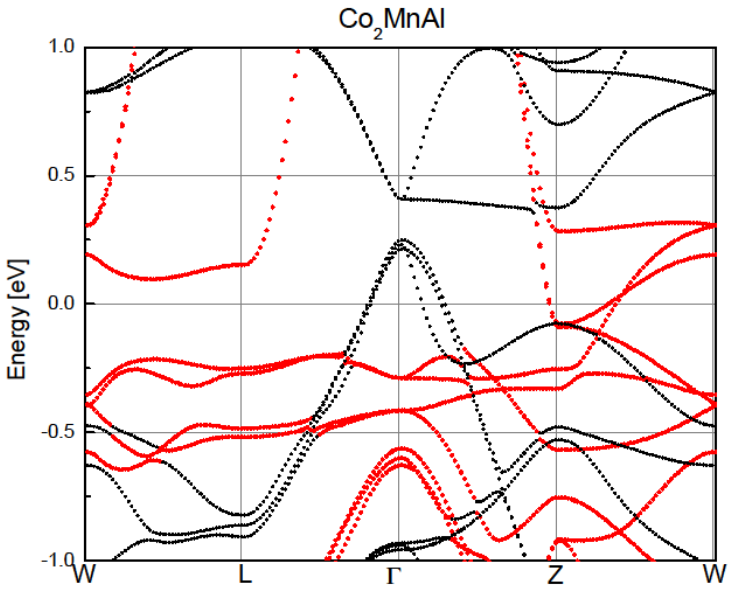
No M dependence – Berry curvature

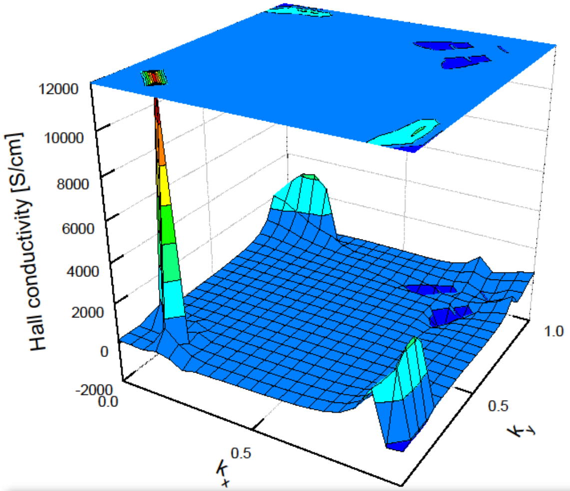
AHE in half metallic ferromagnets

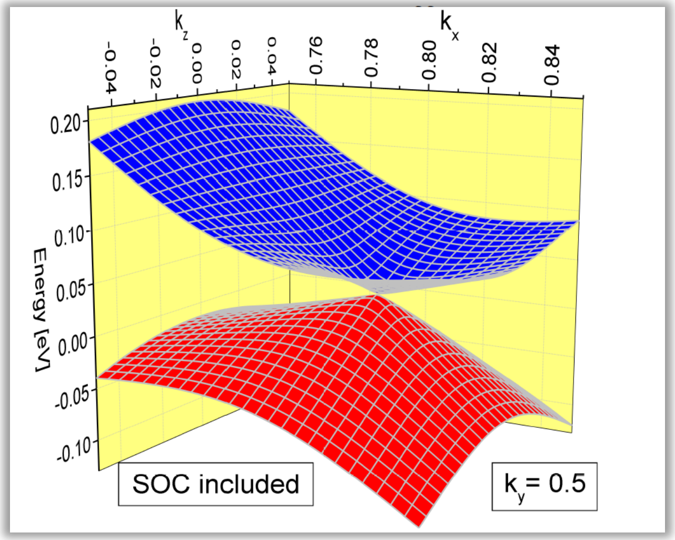
Giant AHE in Co_2MnAl

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

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



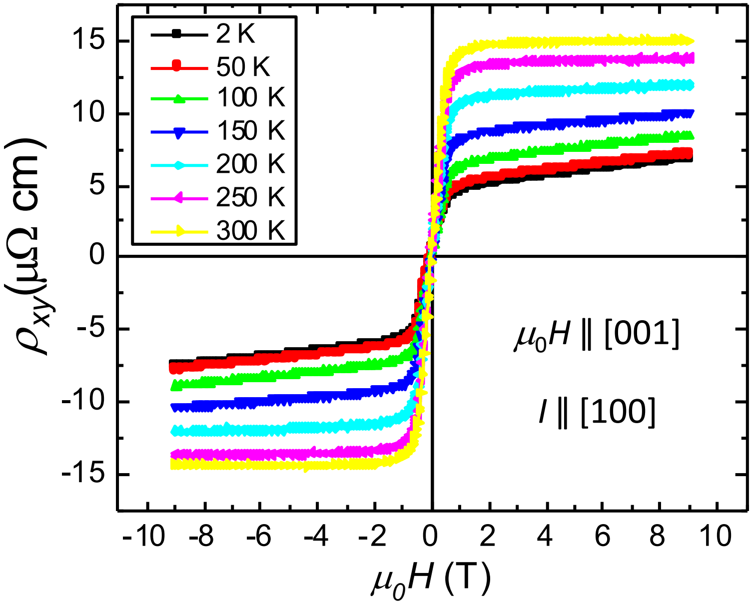


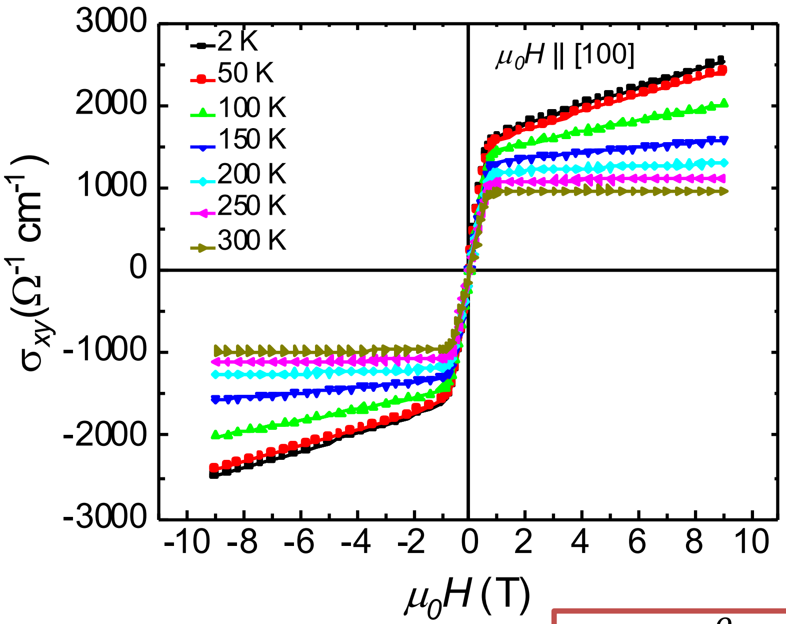


Weyl points are the origin for a large Berry phase and a Giant AHE

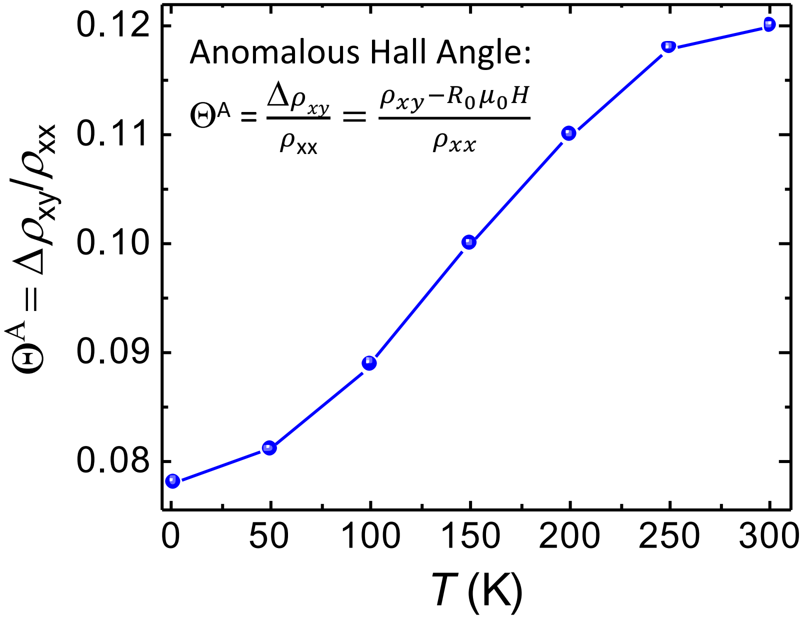
Kübler, Felser, PRB 85 (2012) 012405
Vidal et al. APL. 99 (2011) 132509
Kübler, Felser, EPL 114 (2016) 47005.

Co_2MnGa Hall Measurement





$$\sigma_{xy} = \frac{\rho_{yx}}{\rho_{xx}^2 + \rho_{xy}^2}$$

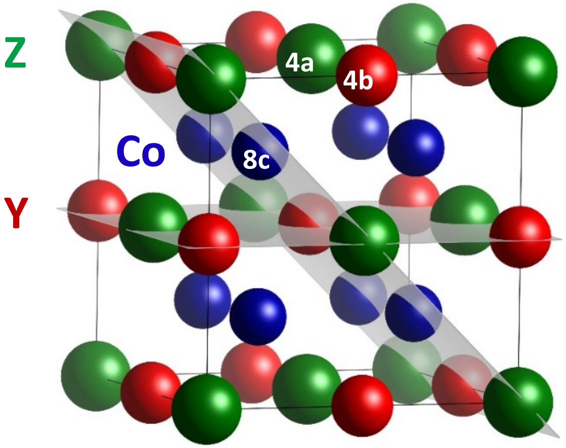


- Anomalous Hall conductivity:

  $|\sigma_{xy}|_{max}$ ~ 1590 Ω^{-1} cm $^{-1}$ at 2 K.
- Carrier concentration (2 K): 2.3×10^{21} cm^{-3}
- Anomalous Hall Angle upto 12% at RT

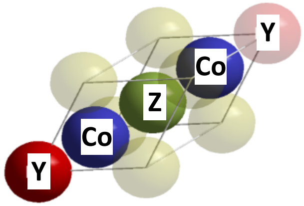
Kaustuv Manna et al.,, arXiv:1712.10174

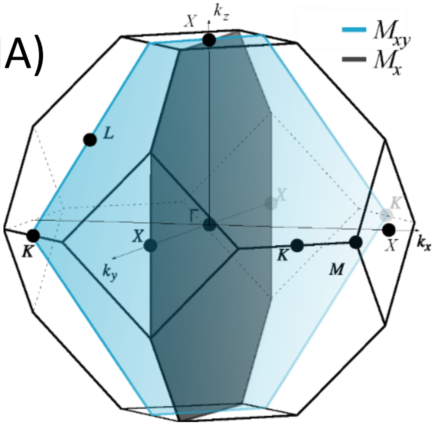
Weyl Fermion in Regular Heusler

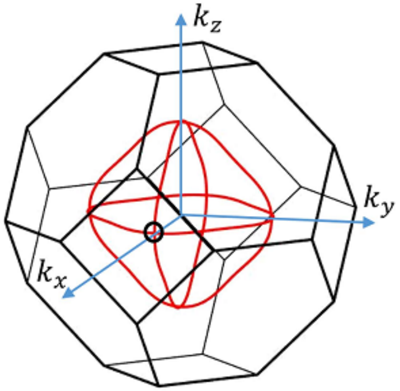


Co_2YZ (Y = IVB or VB; Z = IVA or IIIA)

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



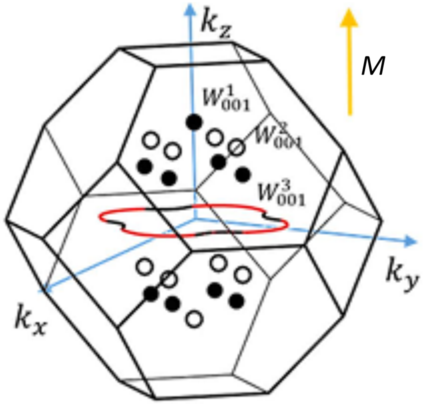




Without SOC

With SOC

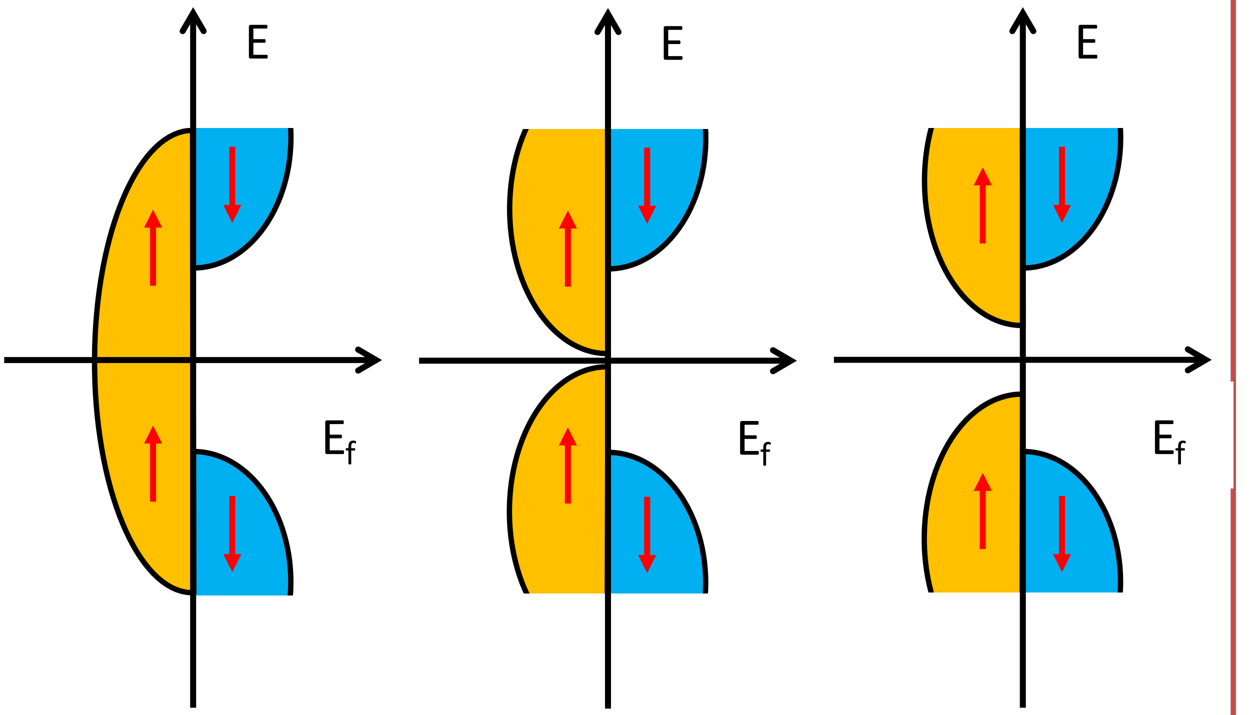
Symmetry and electronic structures depend on the magnetization direction



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

Kaustuv Manna et al.,, arXiv:1712.10174

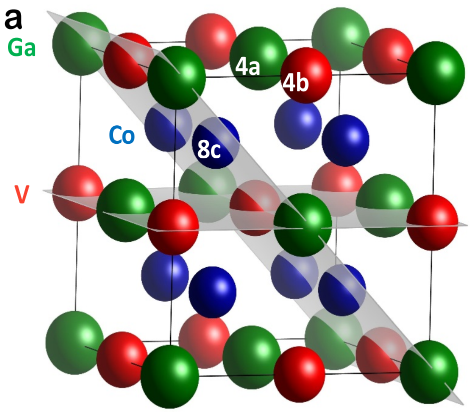


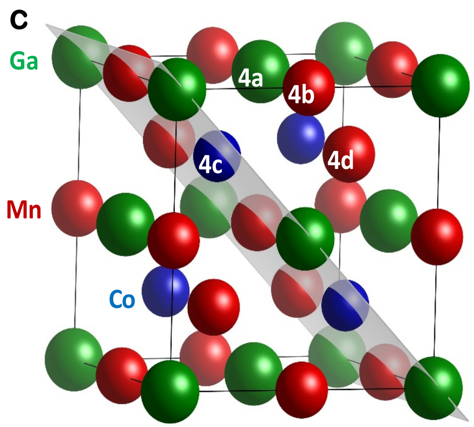
Half-metal

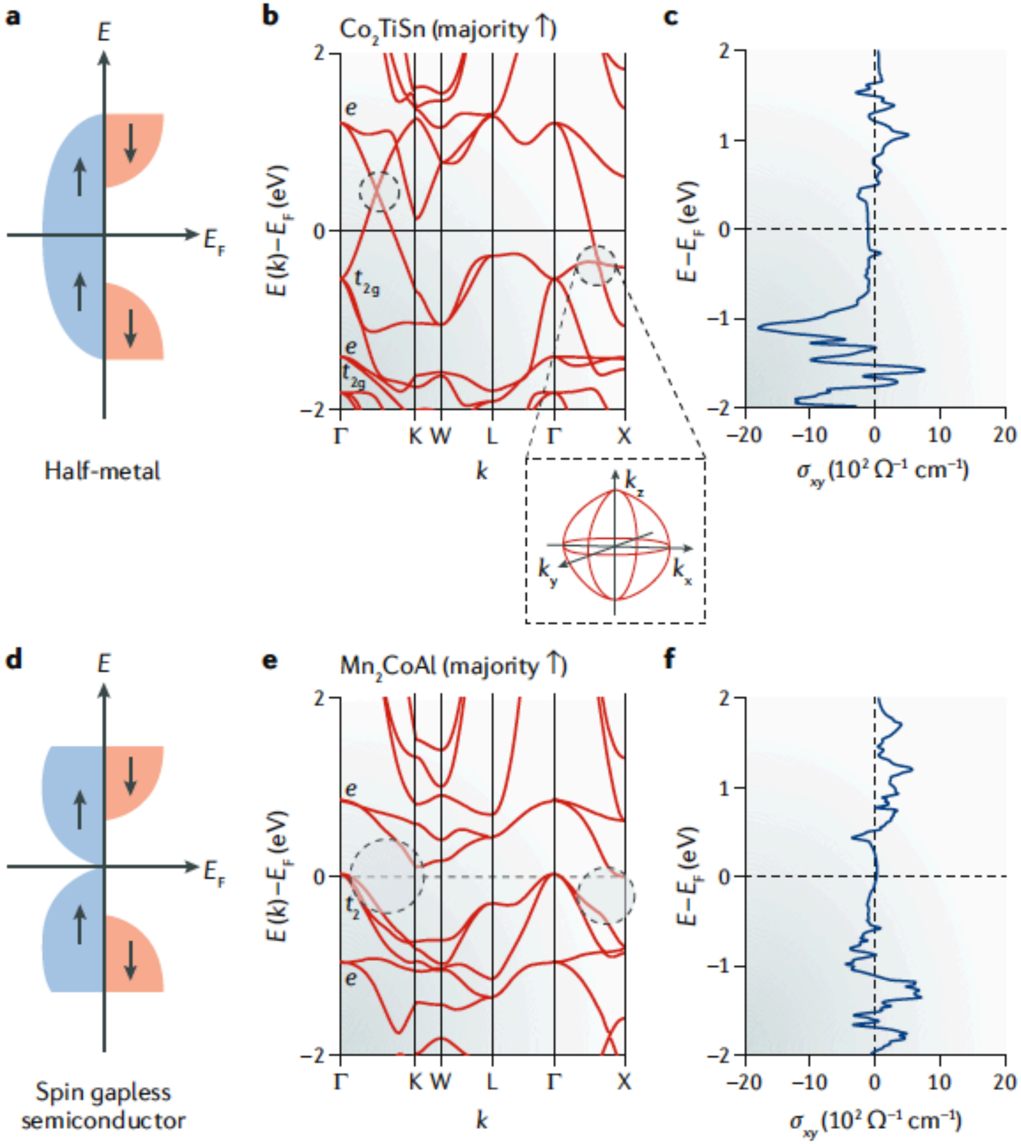
Spin-gapless Semiconductor

Magnetic Semiconductor

Spingapless semiconductors and Weyl semimetals





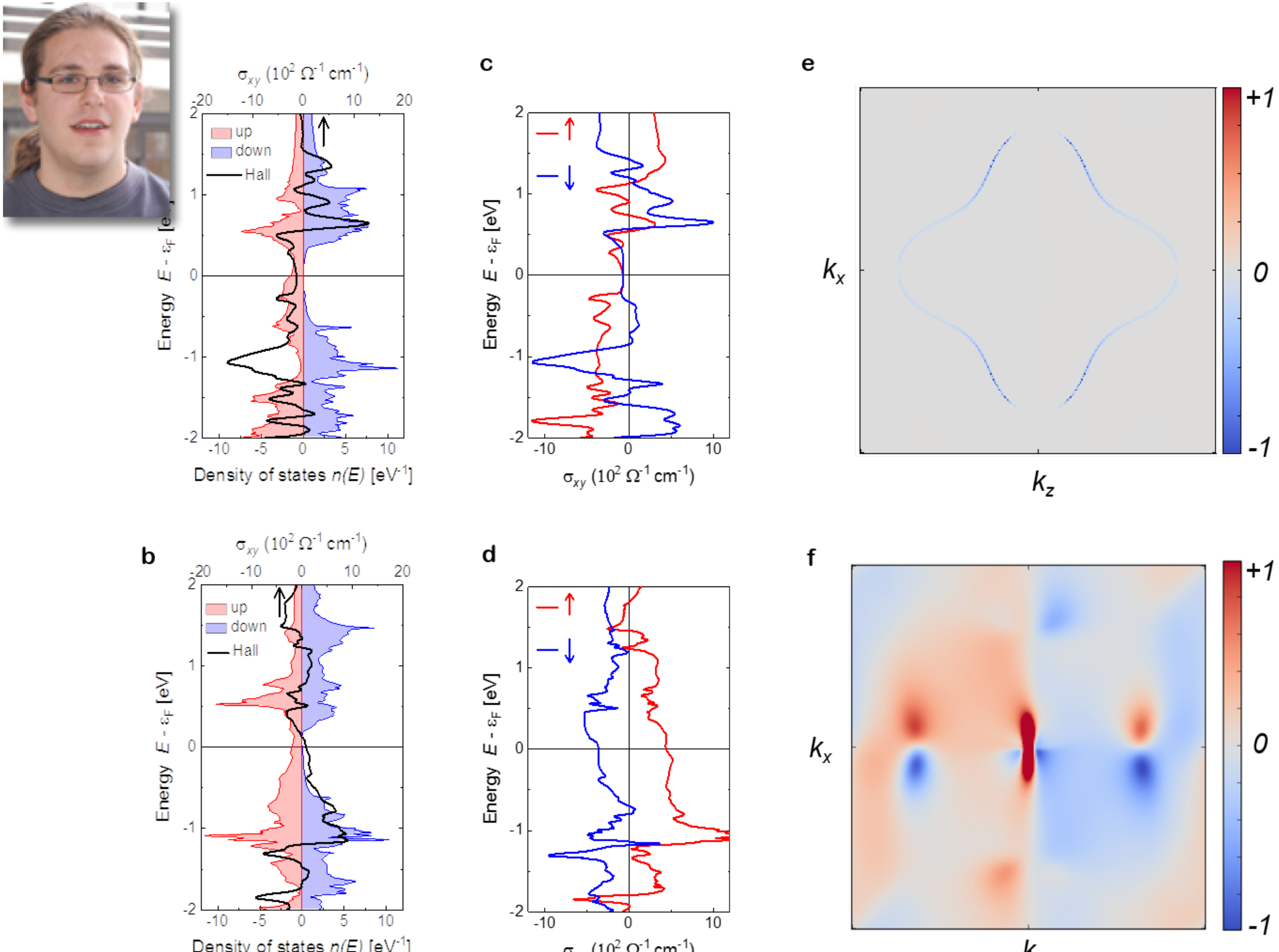


S. Ouardi, G. H. Fecher, J. Kübler, and C. Felser, Physical Review Letter 110 (2013) 100401

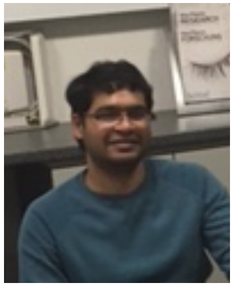
K. Manna et al.,, arXiv:1712.10174

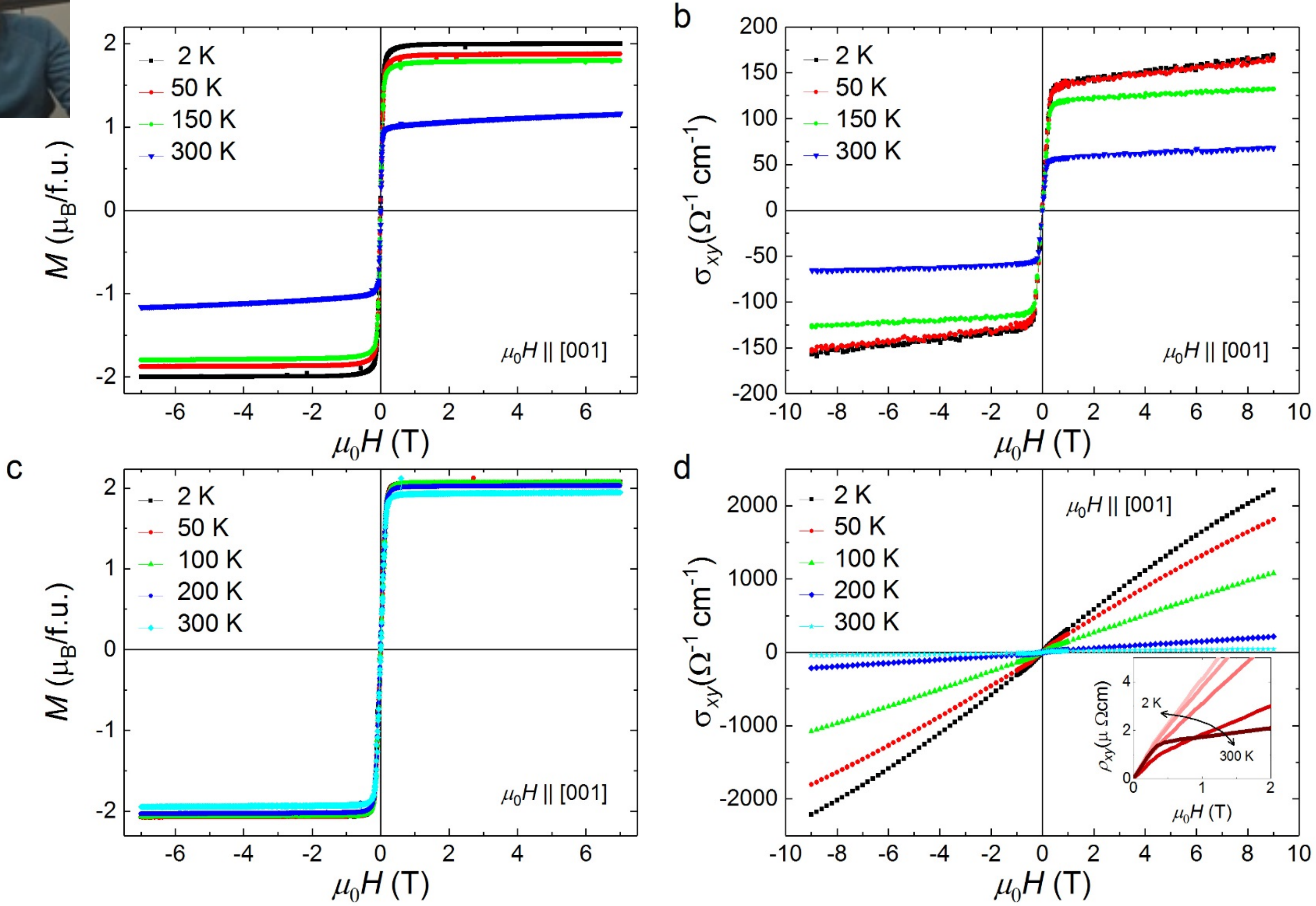
K. Manna et al., Nature Materials Review, in press, arXiv:1802.02838v1

Berry Curvature



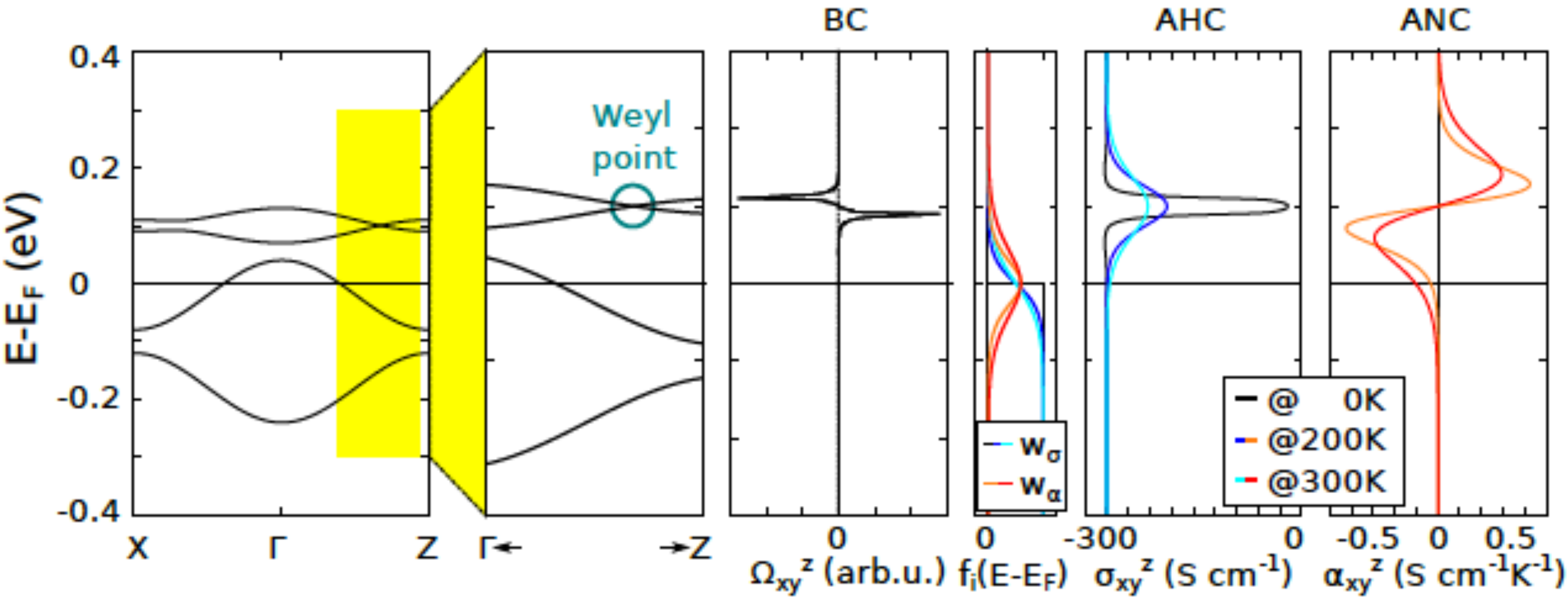
Kaustuv Manna et al.,, arXiv:1712.10174





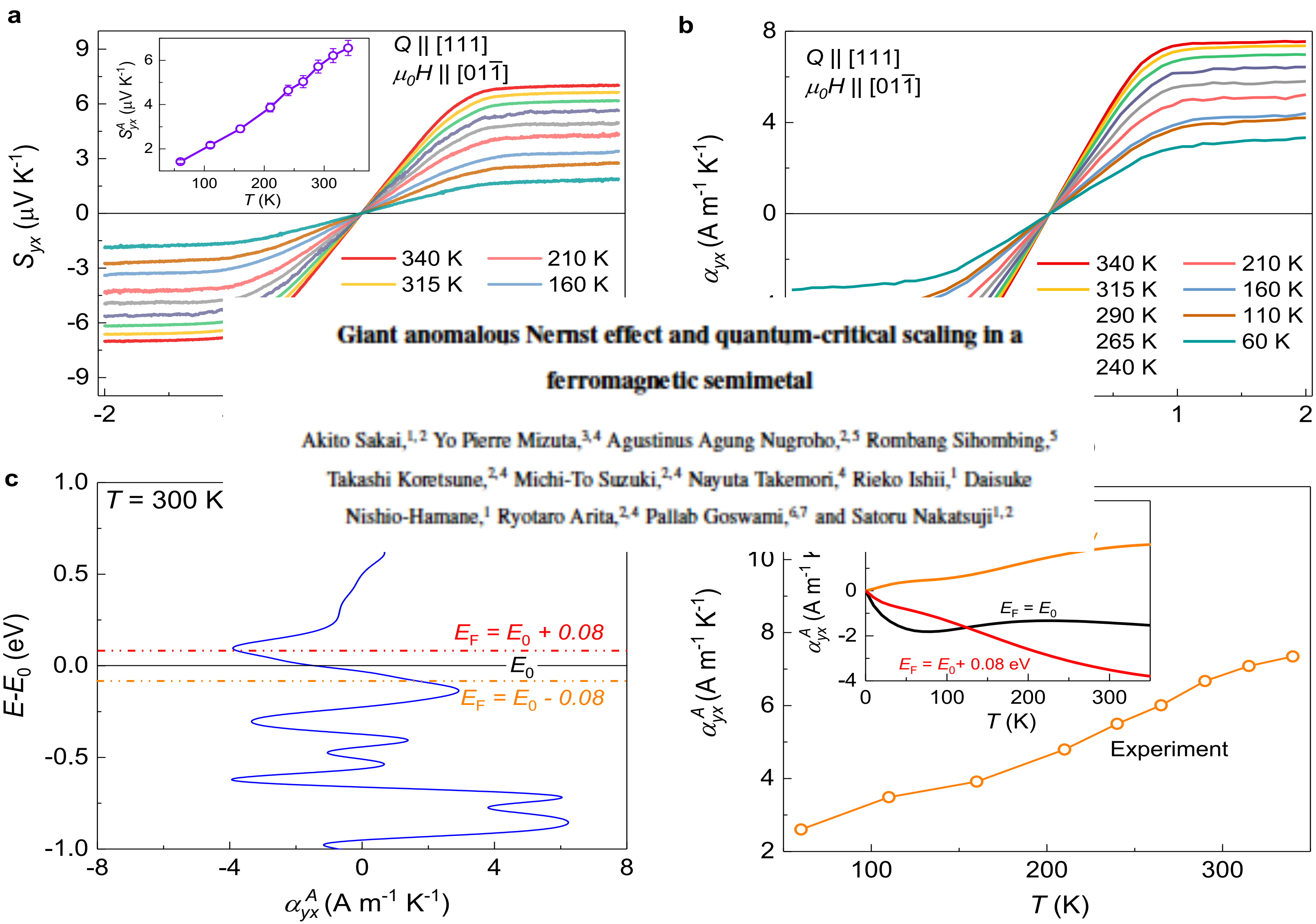
Kaustuv Manna et al.,, arXiv:1712.10174

Co_2MnGa Anomalous Nernst



Jonathan Noky et al., submitted

Co$_2$MnGa Anomalous Nernst

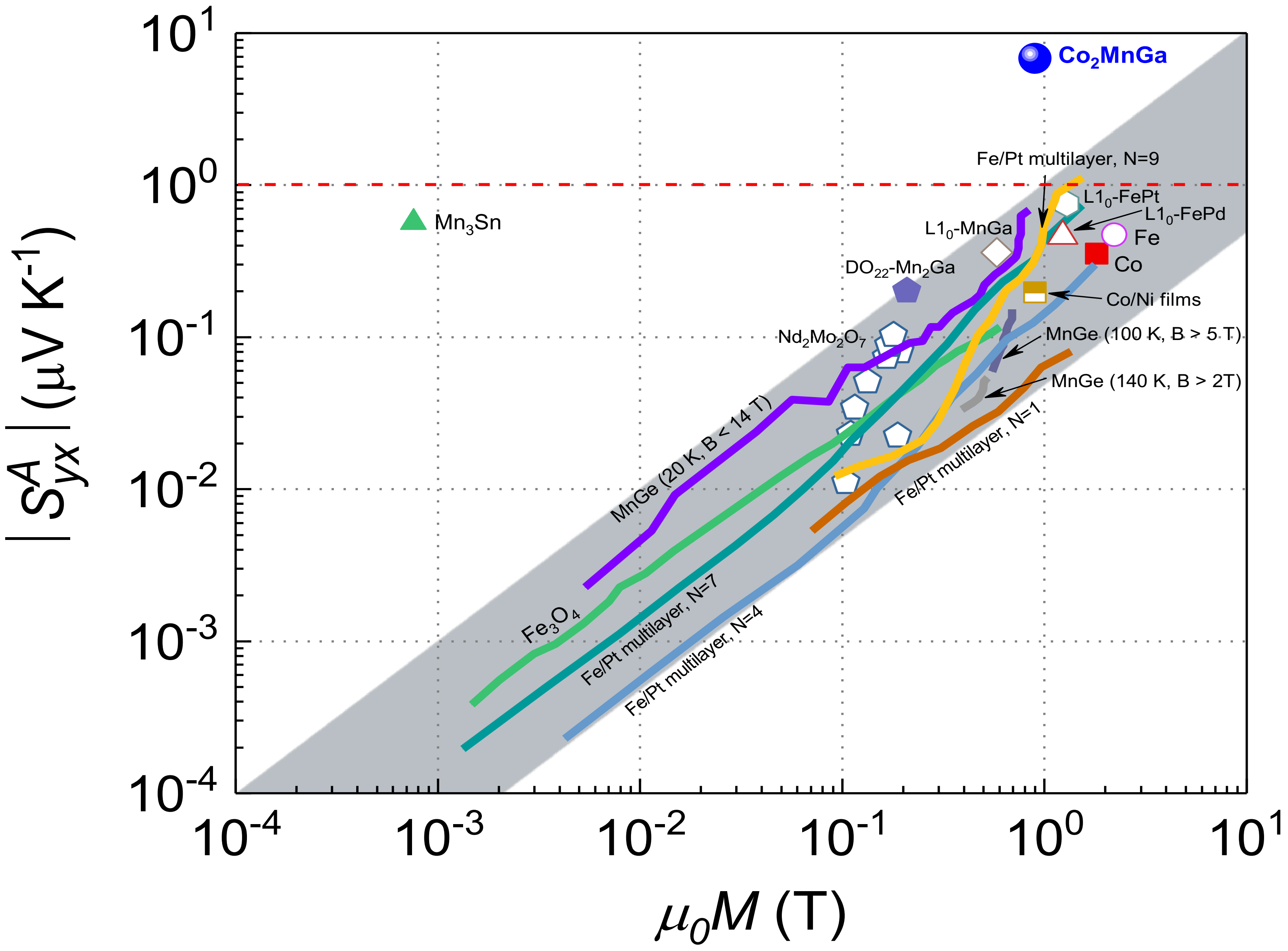


Giant anomalous Nernst effect and quantum-critical scaling in a ferromagnetic semimetal

Akito Sakai,[1,2] Yo Pierre Mizuta,[3,4] Agustinus Agung Nugroho,[2,5] Rombang Sihombing,[5] Takashi Koretsune,[2,4] Michi-To Suzuki,[2,4] Nayuta Takemori,[4] Rieko Ishii,[1] Daisuke Nishio-Hamane,[1] Ryotaro Arita,[2,4] Pallab Goswami,[6,7] and Satoru Nakatsuji[1,2]

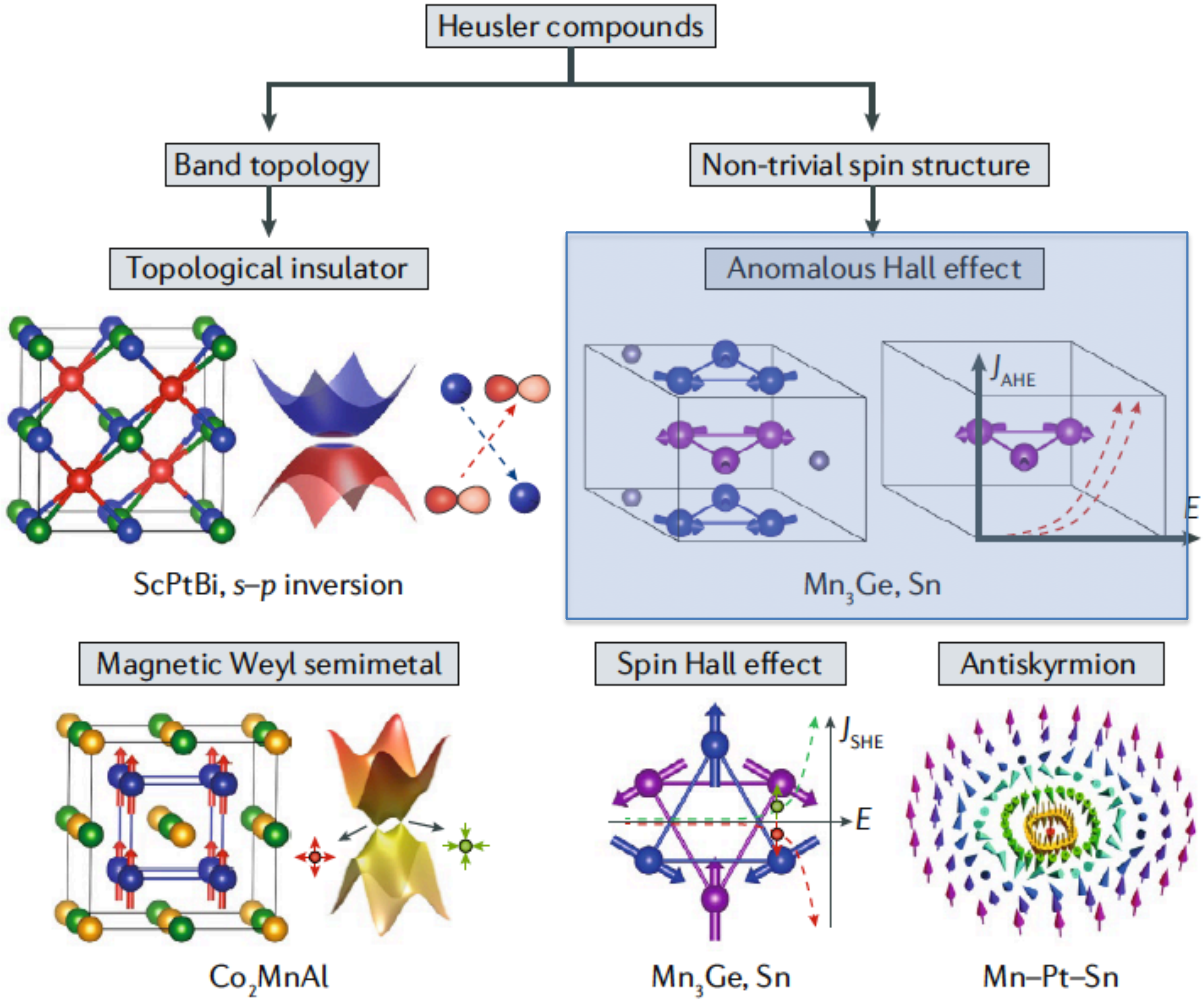
Satya N. Guin, et al., arXiv:1806.06753

Co_2MnGa Anomalous Nernst



Satya N. Guin, arXiv:1806.06753
Jonathan Noky et al., submitted

Magnetism and Topology



Heusler compounds

Band topology

Non-trivial spin structure

Topological insulator

ScPtBi, *s*–*p* inversion

Anomalous Hall effect

Mn$_3$Ge, Sn

Magnetic Weyl semimetal

Co$_2$MnAl

Spin Hall effect

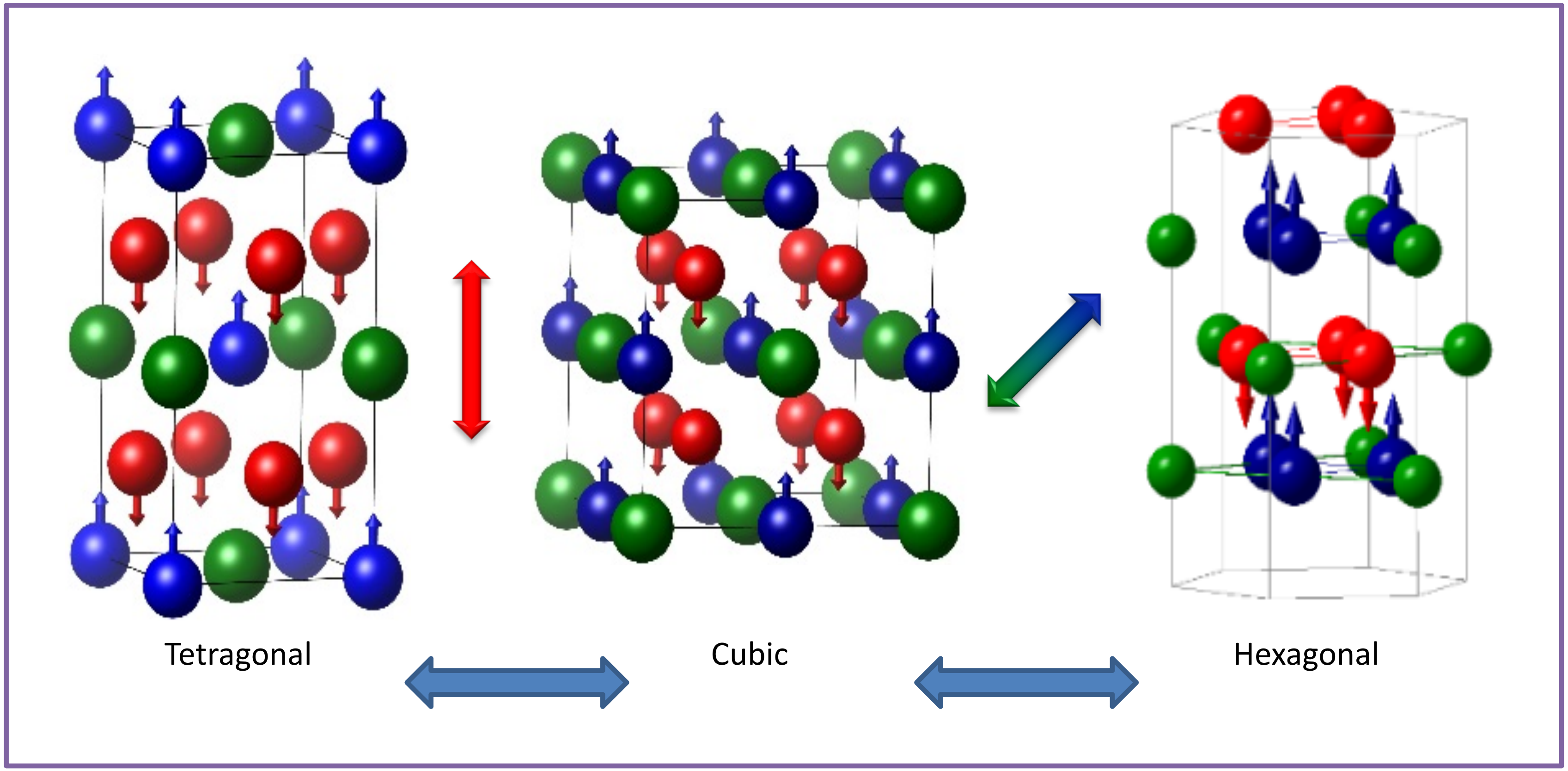
Mn$_3$Ge, Sn

Antiskyrmion

Mn–Pt–Sn

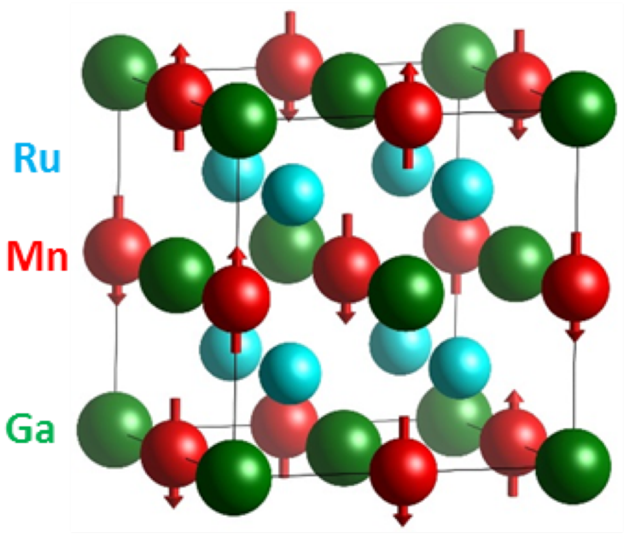
Kaustuv Manna et al., Nature Materials Review, in press, arXiv:1802.02838v1

Tuning the crystal anisotropy

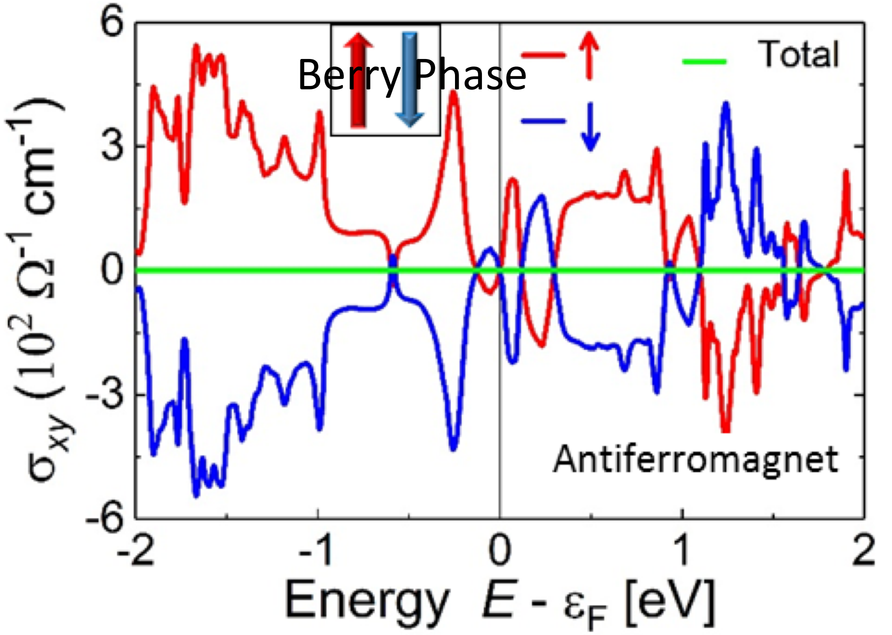


Mn_3Ga Mn_3Ge Mn_3Sn

No AHE in Antiferromagnets



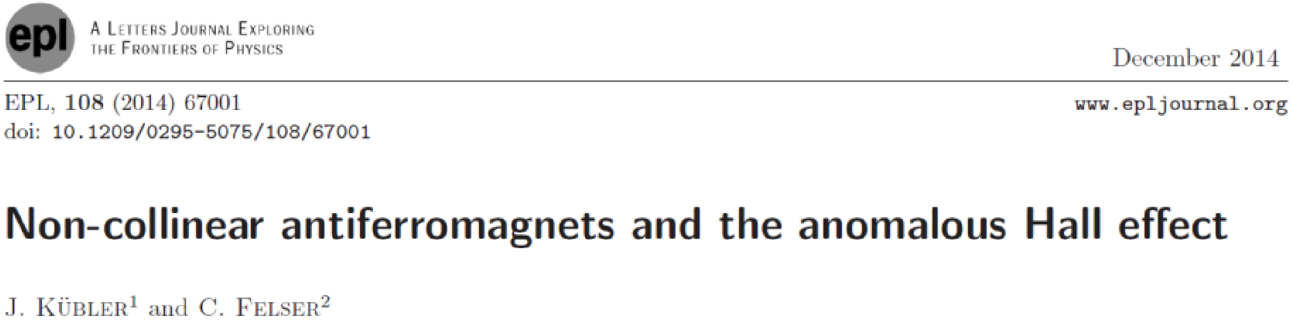
[Ru_2MnSi]



$$\rho_H = R_0 B + \boxed{4\pi R_s\, M}$$

No ! – No Berry phase

Hexagonal Antiferromagnet



A Letters Journal Exploring
the Frontiers of Physics

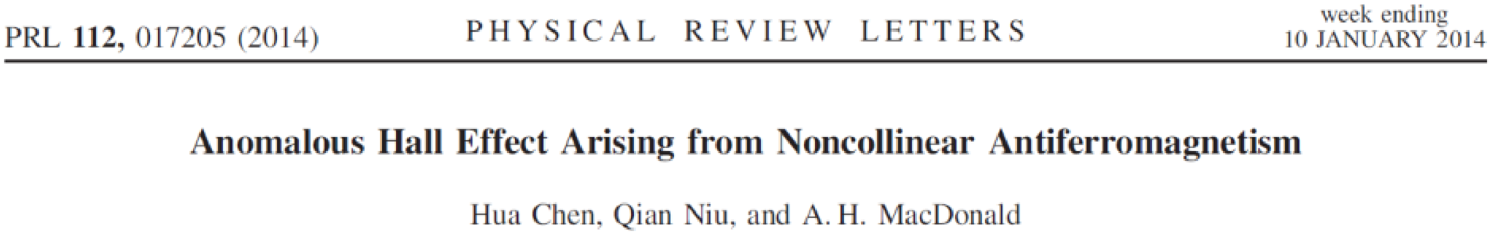
December 2014

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

www.epljournal.org

Non-collinear antiferromagnets and the anomalous Hall effect

J. Kübler[1] and C. Felser[2]



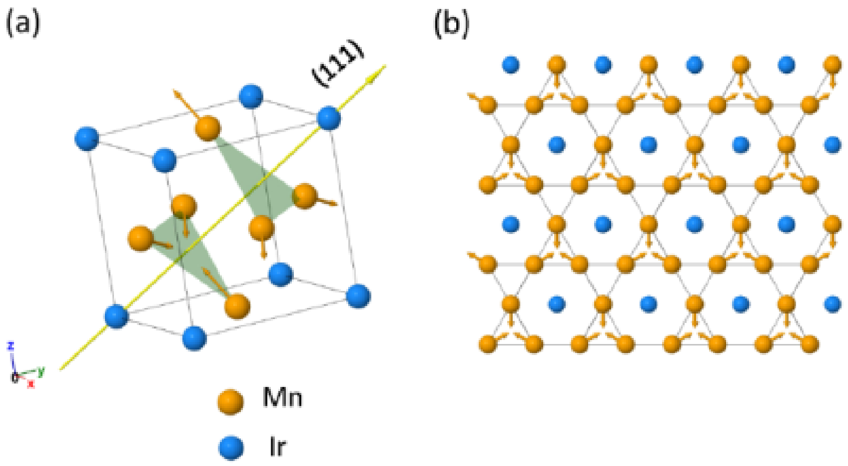
PRL **112,** 017205 (2014)

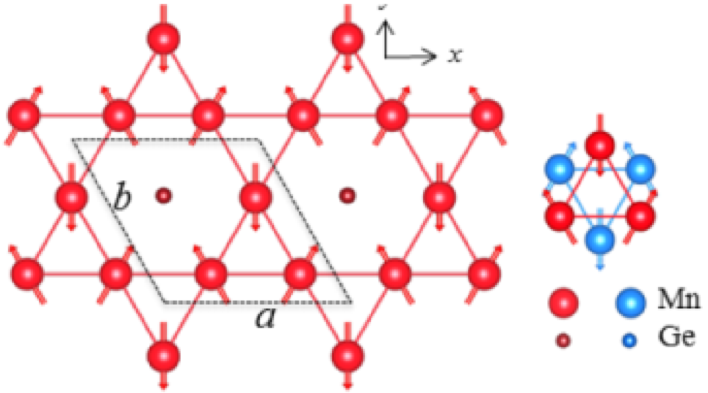
PHYSICAL REVIEW LETTERS

week ending
10 JANUARY 2014

Anomalous Hall Effect Arising from Noncollinear Antiferromagnetism

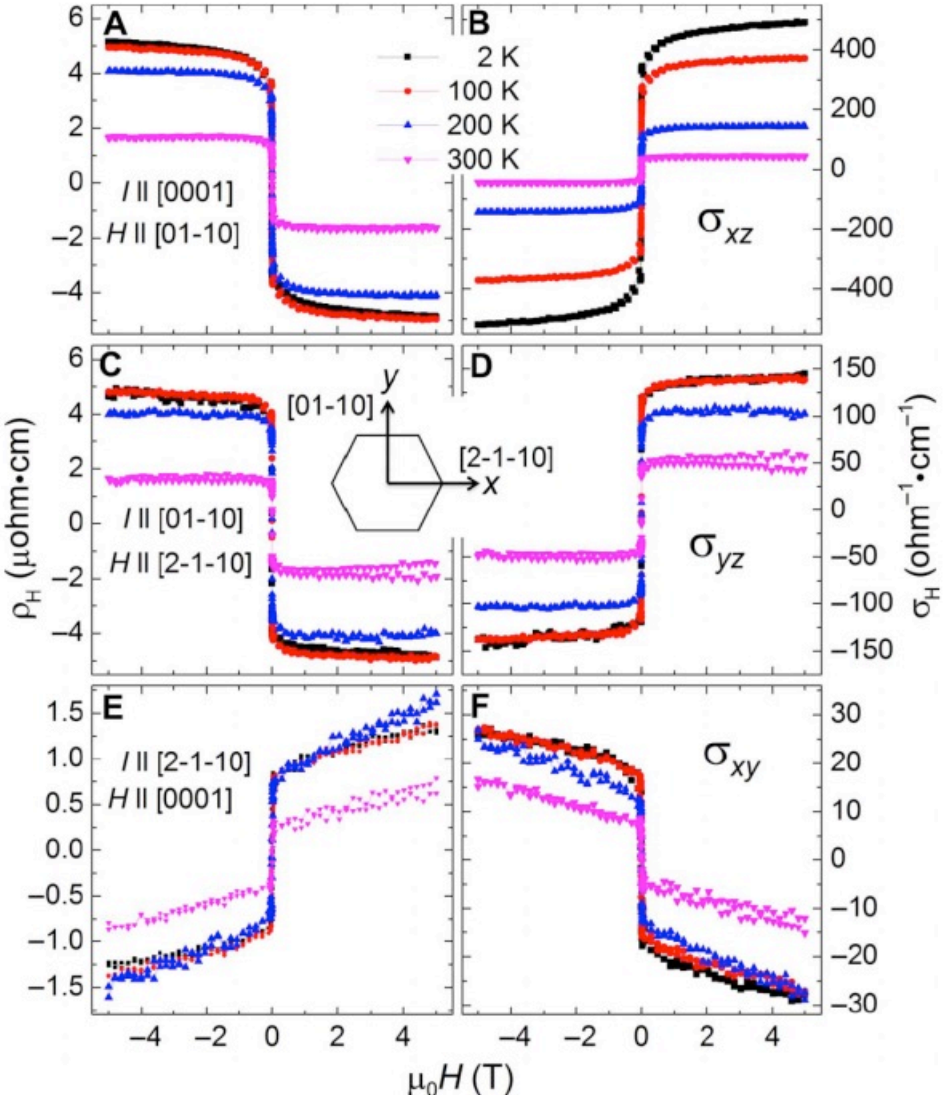
Hua Chen, Qian Niu, and A. H. MacDonald





Chen, Niu, and MacDonald, Phys. Rev. Lett., 112 (2014) 017205
Kübler and Felser EPL 108 (2014) 67001

Non-collinear AFM Mn_3Ge/Mn_3Sn



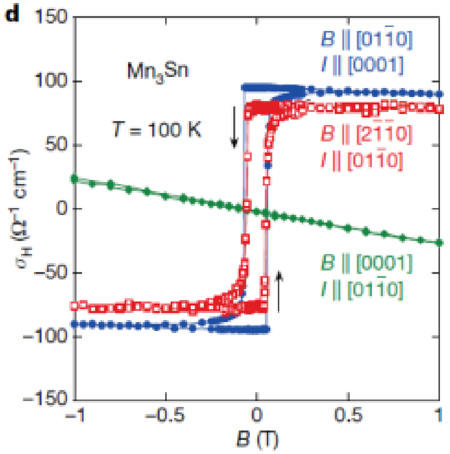
LETTER

doi:10.1038/nature15723

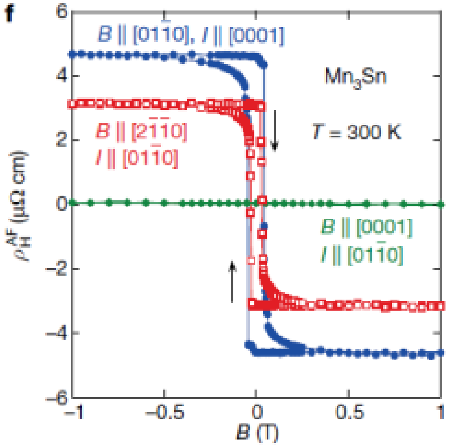
Large anomalous Hall effect in a non-collinear antiferromagnet at room temperature

Satoru Nakatsuji[1,2], Naoki Kiyohara[1] & Tomoya Higo[1]

d



f

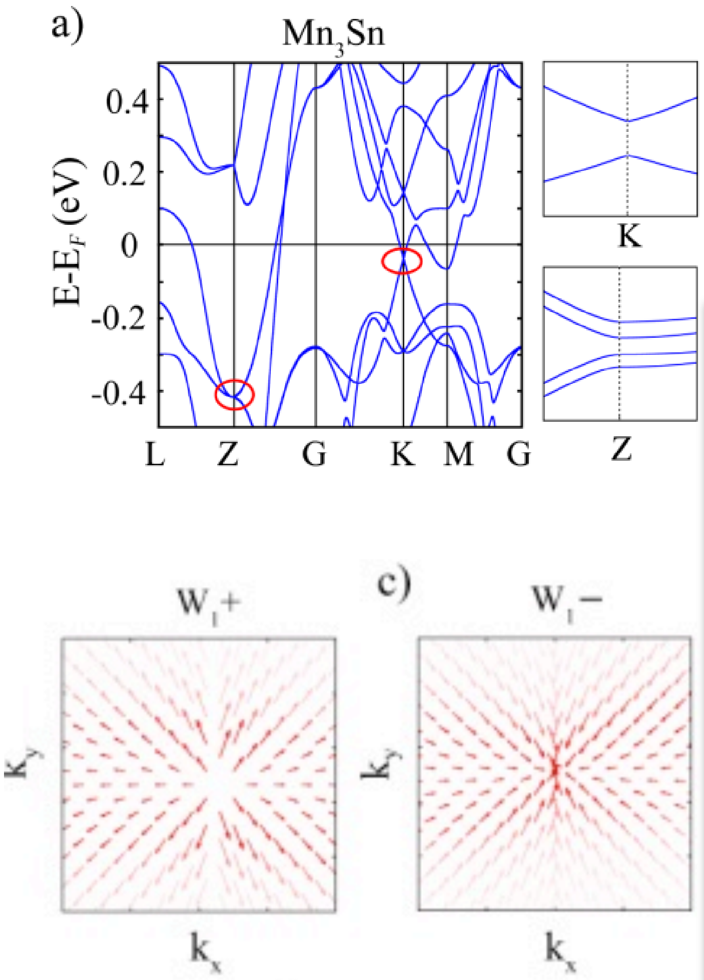


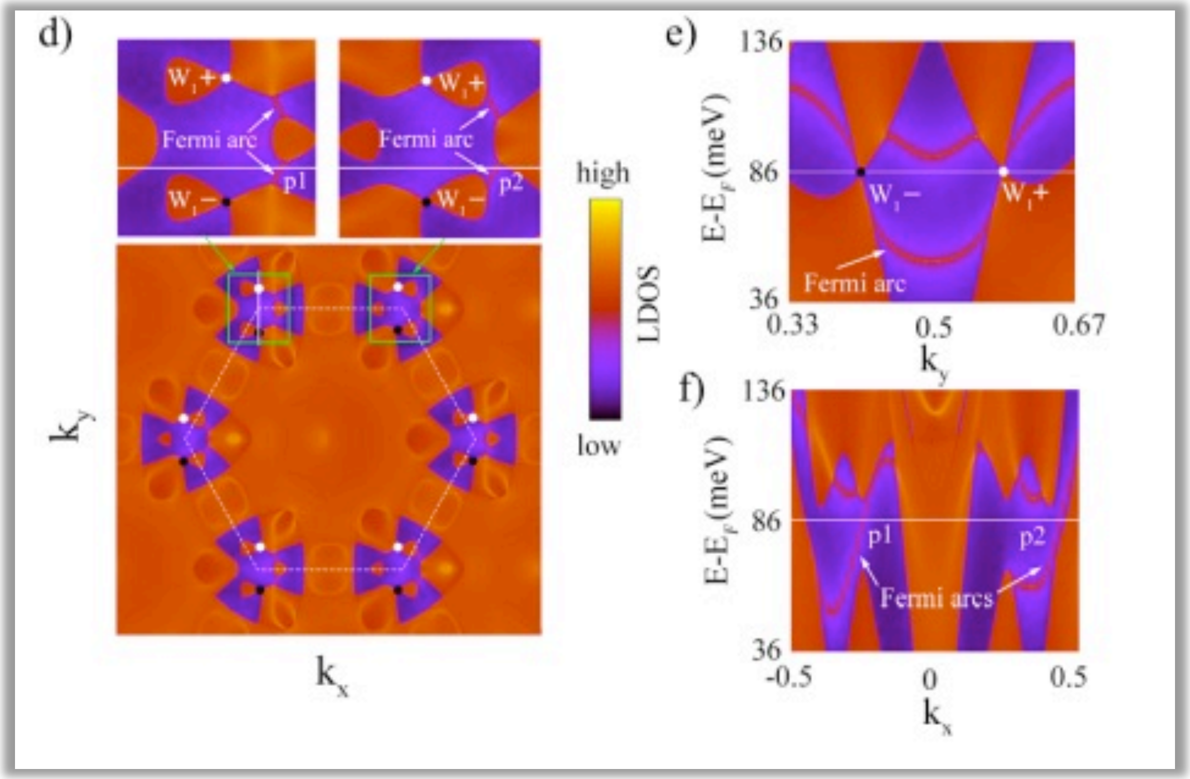
Nayak et al. preprint: arXiv:1511.03128, Science Advances 2 (2016) e1501870

Kiyohara, Nakatsuji, preprint: arXiv:1511.04619,

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

Fermiarcs in the Weyl AFM





Hao Yang, et al. , New J. Phys. 19 (2017) 015008: arXiv:1608.03404

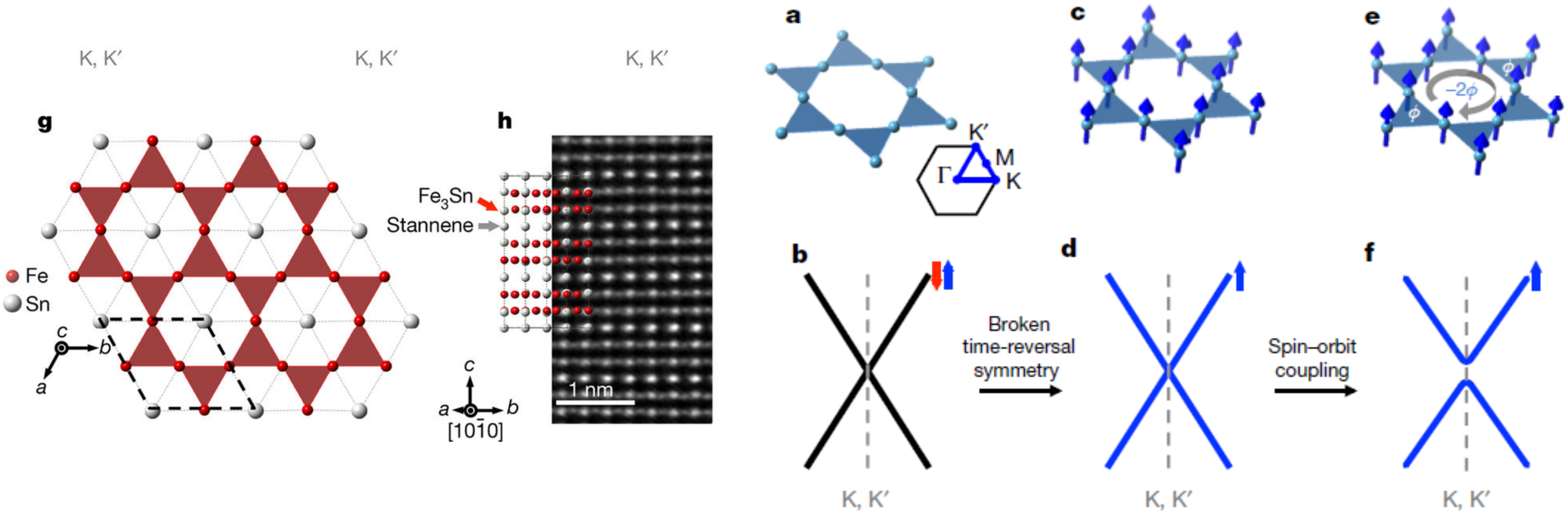
Quantum topological states on Kagome lattice

LETTER

doi:10.1038/nature25987

Massive Dirac fermions in a ferromagnetic kagome metal

Fe_3Sn_2

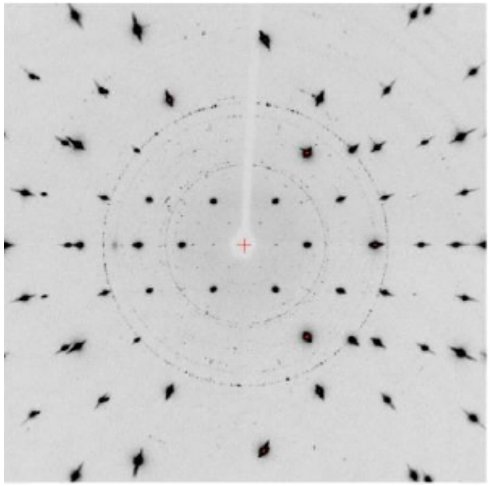


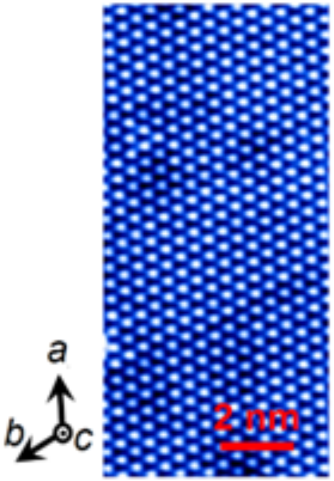
Looking for Weyl fermions on a ferromagnetic Kagomé lattice with out of plane magnetisation.

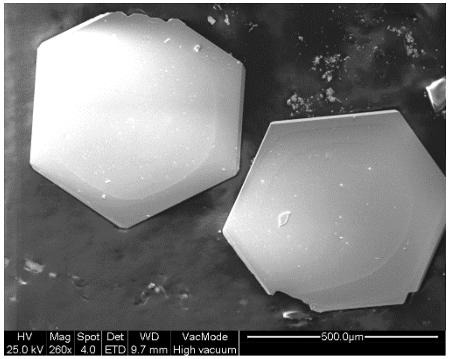
Nature, 2018, doi:10.1038/nature25987

Single crystal growth: $Co_3Sn_2S_2$

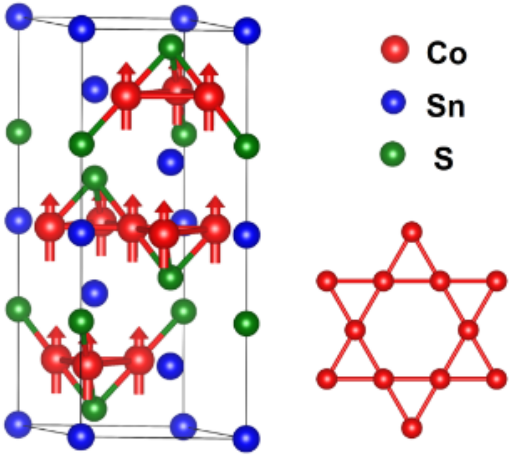
- Self-flux by congruent solidification
- Chemical Vapor Transport
- Bridgeman







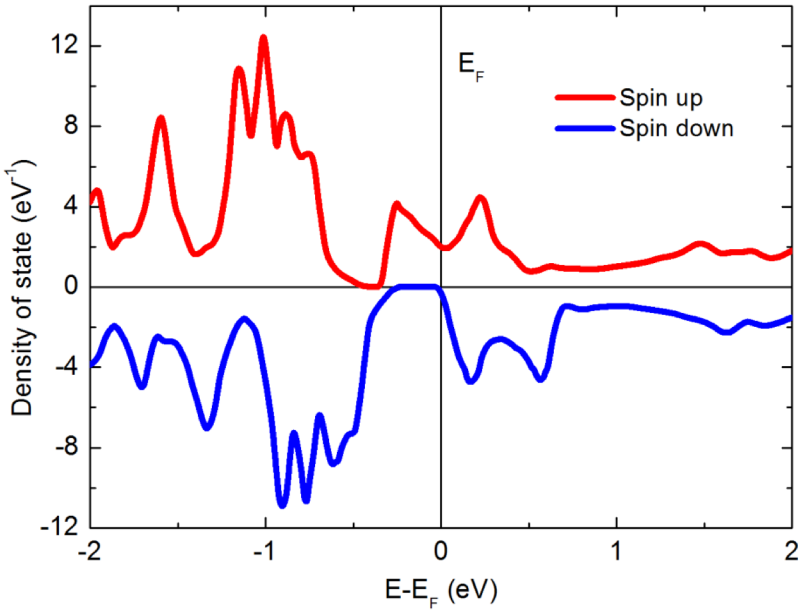
R -3 m: H
Unit cell dimensions
a = 5.3689(5) Å
c = 13.176(2) Å

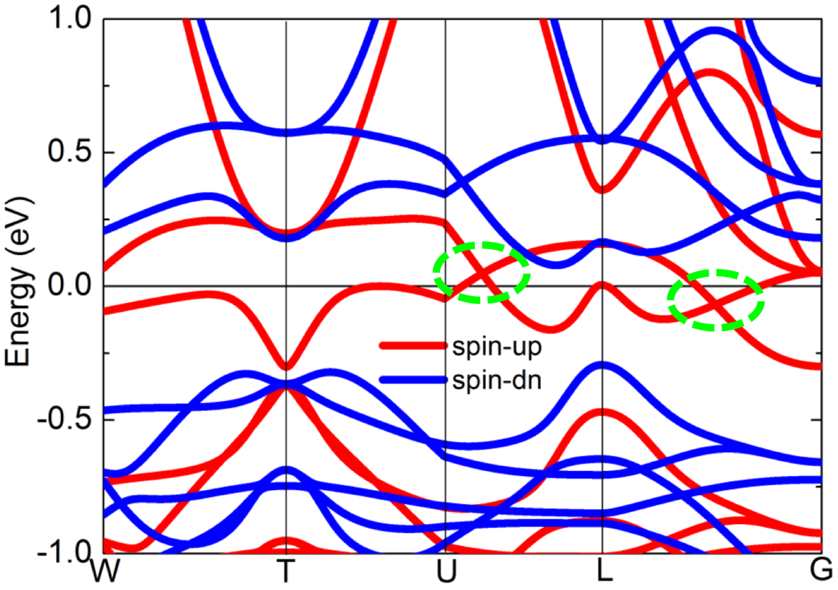


High-quality single crystals

Enke Liu, et al. Nature Physics accepted, preprint arXiv:1712.06722

Electron bands without SOC





spin-down channel insulating, gap 0.35 eV, spin-up channel metallic

Linear crossing around Fermi level

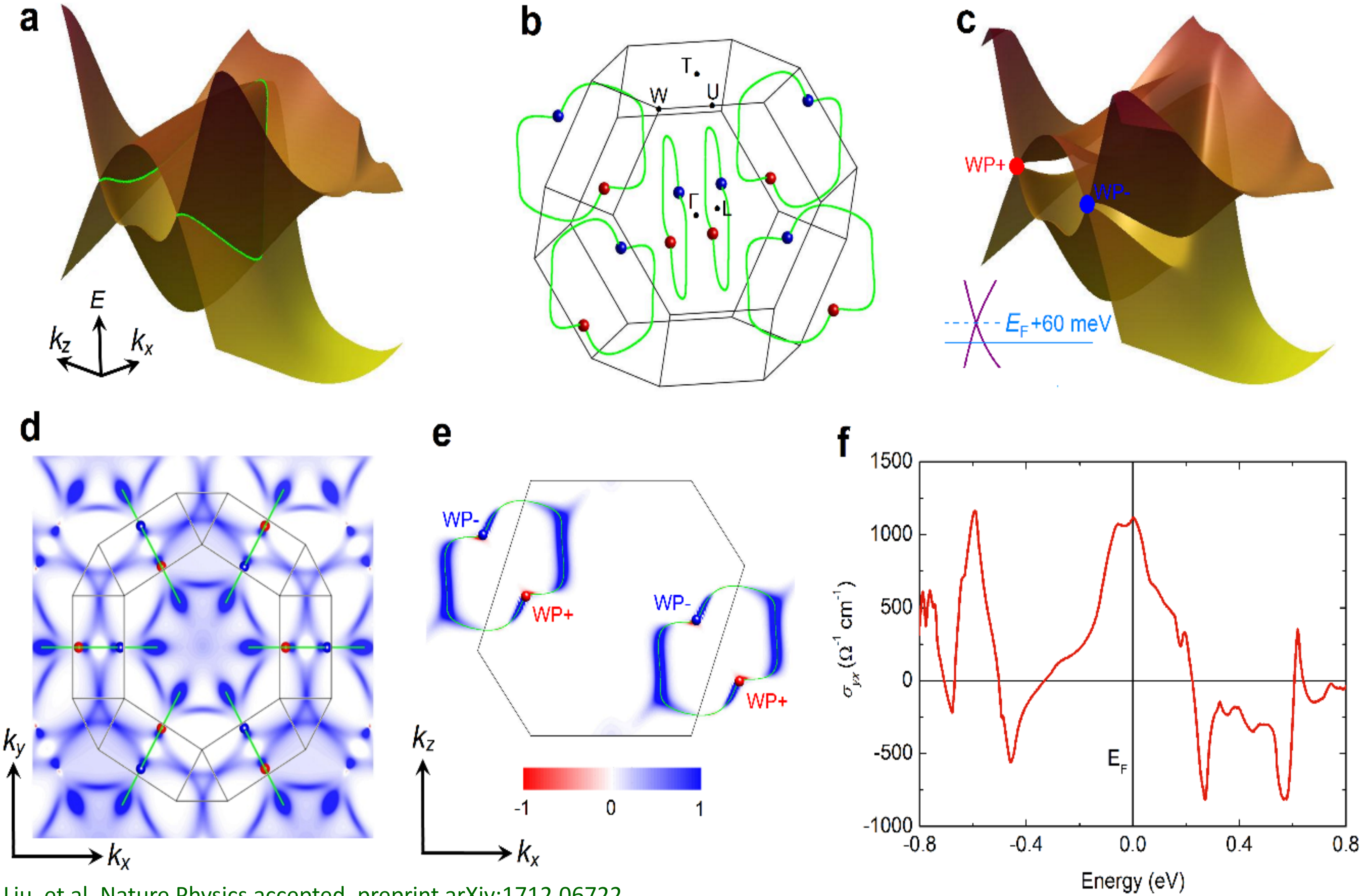
Possible Weyl nodes with SOC?

Calc.: m = 0.89 uB/fu,

Calc.: mCo = 0.30 uB/Co

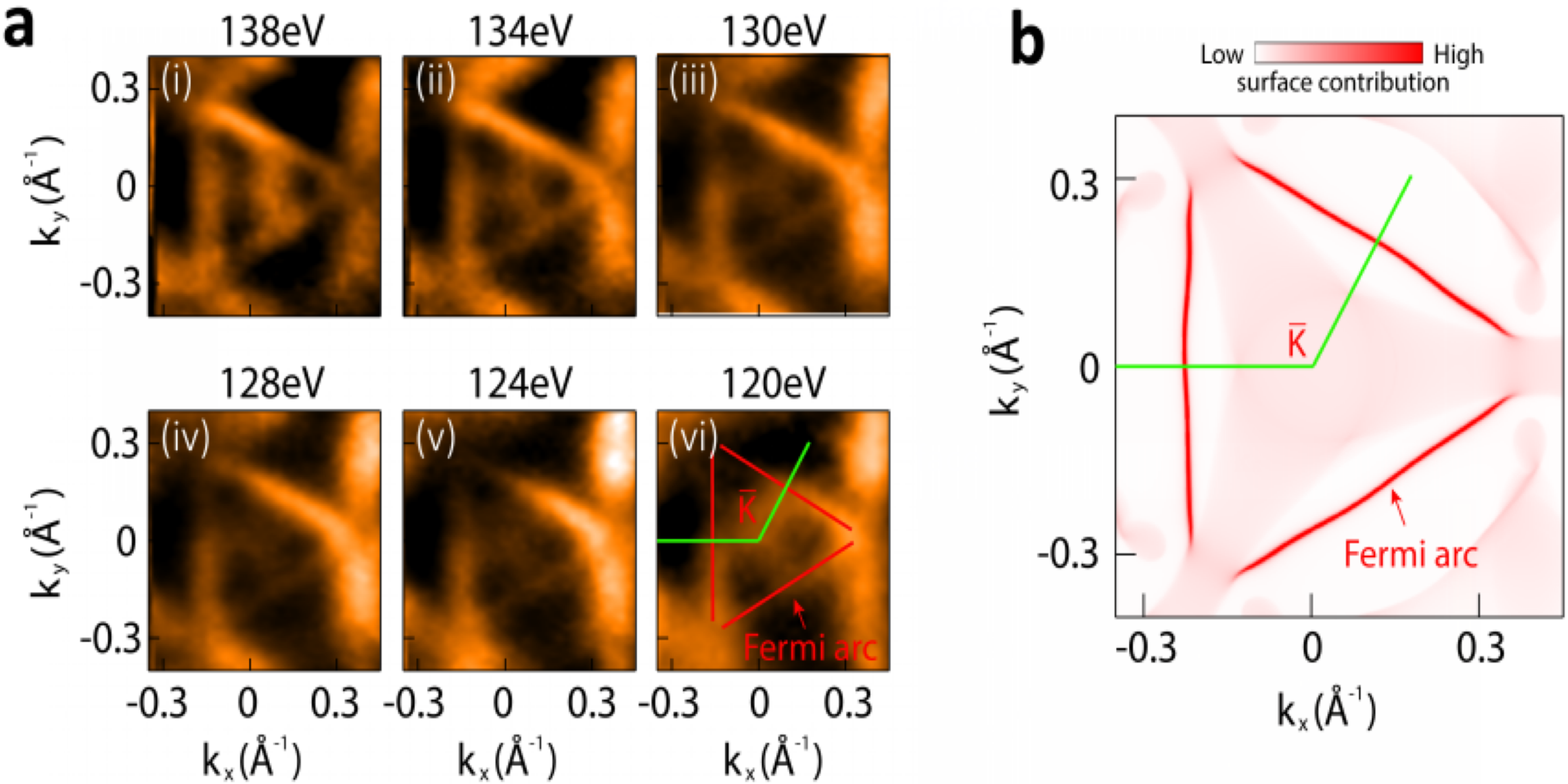
Enke Liu, et al. Nature Physics accepted, preprint arXiv:1712.06722

Prediction of a Weyl



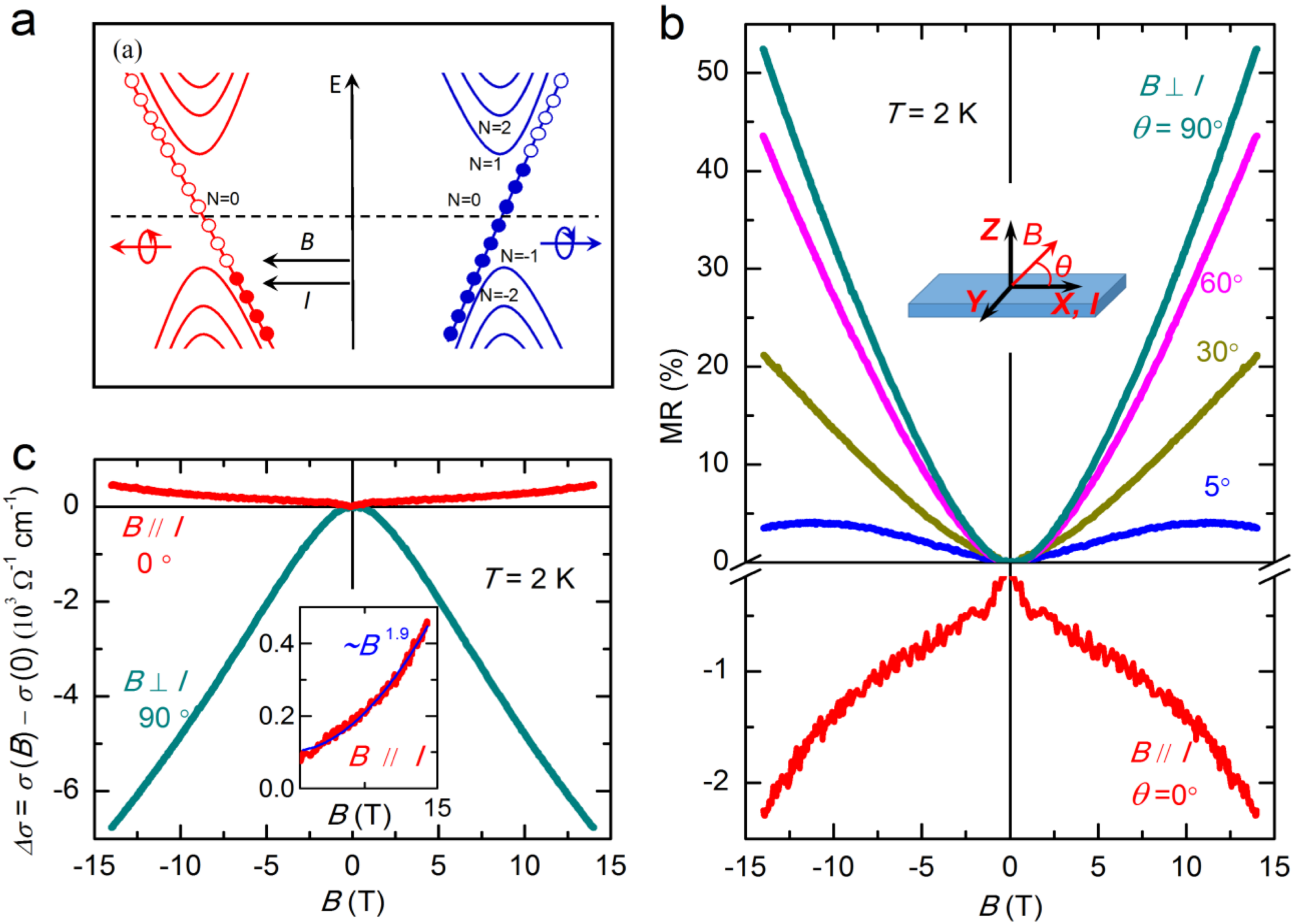
Enke Liu, et al. Nature Physics accepted, preprint arXiv:1712.06722

Fermiarcs



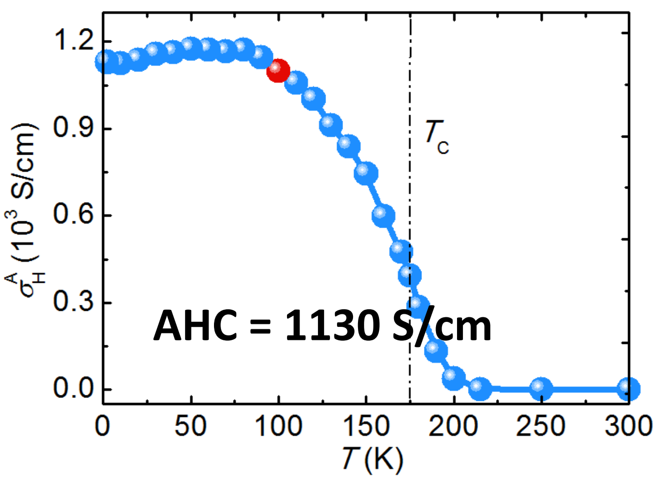
Qiunan Xu, Enke Liu, Yan Sun, arXiv:1801.00136

Chiral Anomaly

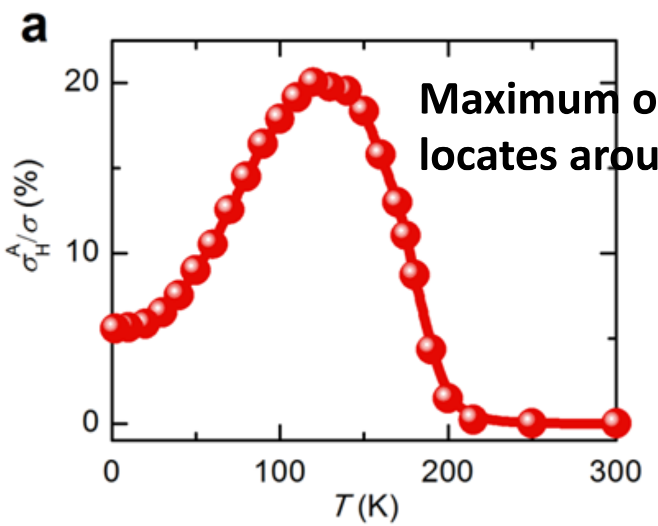


Enke Liu, et al. Nature Physics accepted, preprint arXiv:1712.06722

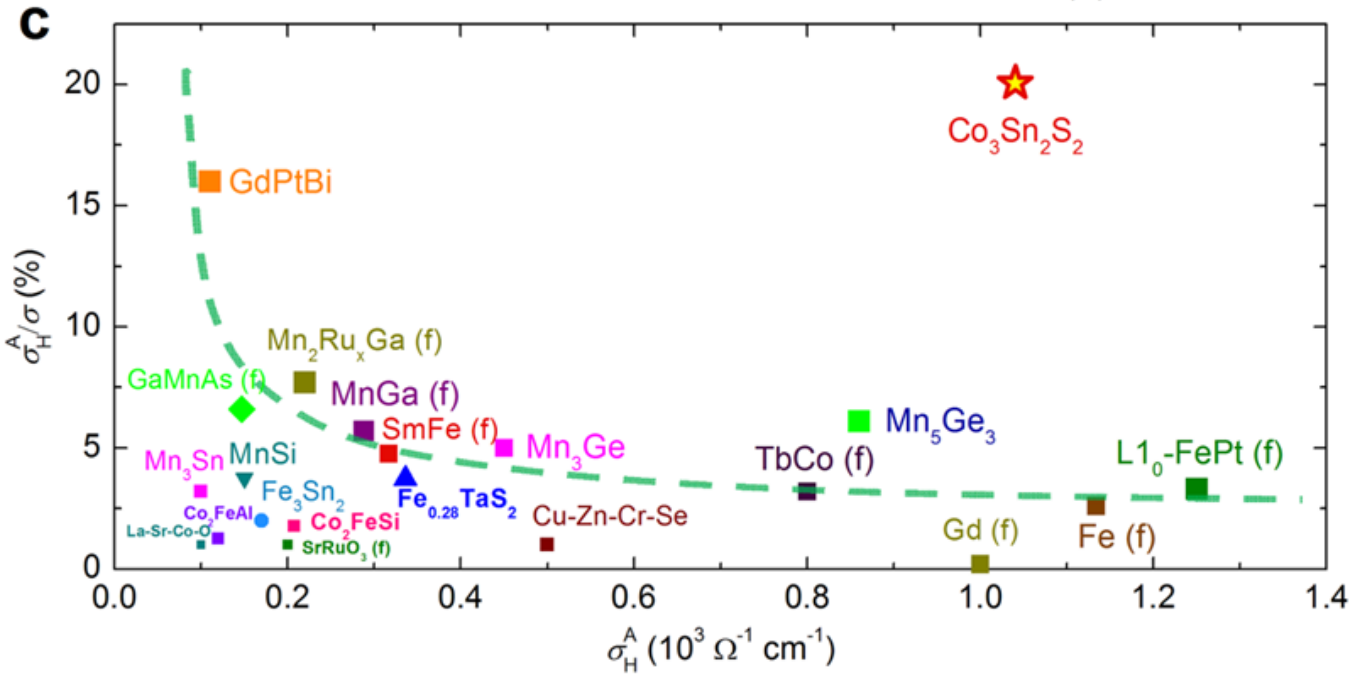
Anomalous Hall conductivity



AHC = 1130 S/cm

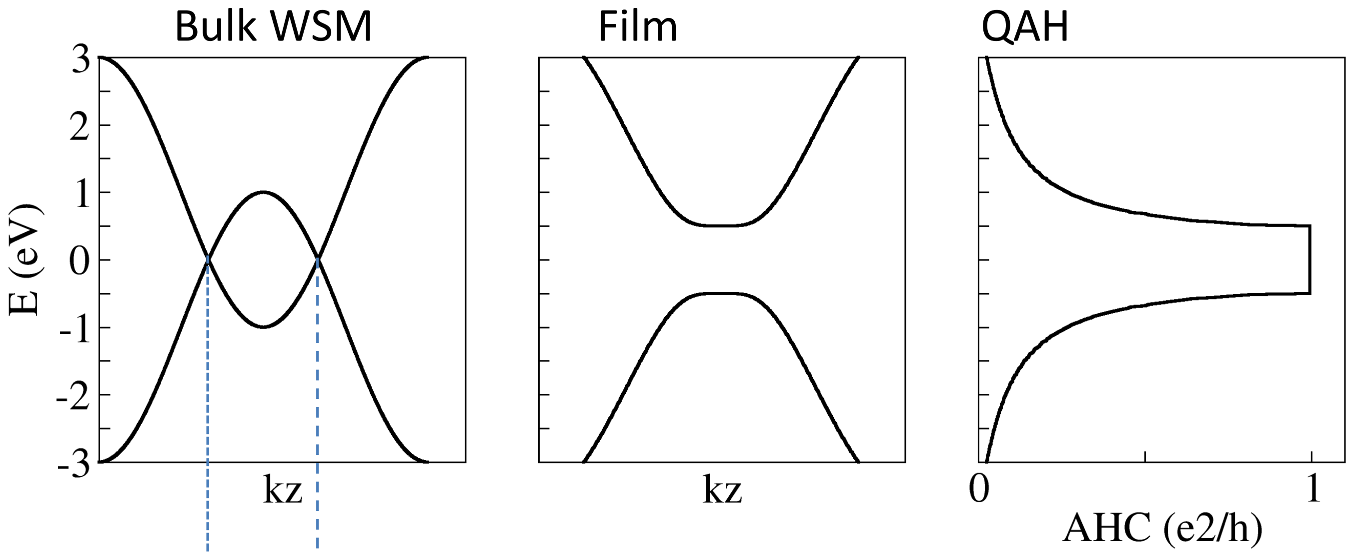


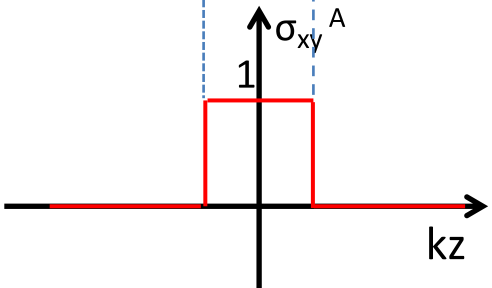
Maximum of AHA of 20 % locates around 120 ~ 150 K

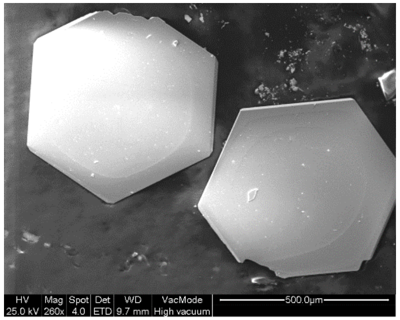


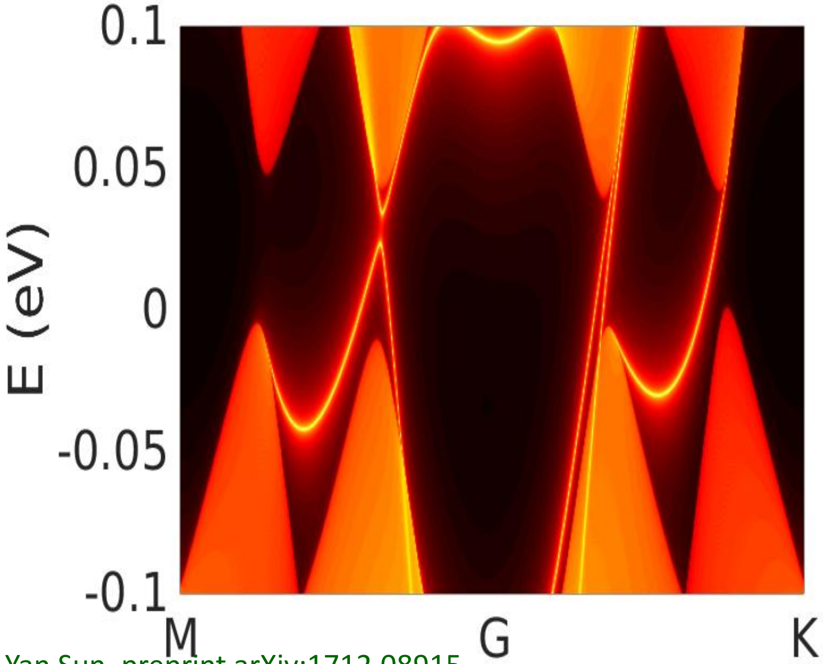
Enke Liu, et al. Nature Physics accepted, preprint arXiv:1712.06722

Quantum Anomalous Hall effect







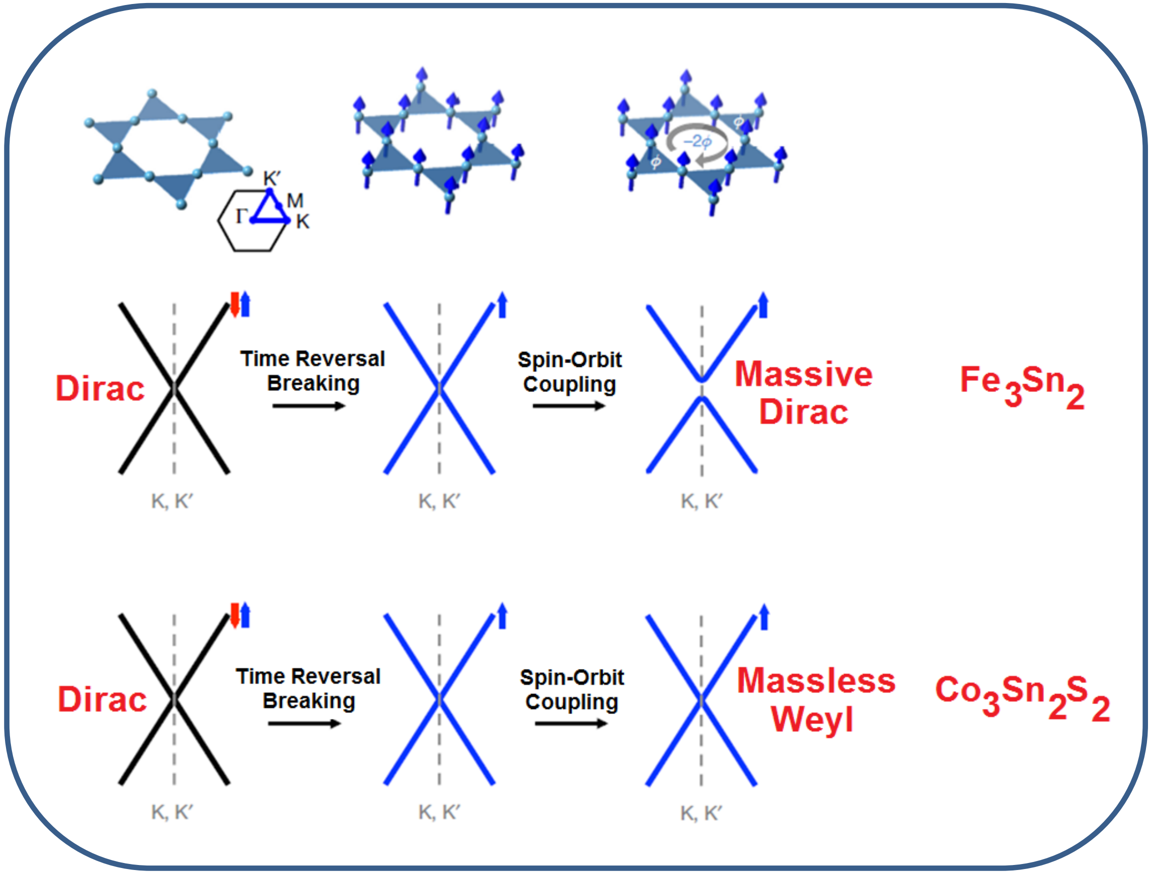


Qiunan Xu, Enke Liu, Wujun Shi, Lukas Muechler, Claudia Felser, Yan Sun, preprint arXiv:1712.08915

LETTER

doi:10.1038/nature25987

Massive Dirac fermions in a ferromagnetic kagome metal



A new progress with Dirac fermions with a tiny band gap on Kagomé lattice, online in Nature two weeks ago.

Nature, 2018, doi:10.1038/nature25987

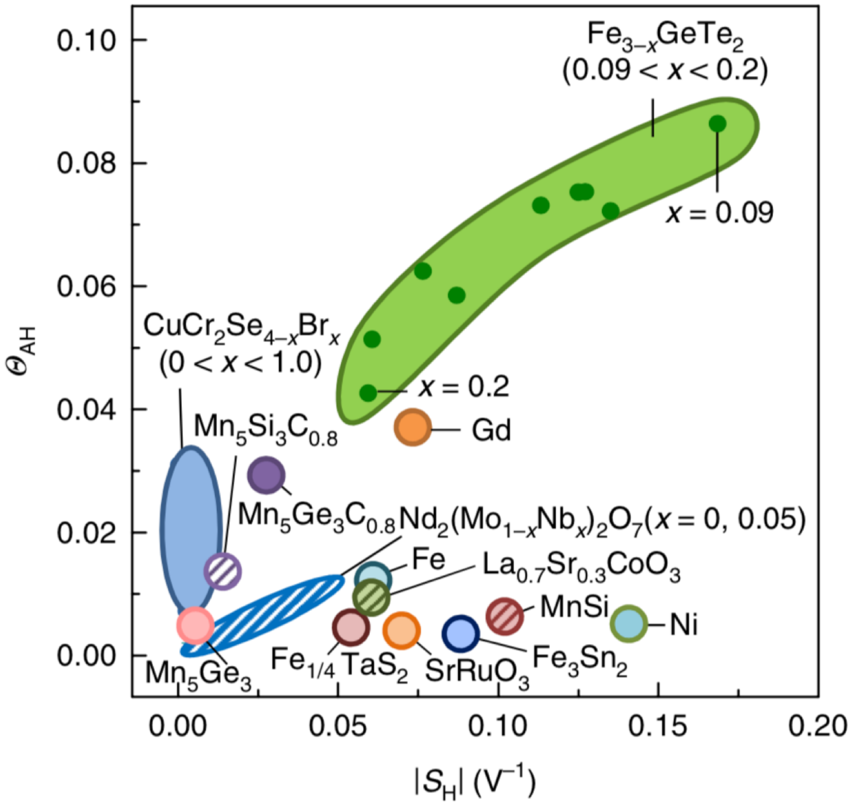
$Co_3Sn_2S_2$ goes even further and for the first time shows the gapless (massless) Weyl fermions in the ferromagnetic Kagome lattice.

Enke Liu, et al. Nature Physics accepted, preprint arXiv:1712.06722

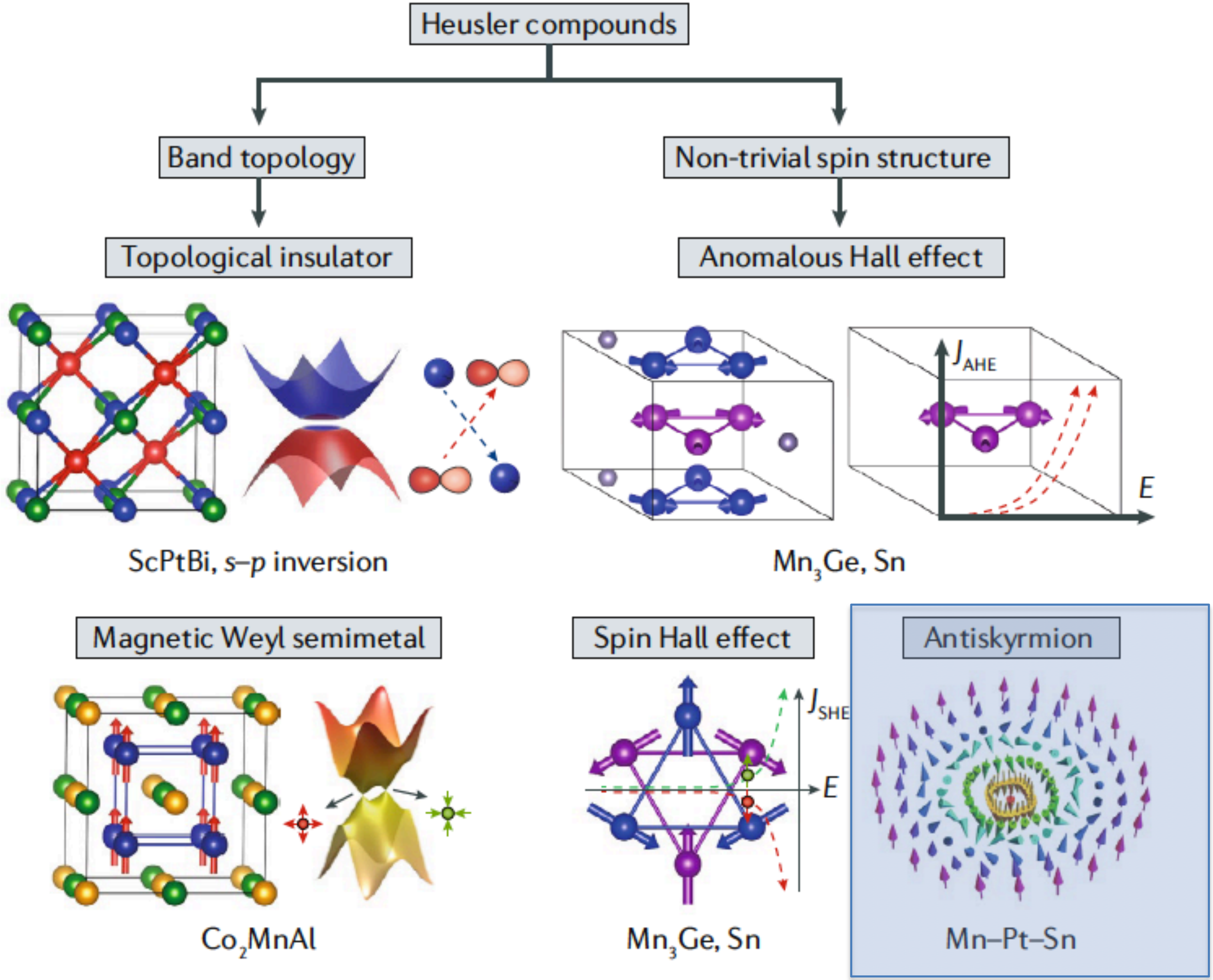
ARTICLES
https://doi.org/10.1038/s41563-018-0132-3
nature materials

Large anomalous Hall current induced by topological nodal lines in a ferromagnetic van der Waals semimetal

Kyoo Kim[1,2,10], Junho Seo[1,3,10], Eunwoo Lee[4,5,6], K.-T. Ko[1,2], B. S. Kim[4,5], Bo Gyu Jang[7], Jong Mok Ok[1,3], Jinwon Lee[1,3], Youn Jung Jo[8], Woun Kang[9], Ji Hoon Shim[7], C. Kim[4,5], Han Woong Yeom[1,3], Byung Il Min[1], Bohm-Jung Yang[4,5,6]* and Jun Sung Kim[1,3]*



Magnetism and Topology



Heusler compounds

Band topology

Topological insulator

ScPtBi, *s*–*p* inversion

Non-trivial spin structure

Anomalous Hall effect

Mn_3Ge, Sn

Magnetic Weyl semimetal

Co_2MnAl

Spin Hall effect

Mn_3Ge, Sn

Antiskyrmion

Mn–Pt–Sn

Kaustuv Manna et al., Nature Materials Review, in press, arXiv:1802.02838v1

Summary

GdPtBi is an ideal Weyl semimetal

In magnetic Weyls we have additional degrees of freedoms –
Co2MnGa
Co3Sn2S2

Large Berry curvatures lead to large AHE and ANE

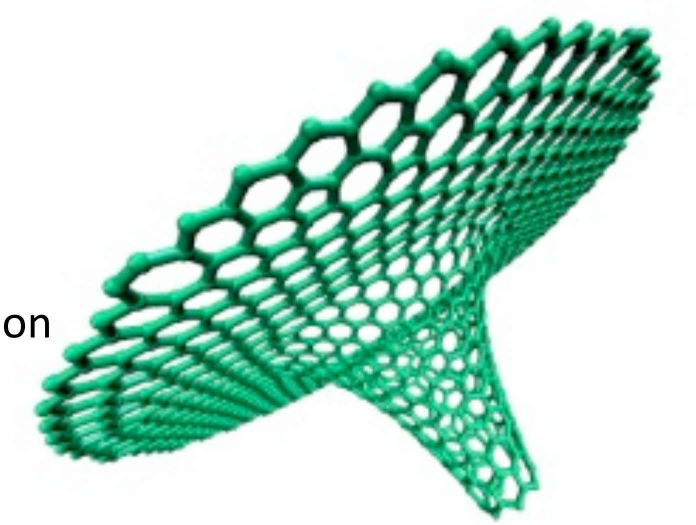
and in the 2D limit to a QAH effect – for room temperature applications

Berry curvatures in zero moment compounds:
Mn_3Sn
Ti_2MnGa

Is there a relation between real space? Skyrmion

New topological physics, hydrodynamics …

… much more to do!



arXiv:1511.07672v1

Single Crystals available

BaCr2As2
BaCrFeAs2

CaPd3O4
SrPd3O4
BaBiO3

Bi2Te2Se
Bi2Te3
Bi2Se3
BiSbTe2S
BiTeI
BiTeBr
BiTeCl

LaBi, LaSb
GdBi, GdSb

HfSiS
ZrSiS

Bi4I4

BaSn2

AlPt
GdAs
CoSi

MoP
WP

TaP
NbP
NbAs
TaAs
NbP-Mo
NbP-Cr
TaP-Mo
TaAsP

CrNb3S6
V3S4
Cd3As2

MnP
MnAs

MoSe2-xTex
MoTe2-xSex
MoTe2 (T´/2H)

PtTe2
PtSe2
PdTe2
PdSe2
OsTe2
RhTe2
TaTe2
NbTe2
WSe2
HfTe5
MoTe2
TaS2
PdSb2
CuxWTe2
FexWTe2
WTe2
Co0,4TaS2
Fe0,4TaS2

Ag2Se
IrO2
OsO2
ReO2
WP2
MoP2

VAl3
Mn3Ge
Mn3Ir
Mn3Rh
Mn3Pt
[illegible]

YPtBi
NdPtBi
GdPtBi
YbPtBi
ScPdBi
YPdBi
ErPdBi
GdAuPb
TmAuPb
AuSmPb
AuPrPb
AuNdPb
[illegible]
uLuSn
AuYSn
ErAuSn
EuAuBi

CaAgAs

KMgSb
KMgBi
KHgSb
KHgBi
LiZnAs
LiZnSb

YbMnBi2
Ni2Mn1.4In0.6
YFe4Ge2

Mn1.4PtSn

CuMnSb
CuMnAs

Co2Ti0.5V0.5Sn
Co2VAl0.5Si0.5
Co2Ti0.5V0.5Si
Mn2CoGa
Co2MnGa
Co2Al9
Co2MnAl
Co2VGa0.5Si0.5
Co2TiSn
Co2VGa
Co2V0.8Mn0.2Ga
CoFeMnSi

Thank you!