

Magnetic Weyl Semimetals

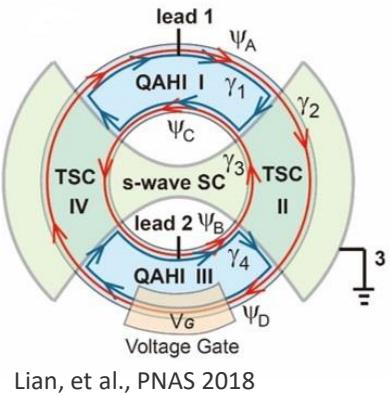


MAX-PLANCK-GESELLSCHAFT

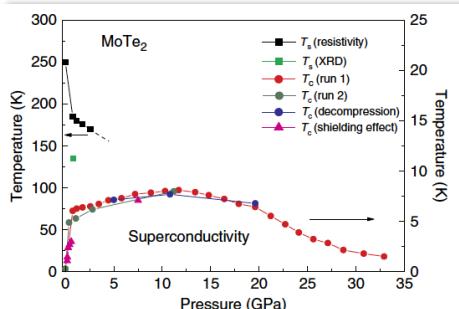
Claudia Felser



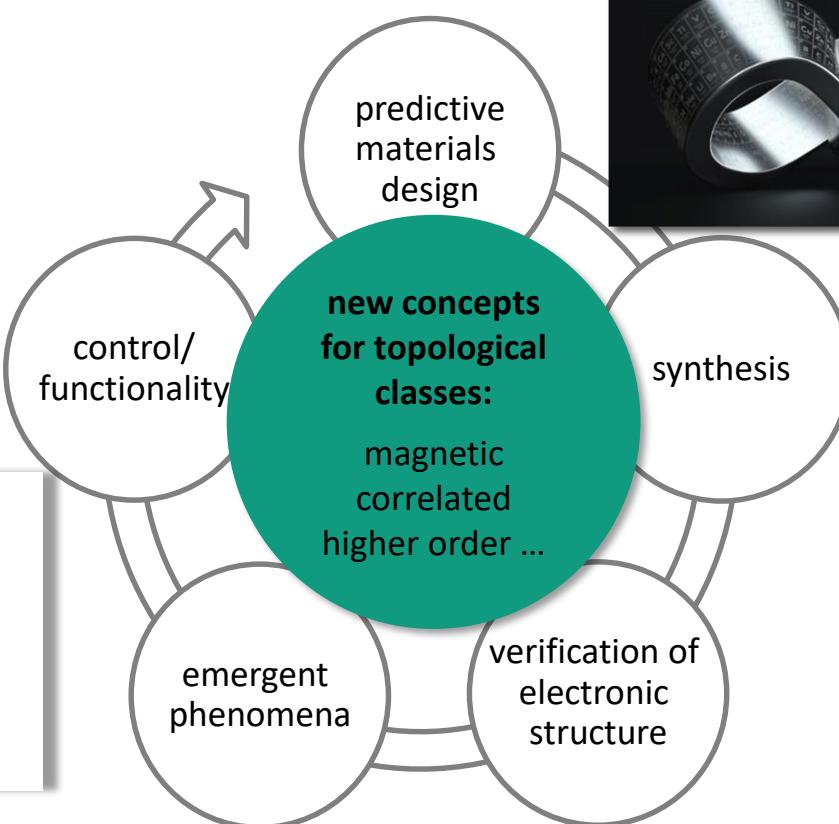
the concept



Lian, et al., PNAS 2018



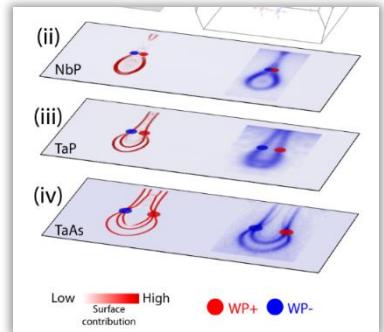
Qi et al. Nat. Com. (2016)



© Nature



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

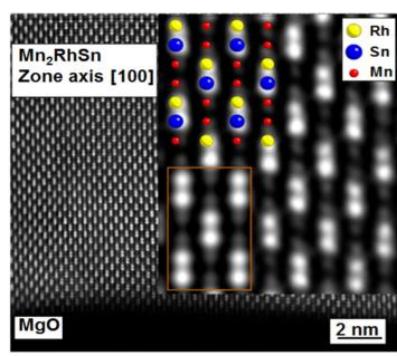
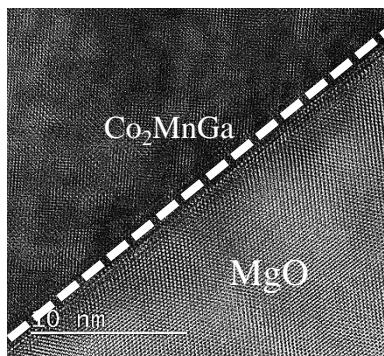
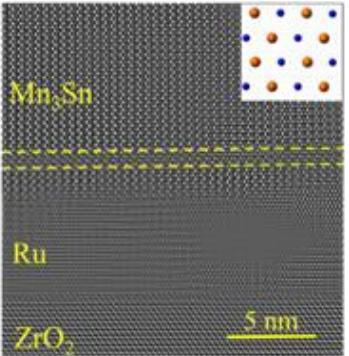
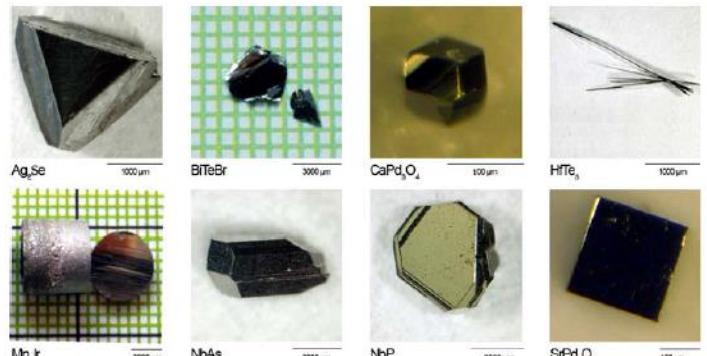
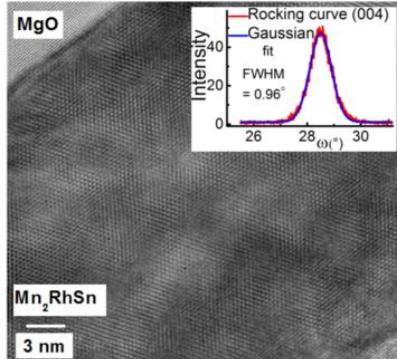


Liu et al. Nat. Mat. (2016)

the materials

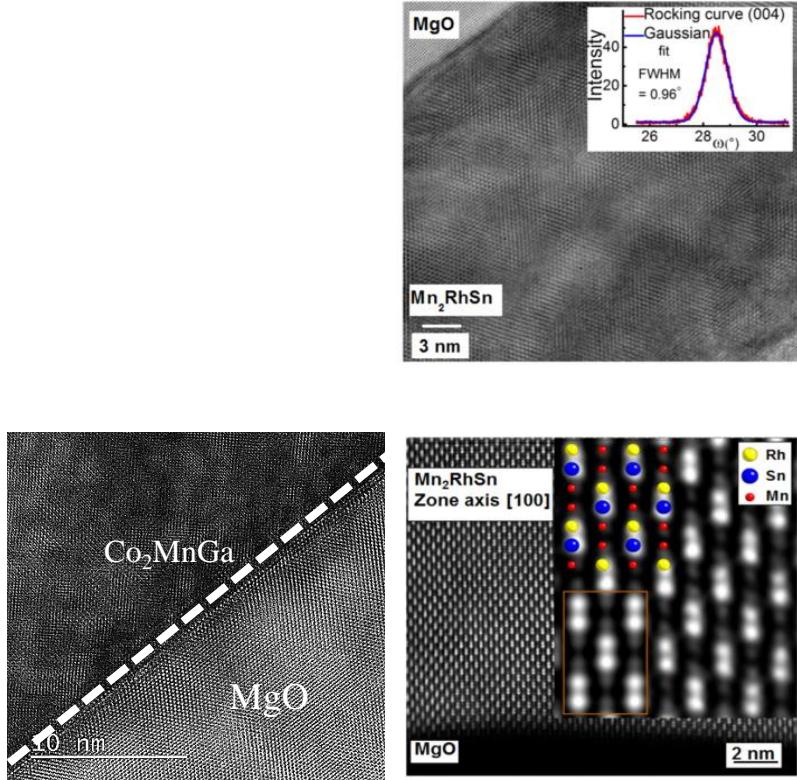
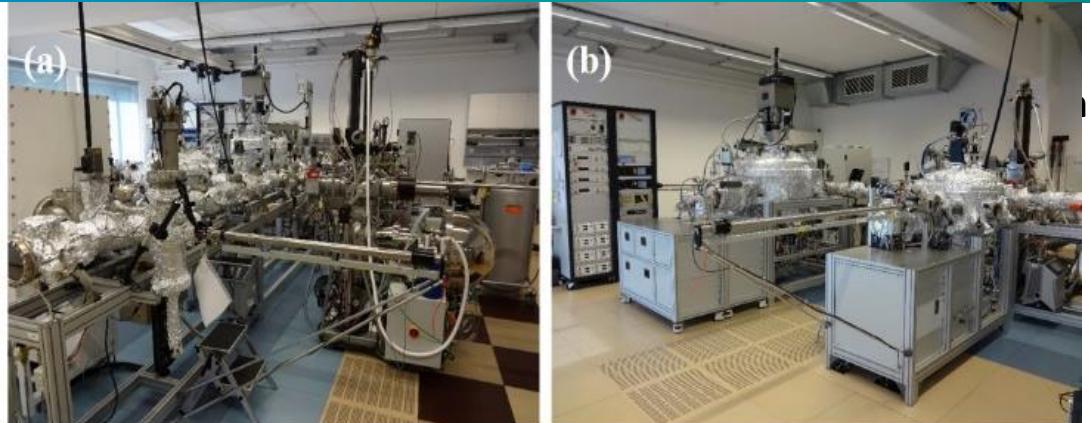


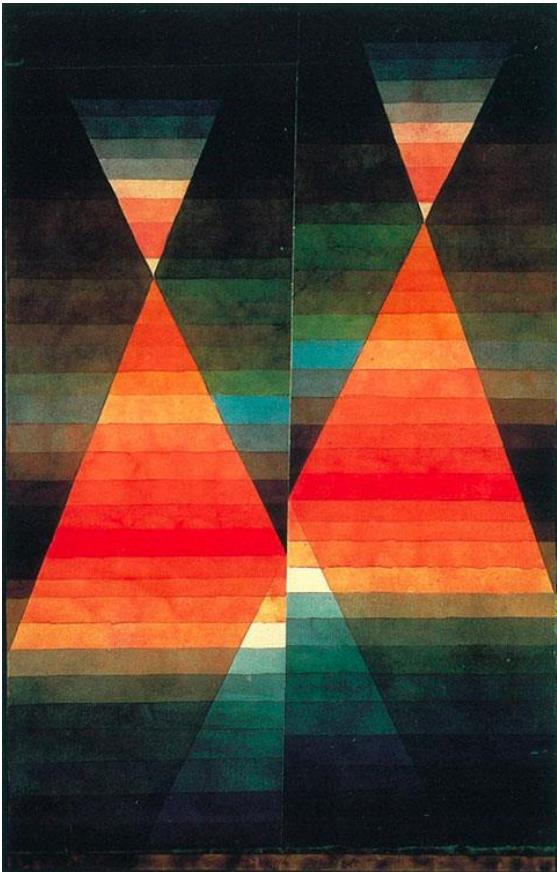
- explorative search for new materials & predictive design
- high quality **single crystal growth**
- epitaxial growth of ultrathin films and heterostructures
- 2D materials and micro/nano structures





the materials



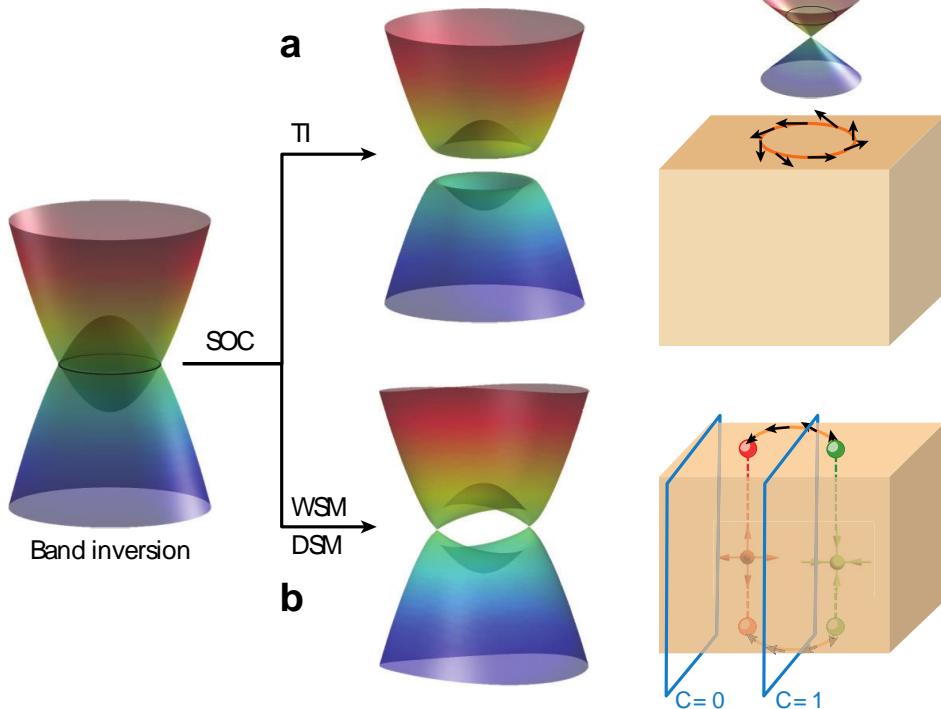


Weyl semimetals

Breaking time reversal symmetry



Weyl semimetals

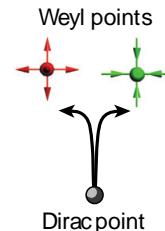
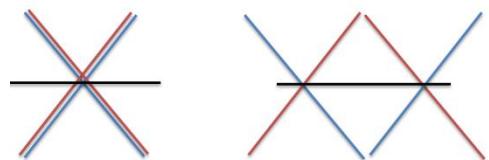


Breaking symmetry

- Inversion symmetry (Strain)

Breaking time reversal symmetry

- Magnetic field

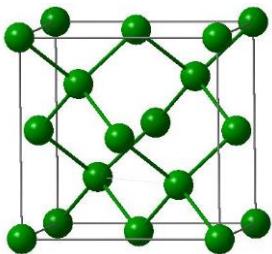


- Dirac points at high symmetry
- Weyl points at low symmetry
- All crossings in ferromagnets: Weyl points**



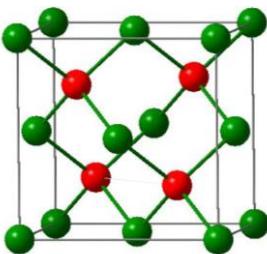
the Heusler family

Diamond

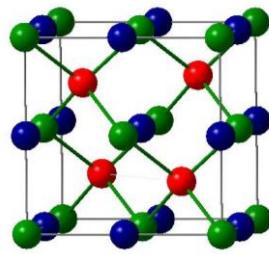


C	N
2.55	3.04
Si	P
1.90	2.19
Ge	As
2.01	2.18
Sn	Sb
1.96	2.05

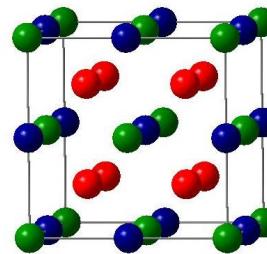
ZnS



Heusler $X\text{Y}\text{Z}$ C1_b



X_2YZ L2₁



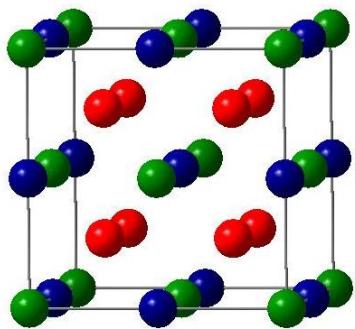
H	2.20
Li	0.98
Be	1.57
Na	0.93
Mg	1.31
K	0.82
Ca	1.00
Sc	1.36
Ti	1.54
V	1.63
Cr	1.66
Mn	1.55
Fe	1.83
Co	1.88
Ni	1.91
Cu	1.90
Zn	1.65
Ga	1.81
Ge	2.01
As	2.18
Se	2.55
Br	2.96
Kr	3.00

B	C	N	O	F	Ne
2.04	2.55	3.04	3.44	3.98	
Al	Si	P	S	Cl	Ar
1.61	1.90	2.19	2.58	3.16	
In	Sn	Sb	Te	I	Xe
1.78	1.96	2.05	2.10	2.66	2.60
Hf	Ta	W	Re	Os	
1.30	1.50	1.70	1.90	2.20	
Ru	Rh	Pd	Ag	Cd	
2.20	2.28	2.20	1.93	1.69	
Ir	Pt	Au	Hg	Tl	
2.20	2.20	2.40	1.90	1.80	
Ac	Th	Pa	U	Np	
1.10	1.30	1.50	1.70	1.30	
Sm	Eu	Gd	Tb	Dy	
1.13	1.17	1.20	1.20	1.10	
Pr	Ho	Er	Tm	Yb	
1.12	1.23	1.24	1.25	1.10	
Ce	Lu				
1.13	1.27				
1.10					



from semiconductors to half metals

X_2YZ



Fe_2

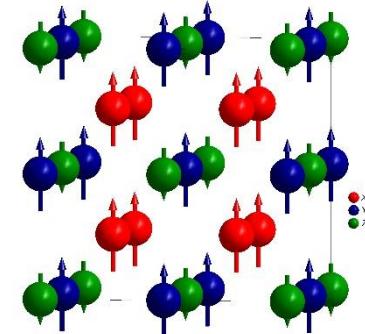
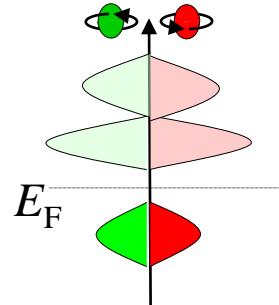
V

Al

$$2 * 8 + 5 + 3 = 24$$



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

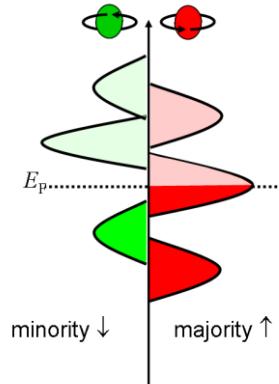


Co_2

Mn

Ga

$$2 * 9 + 7 + 3 = 24 + 4$$



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

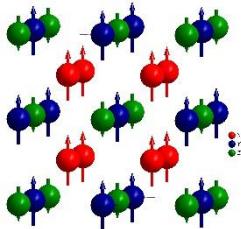
Balke et al. Solid State Com. **150** (2010) 529

Kübler et al., Phys. Rev. B **76** (2007) 024414

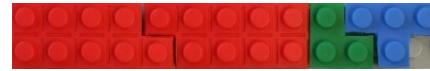
tuning exchange



X_2YZ



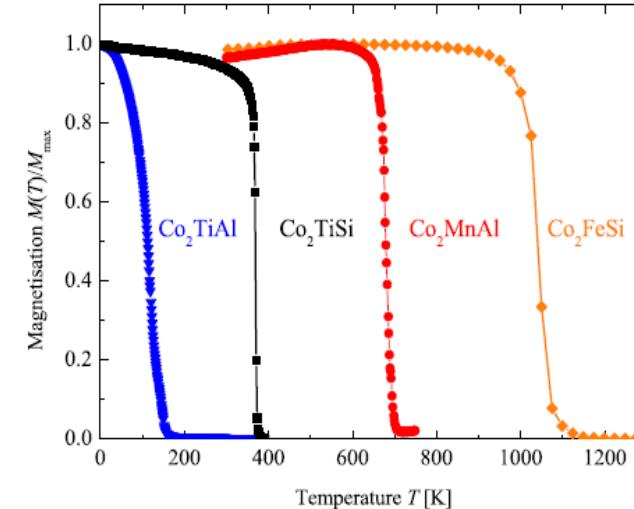
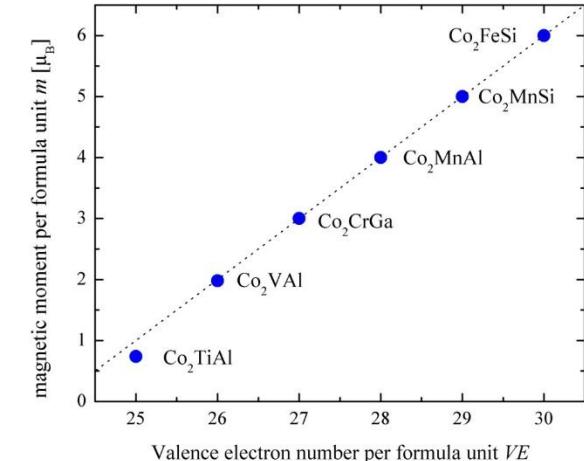
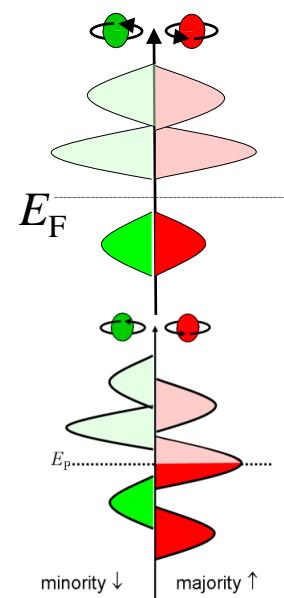
$\text{Co}_2\text{TiAl}: 2 \times 9 + 4 + 3 = 25 \quad \text{Ms} = 1m_B$



$\text{Co}_2\text{MnGa}: 2 \times 9 + 7 + 3 = 28 \quad \text{Ms} = 4m_B$



$\text{Co}_2\text{FeSi}: 2 \times 9 + 8 + 4 = 30 \quad \text{Ms} = 6m_B$



Kübler *et al.*, PRB **28**, 1745 (1983)

de Groot RA, et al. PRL **50** 2024 (1983)

Galanakis *et al.*, PRB **66**, 012406 (2002)

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Balke *et al.* Solid State Com. **150** (2010) 529

Kübler *et al.*, Phys. Rev. B **76** (2007) 024414

Heusler and Weyl



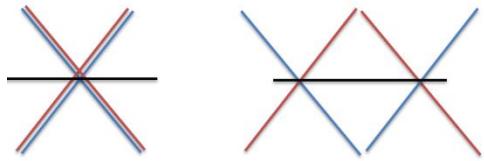
Breaking symmetry

- Inversion symmetry (Strain)



Breaking time reversal symmetry

- Magnetic field



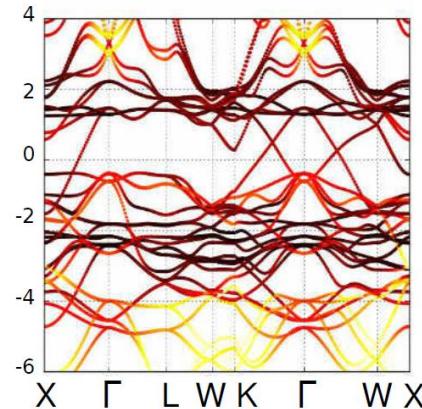
- Dirac points at high symmetry
- Weyl points at low symmetry
- All crossings in ferromagnets:
Weyl points

Co₂TiSn

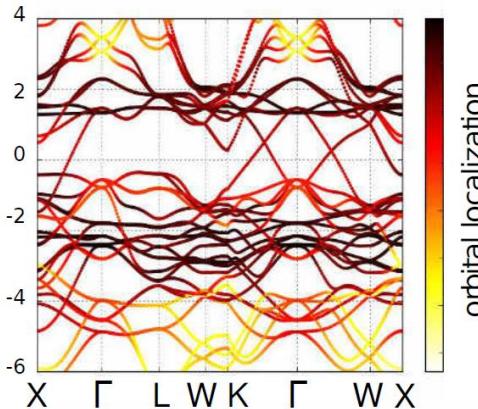
$$\text{Co}_2\text{TiSi}: 2 \times 9 + 4 + 4 = 26 \text{ Ms} = 2\mu_B$$



TiCo₂Ge



TiCo₂Si



orbital localization

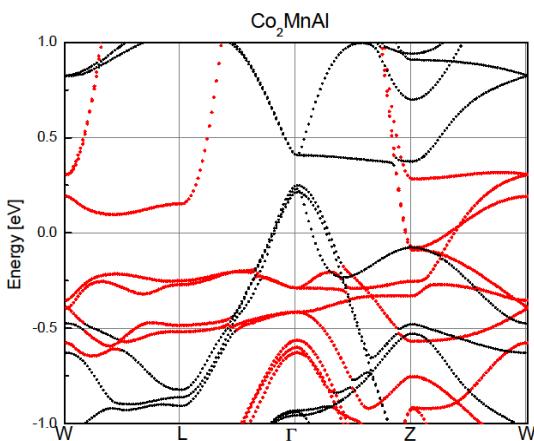


Heusler, Weyl and Berry

Giant AHE in Co₂MnAl

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

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



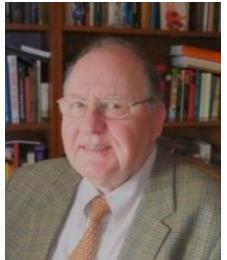
$$\sigma_{xy}^A(\mu) = ie^2 \left(\frac{1}{2\pi} \right)^3 \int dk \sum_{E(n,k) < \mu} f(n, k, \mu) \Omega_{n,xy}(k),$$

Compound ^a	N_V	a (nm)	M^{exp}	M^{calc}	σ_{xy}	P (%)
Co ₂ VGa	26	0.5779	1.92	1.953	66	65
Co ₂ CrAl	27	0.5727	1.7	2.998	438	100
Co ₂ VSn	27	0.5960	1.21	1.778	-1489	35
Co ₂ MnAl	28	0.5749	4.04	4.045	1800	75
Rh ₂ MnAl	28	0.6022		4.066	1500	94
Mn ₂ PtSn ^b	28	0.4509 (1.3477)		6.66	1108	91
Co ₂ MnSn	29	0.5984	5.08	5.00	118	82
Co ₂ MnSi	29	0.5645	4.90	4.98	228	100

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

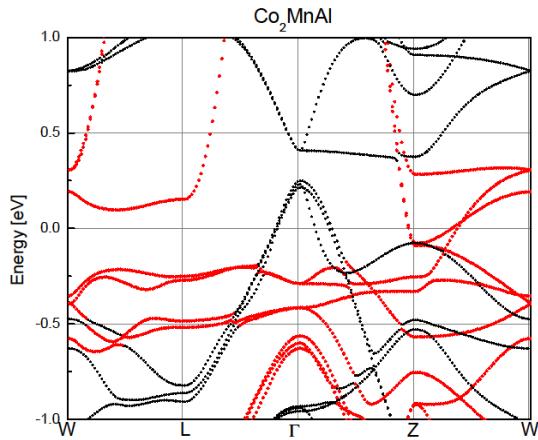


Heusler, Weyl and Berry



Giant AHE in Co₂MnAl

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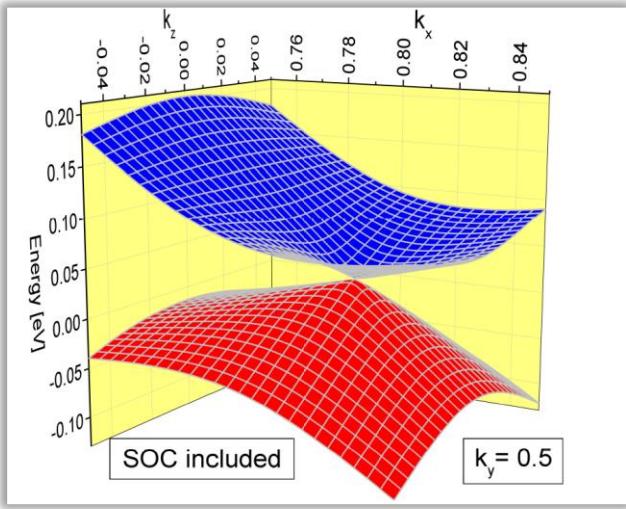
Co₂MnGa

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

PHYSICAL REVIEW B 85, 012405 (2012)

Berry curvature and the anomalous Hall effect in Heusler compounds

Jürgen Kübler^{1,*} and Claudia Felser²

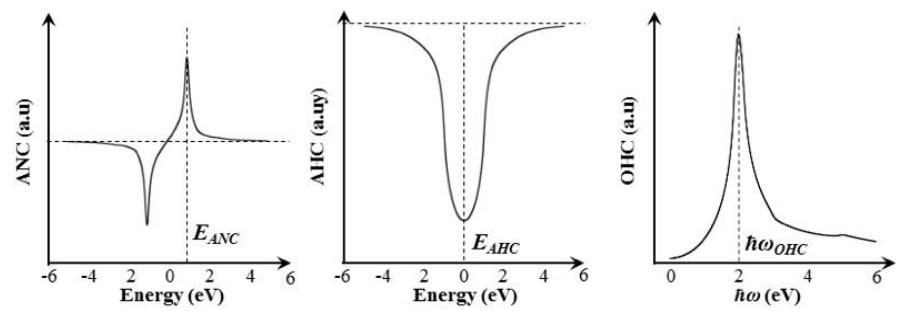
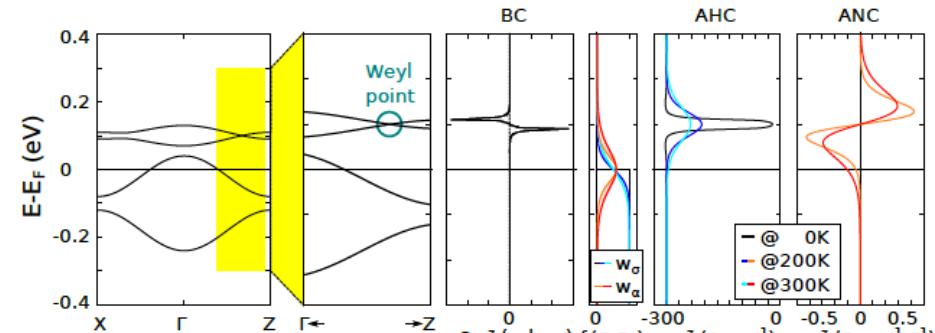
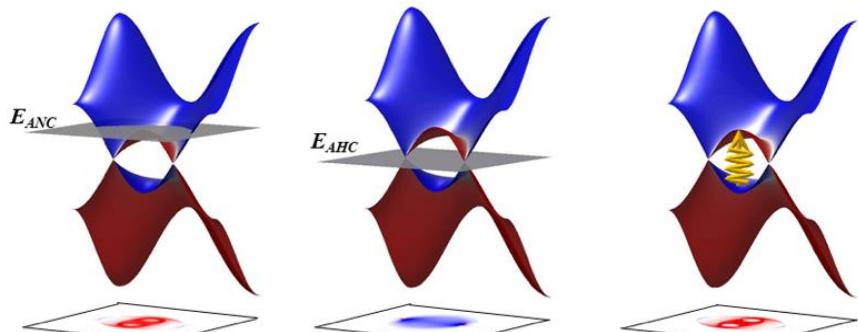
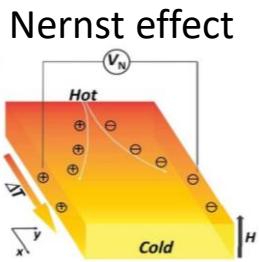




Berry curvature design

Berry curvature design

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



Thermoelectric effect

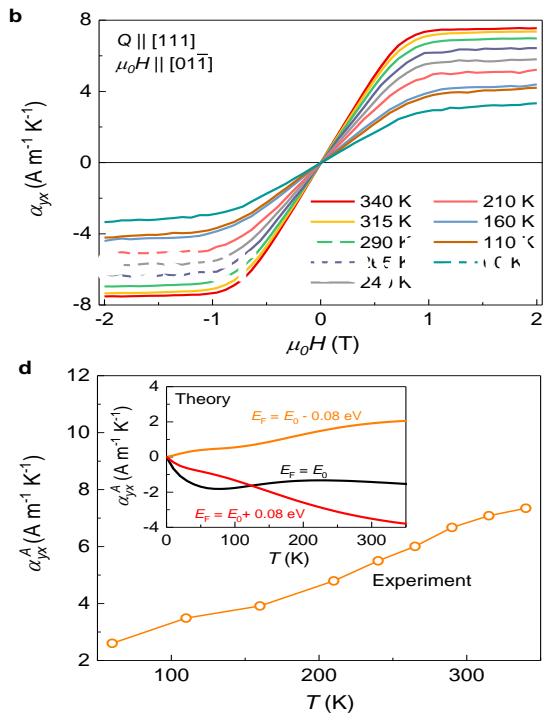
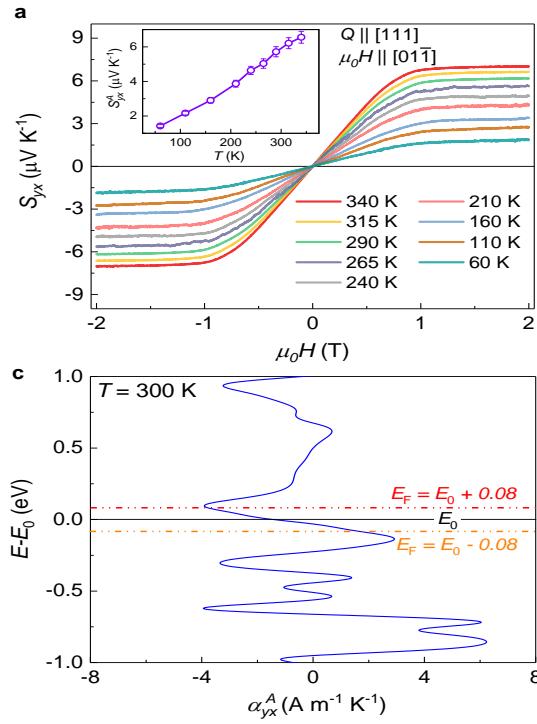
Anomalous Hall effect

Magneto-optic effect



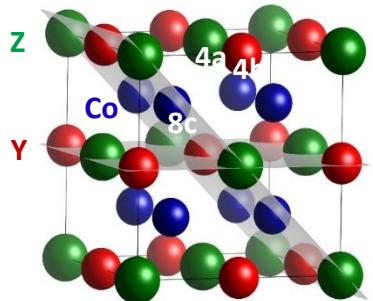
Nernst effect

Co₂MnGa

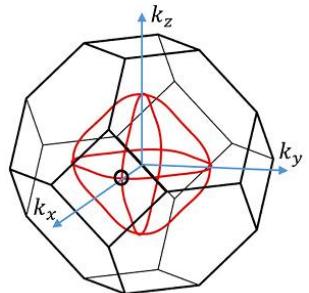
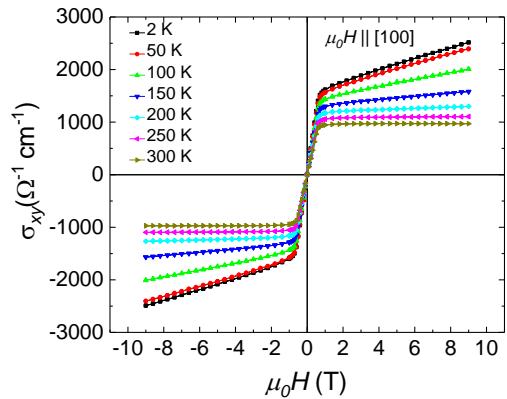
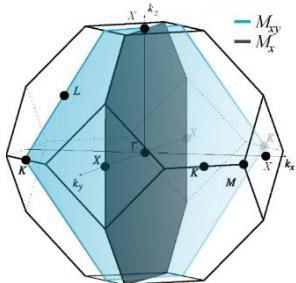




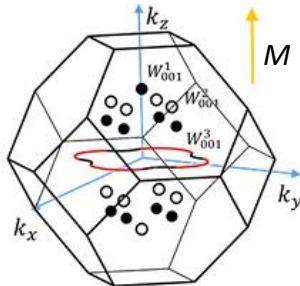
Heusler, Weyl and Berry



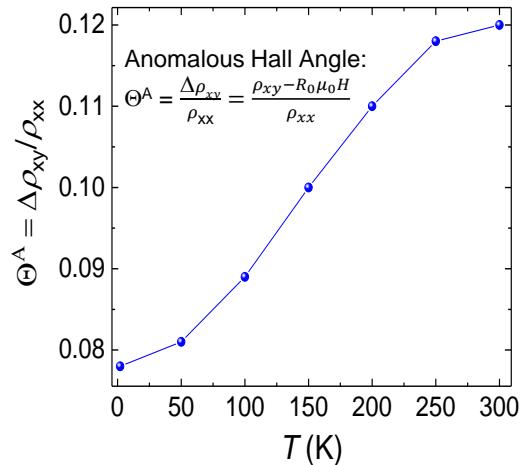
Co_2YZ (Y = IVB or VB; Z = IVA or IIIA)
 L_2I space group 225 ($\text{Fm}\bar{3}\text{m}$)



With SOC
Symmetry and electronic structures depend on the magnetization direction

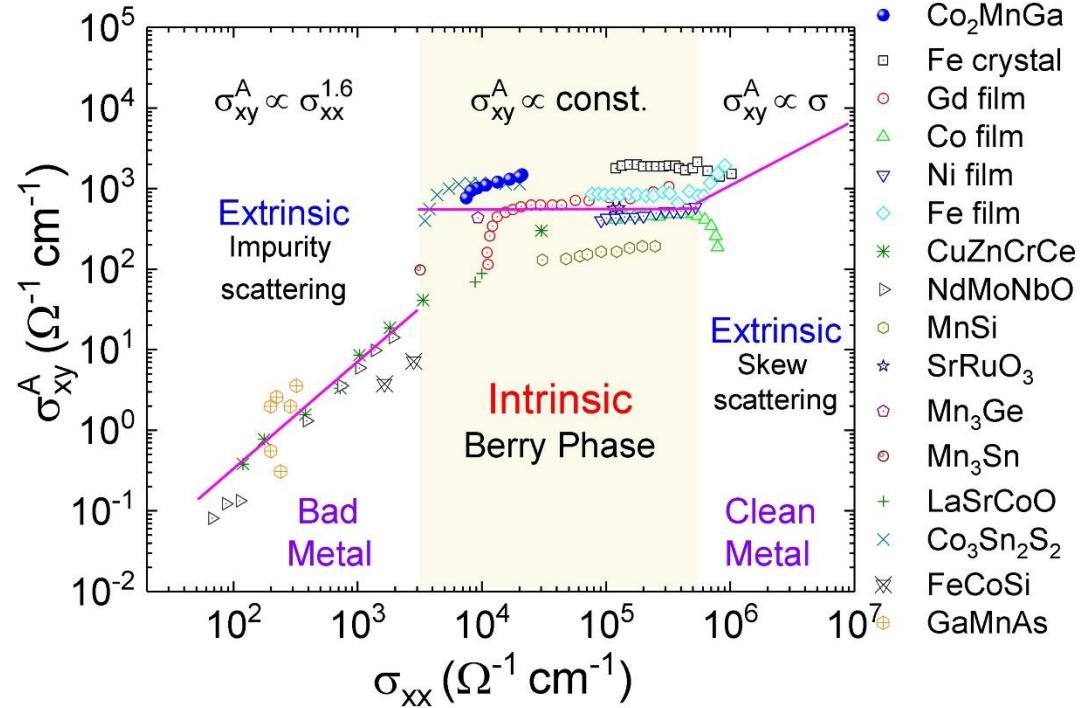
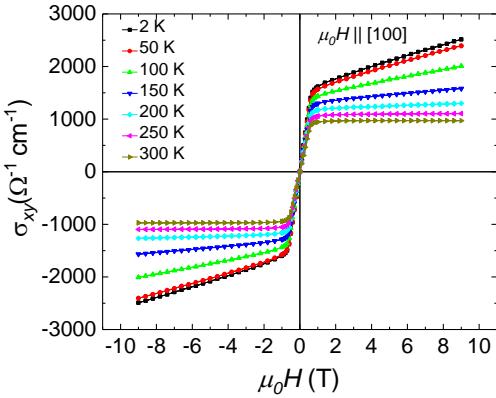
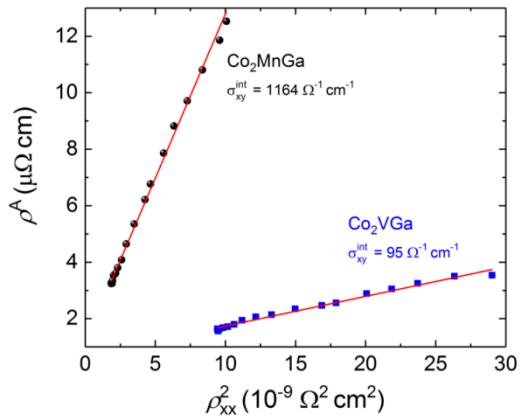


Phys. Rev. Lett. 117, 236401 (2016)
Sci. Rep. 6, 38839 (2016)



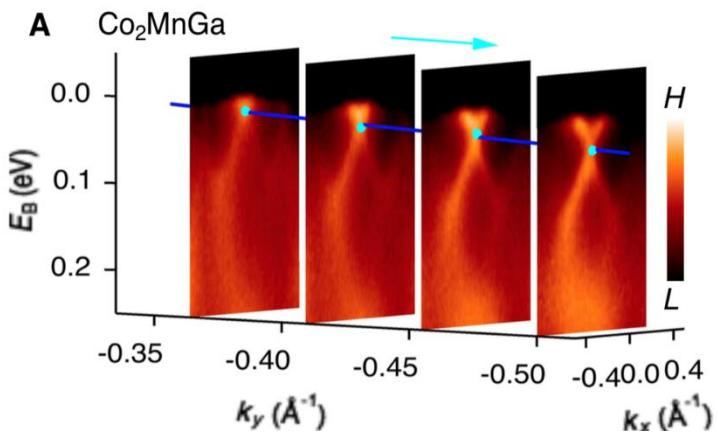
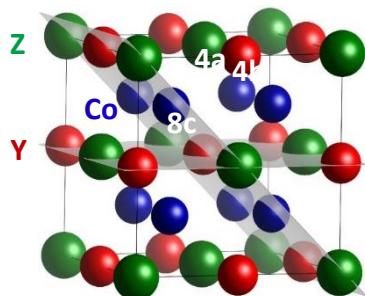
- nodal line is formed in the plane when bands of opposite mirror eigenvalues cross.
- Mirror planes are related to each other by the rotations

Heusler, Weyl and Berry

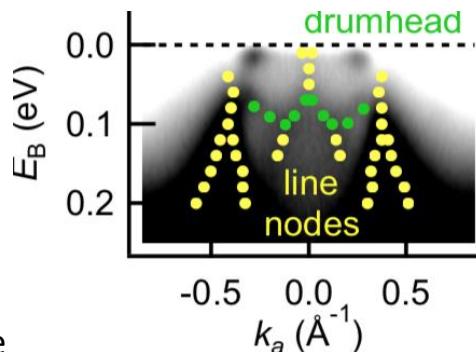
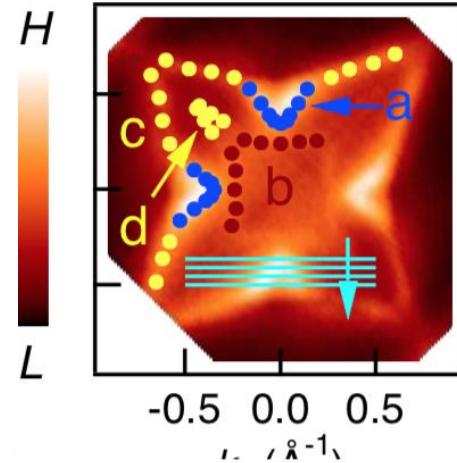




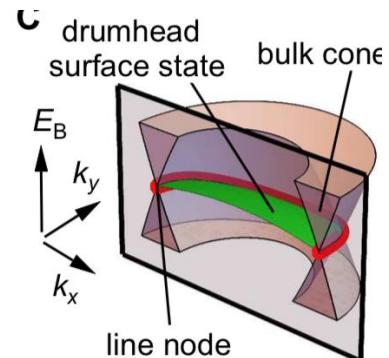
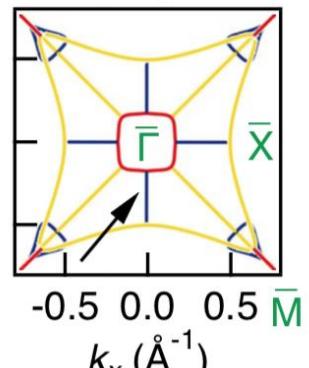
Co₂MnGa – ferromagnetic nodal line



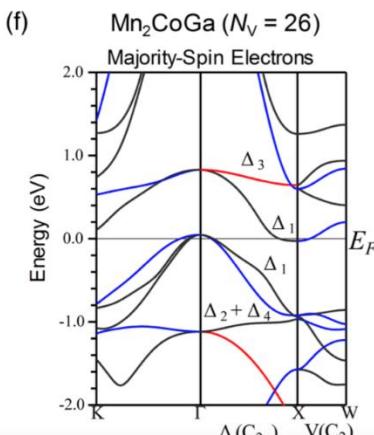
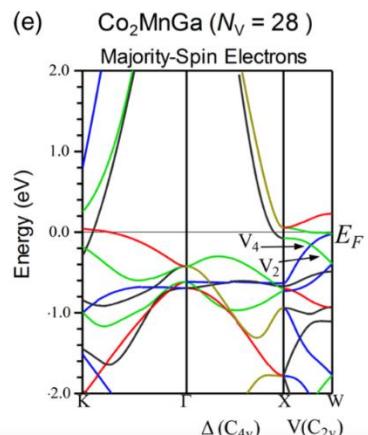
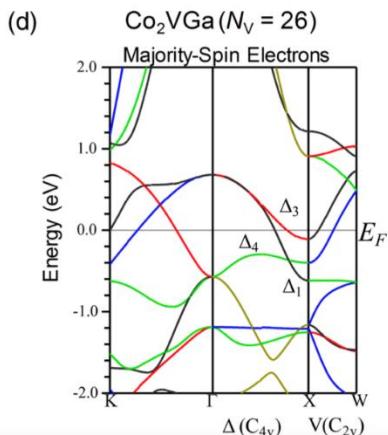
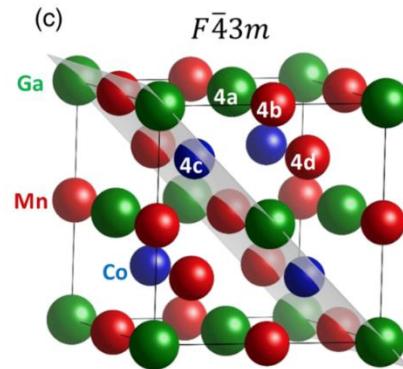
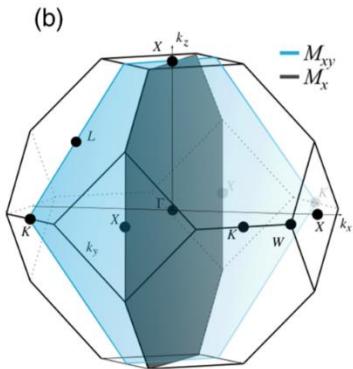
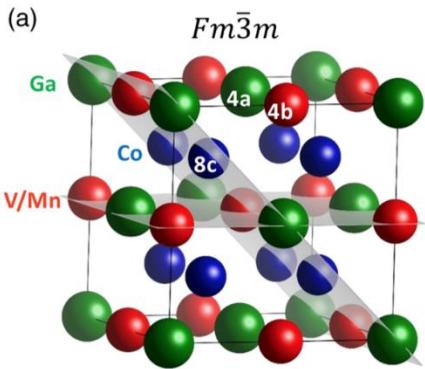
Series of ARPES cuts through the candidate line node



DFT, Weyl lines

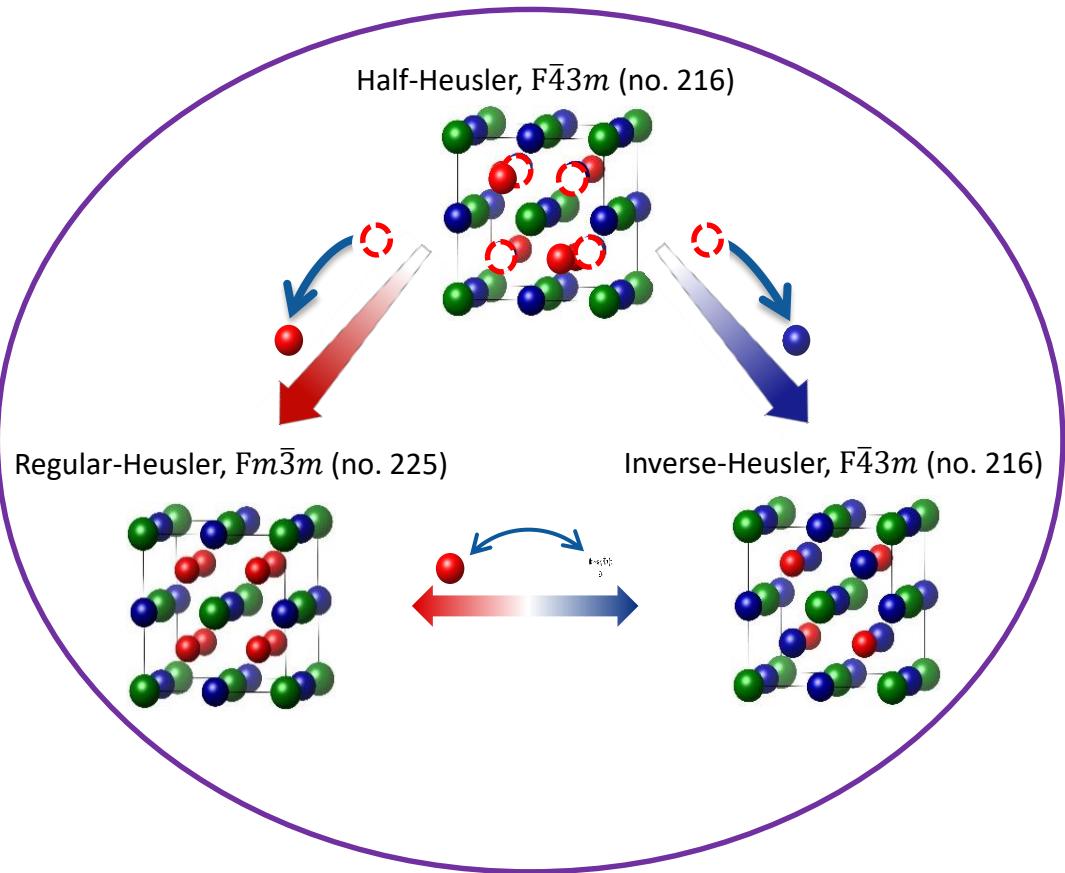


Heusler, Weyl and Berry





no inversion symmetry
topology !

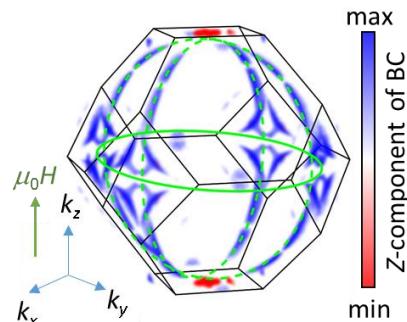
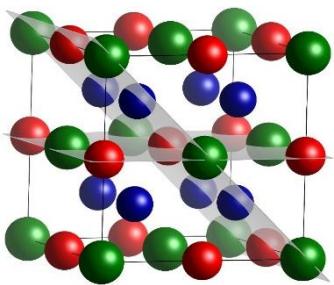




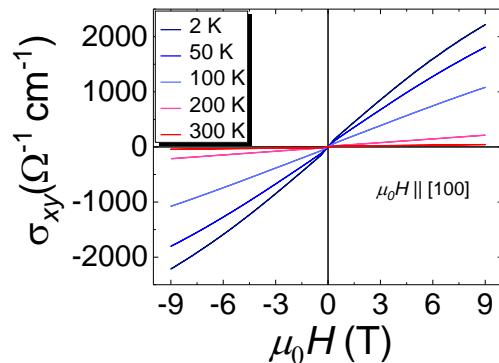
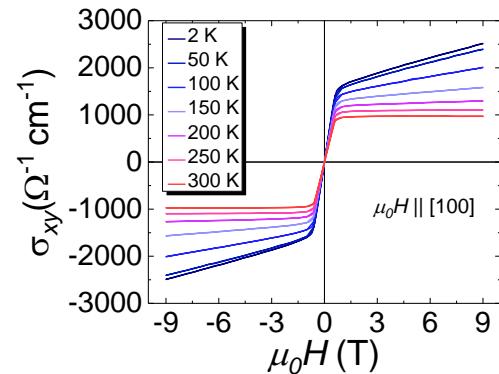
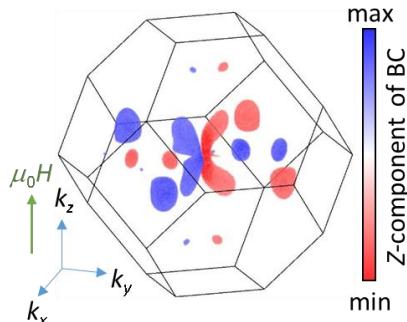
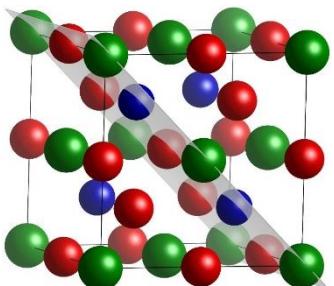
Heusler, Weyl and Berry

playing with symmetry: from Weyl to spingapless semiconductor

Co₂MnGa



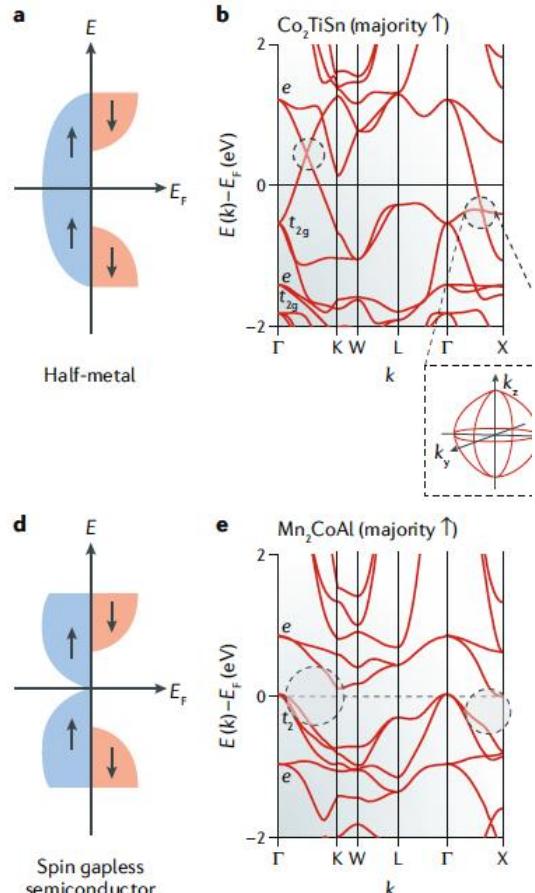
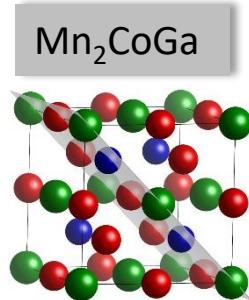
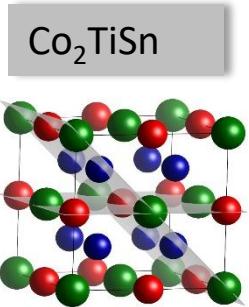
Mn₂CoGa





Heusler, Weyl and Berry

playing with symmetry: from Weyl to spingapless semiconductor



Ouardi, Fecher, Kübler, and Felser, Physical Review Letter 110 (2013) 100401

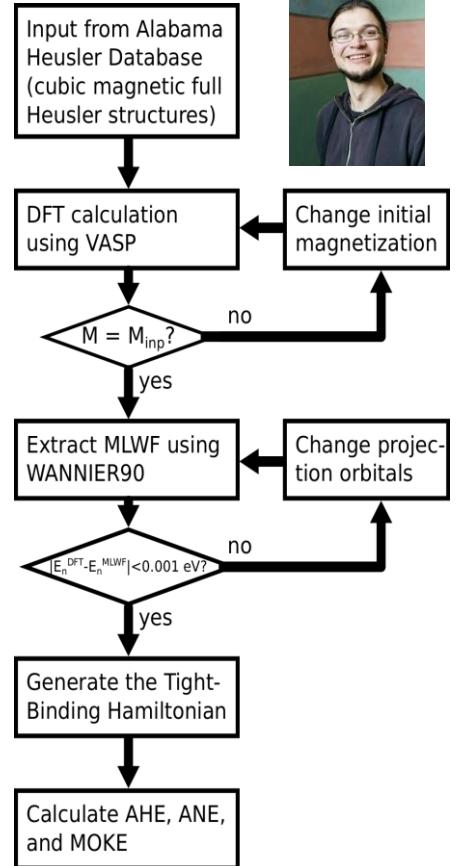
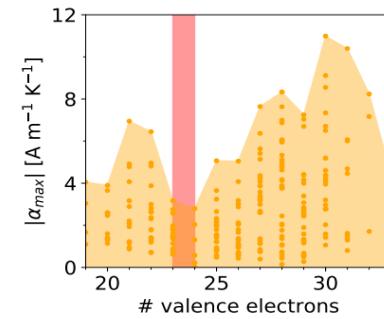
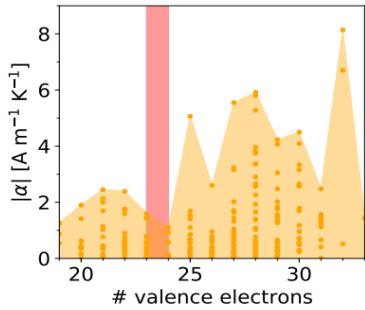
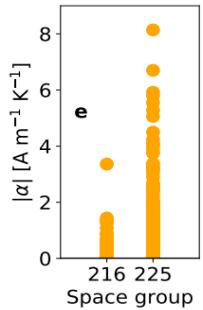
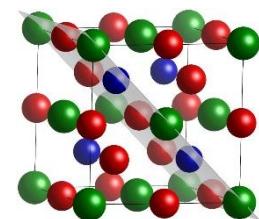
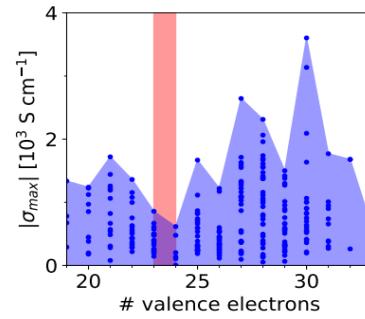
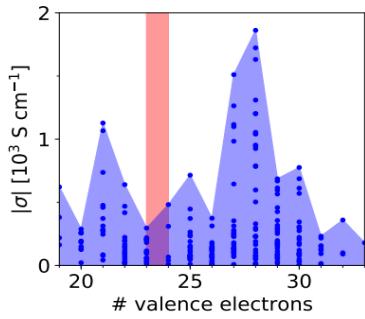
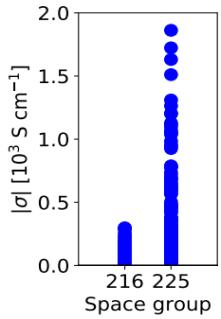
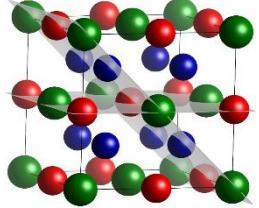
Manna et al., Phys. Rev. X 8 (2018) 041045, arXiv:1712.10174

Manna et al., Nature Review Materials, 3 (2018) 244 arXiv:1802.02838v1



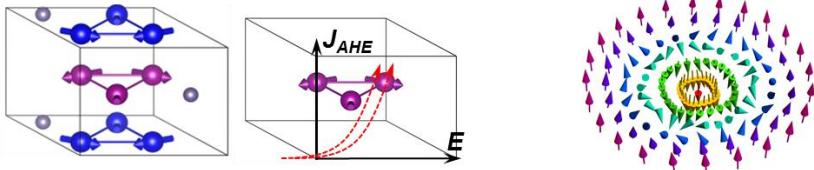
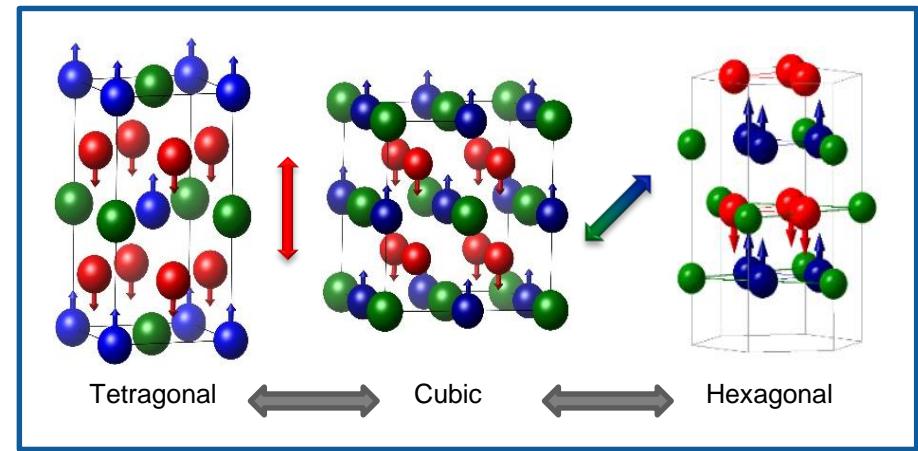
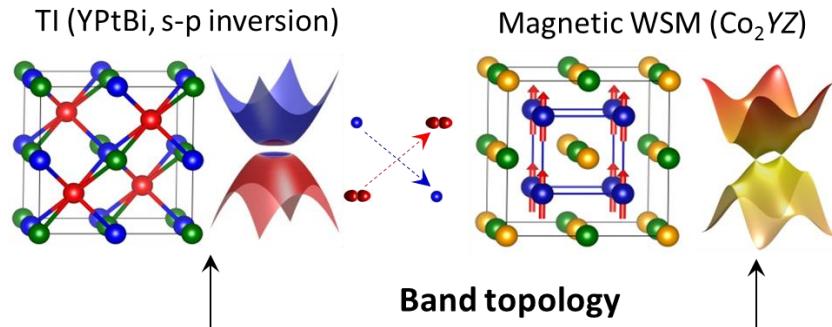
high throughput

playing with symmetry:





Heusler, Weyl and Berry



Mn_3Ga Mn_3Ge Mn_3Sn



Heusler, Weyl and Berry

PRL 112, 017205 (2014)

PHYSICAL REVIEW LETTERS

week ending
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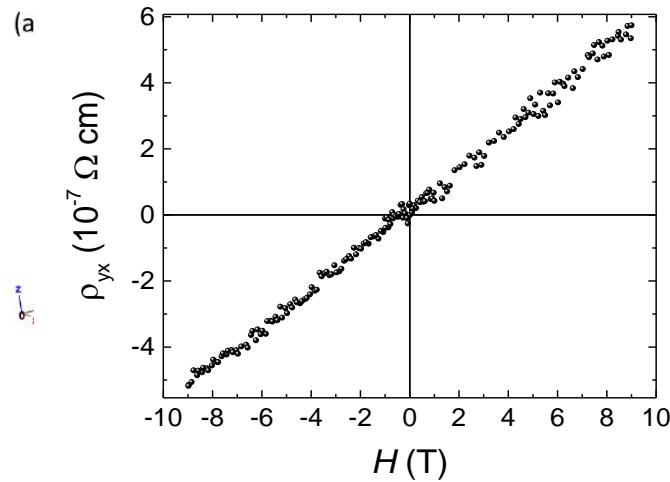
A LETTERS JOURNAL EXPLORING
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December 2014

www.epljournal.org

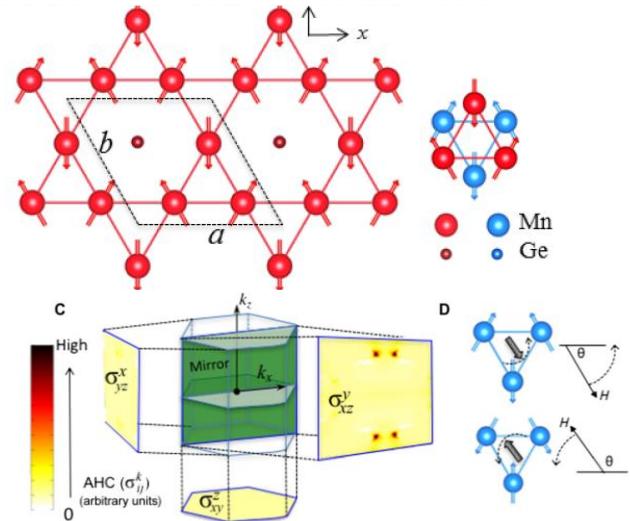
Anomalous Hall Effect Arising from Noncollinear Antiferromagnetism

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



Non-collinear antiferromagnets and the anomalous Hall effect

J. KÜBLER¹ and C. FELSER²

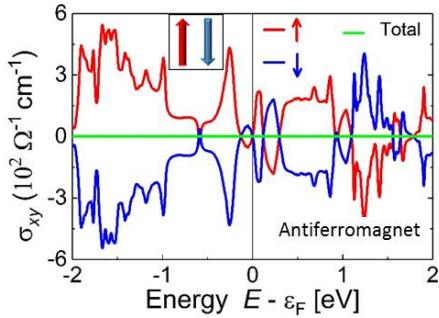
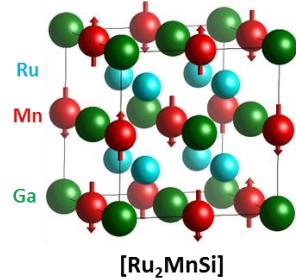


For the planar cases the AHC is connected with Weyl points in the energy- band structure.

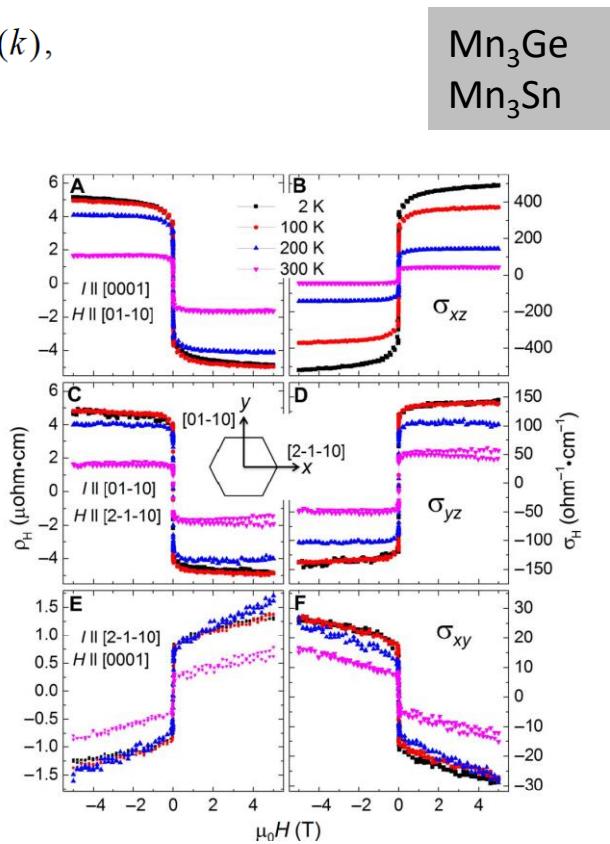


Heusler, Weyl and Berry

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



The anomalous Hall conductivity in an antiferromagnetic metal is zero



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

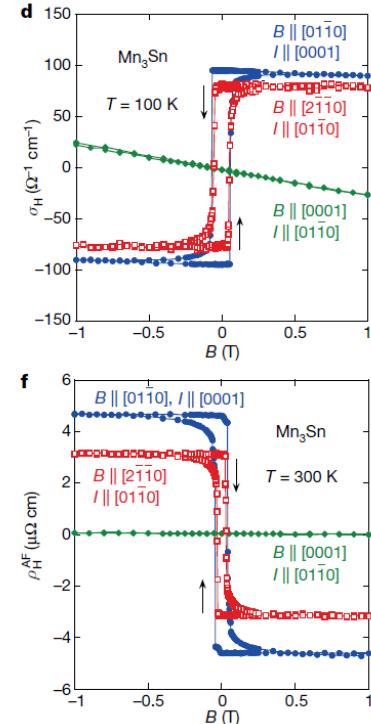
Kiyohara, Nakatsuji, preprint: arXiv:1511.04619

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doi:10.1038/nature15723

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

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



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



Nernst effect in Mn_3Sn

PRL 119, 056601 (2017)

PHYSICAL REVIEW LETTERS

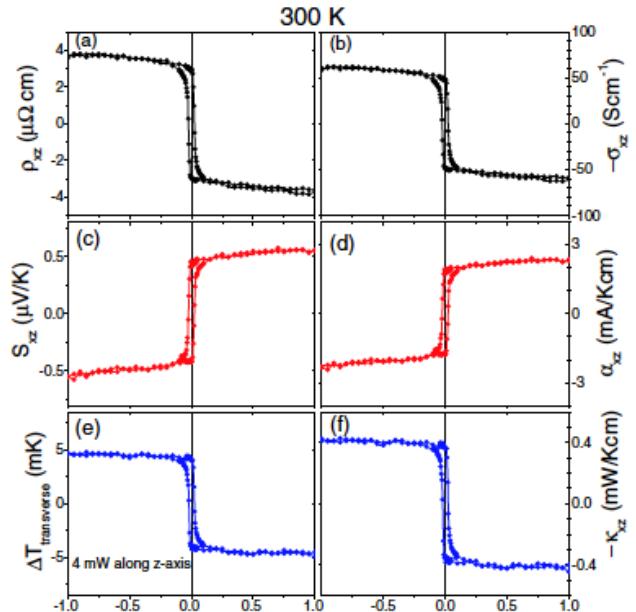
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4 AUGUST 2017nature
physics

LETTERS

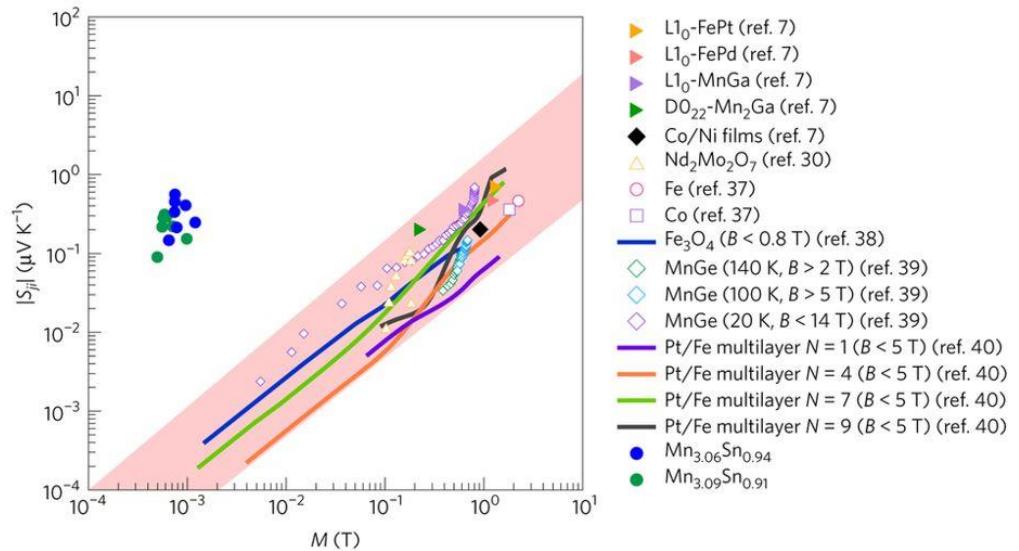
PUBLISHED ONLINE: 24 JULY 2017 | DOI: 10.1103/PhysRevLett.119.056601

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
 Xinfang Tu,¹ Zhenwei Zhu,^{1,*} and Kamran Behnia^{1,2,†}



a) Hall resistivity, ρ_{xz} ; b) Hall conductivity, σ_{xz} , extracted from ρ_{xz} , ρ_{xx} , and ρ_{zz} ; c) Nernst signal, S_{xz} ; d) Transverse thermoelectric conductivity, α_{xz} ,



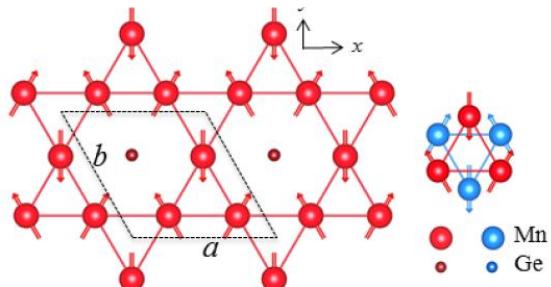
Magnetization dependence of the spontaneous Nernst effect for ferromagnetic metals and Mn_3Sn

Large anomalous Nernst effect at room temperature in a chiral antiferromagnet

Muhammad Ikhlas^{1†}, Takahiro Tomita^{1†}, Takashi Koretsune^{2,3}, Michi-To Suzuki²,
 Daisuke Nishio-Hamane¹, Ryotaro Arita^{2,4}, Yoshichika Otani^{1,2,4} and Satoru Nakatsuji^{1,4*}



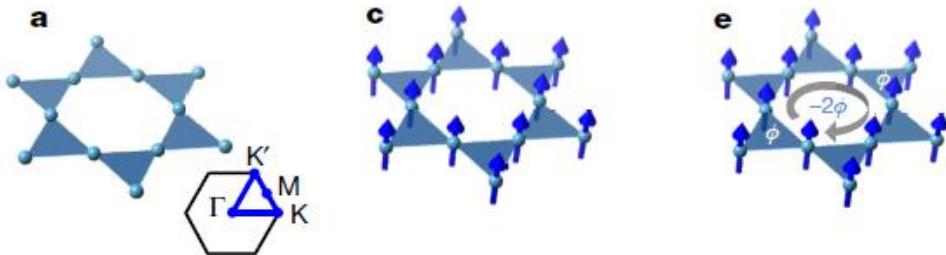
Kagome lattice



LETTER

doi:10.1038/nature25987

Massive Dirac fermions in a ferromagnetic kagome metal



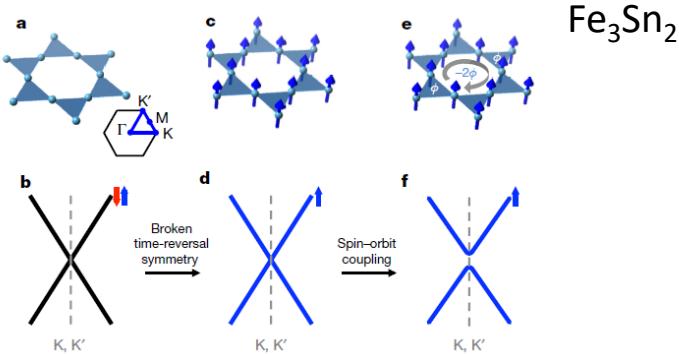


Kagome lattice

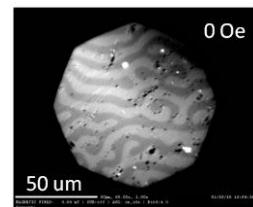
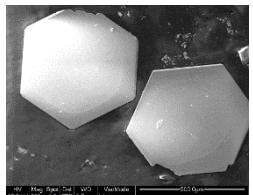
LETTER

doi:10.1038/nature25987

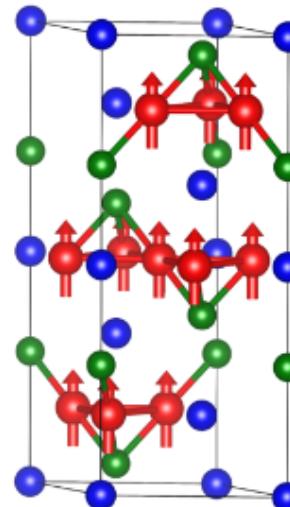
Massive Dirac fermions in a ferromagnetic kagomé metal



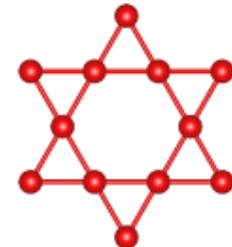
Fe_3Sn_2



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

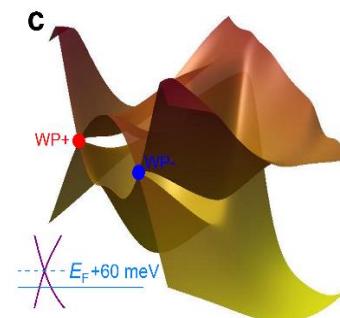
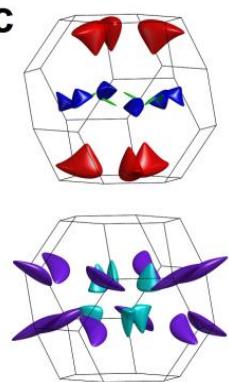
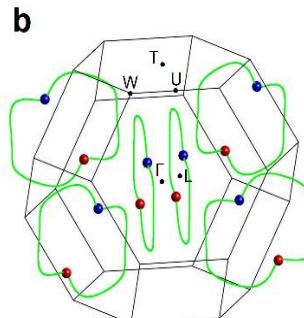
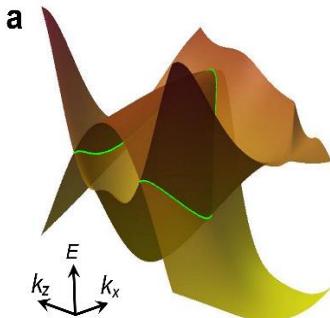
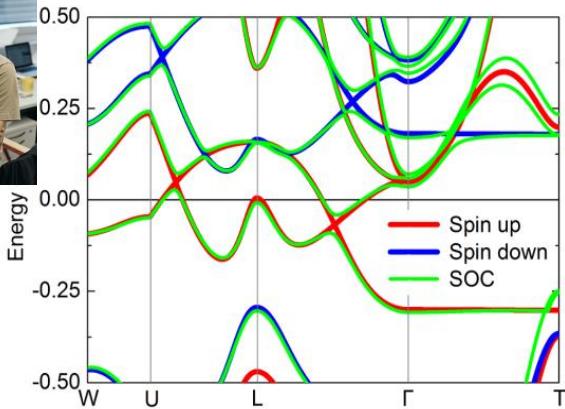


Co
Sn
S



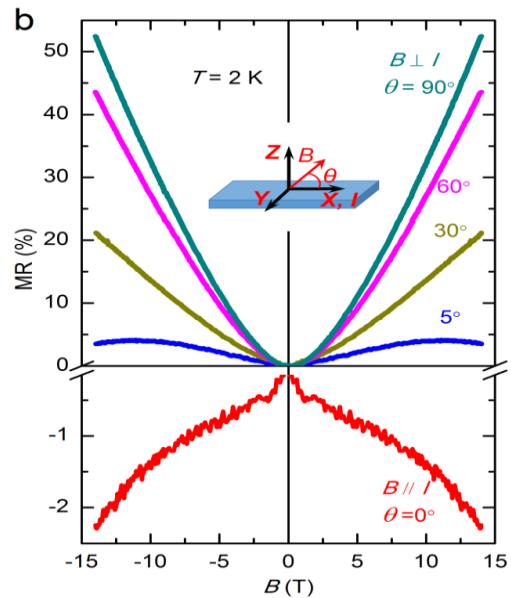


Weyl and Berry



Weyl points are close to EF
Hard magnetic behaviour

transport: chiral anomaly

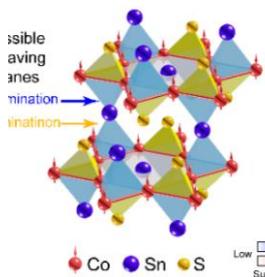
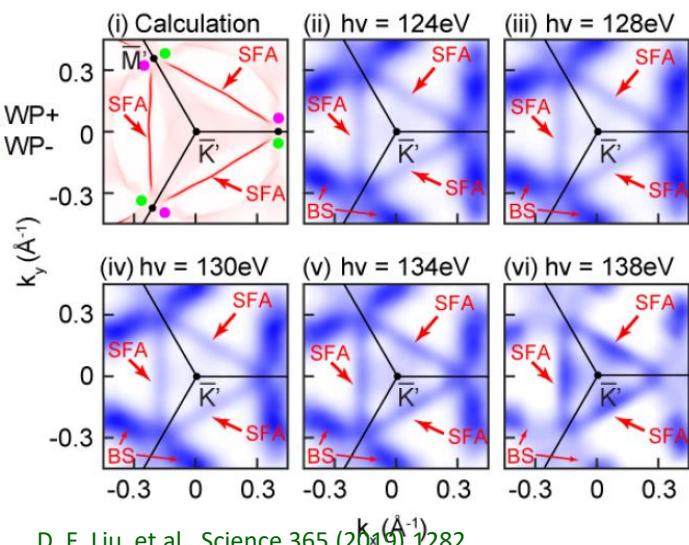




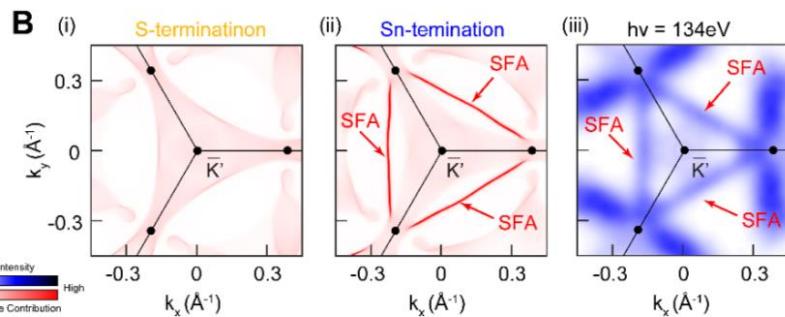
Weyl and Berry



STM and ARPES confirms Weyl and Fermiarcs



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Co Sn S

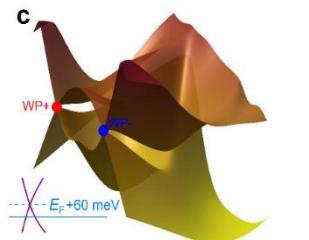
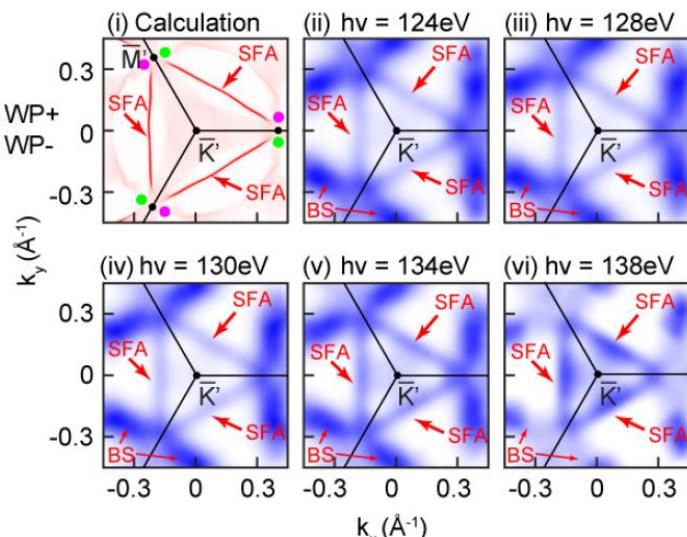




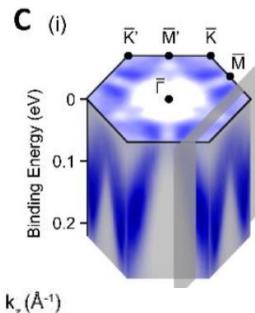
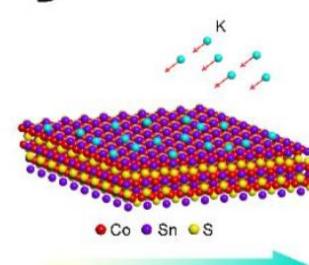
Weyl and Berry



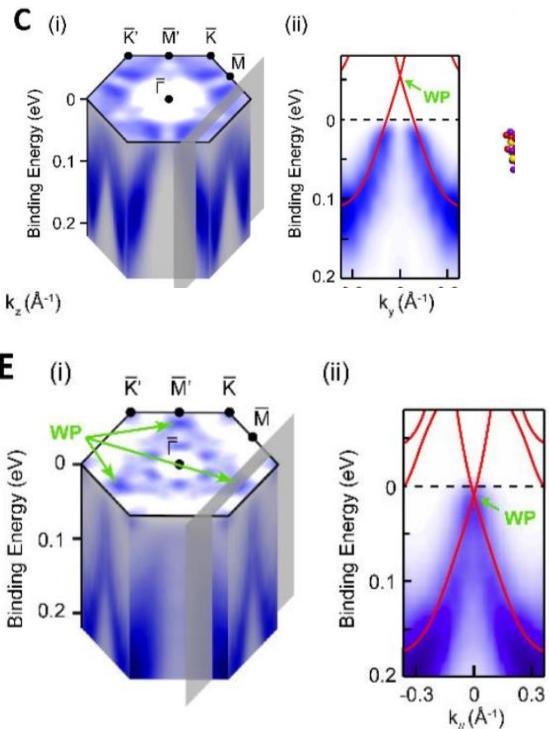
STM and ARPES confirms Weyl and Fermiarcs



D

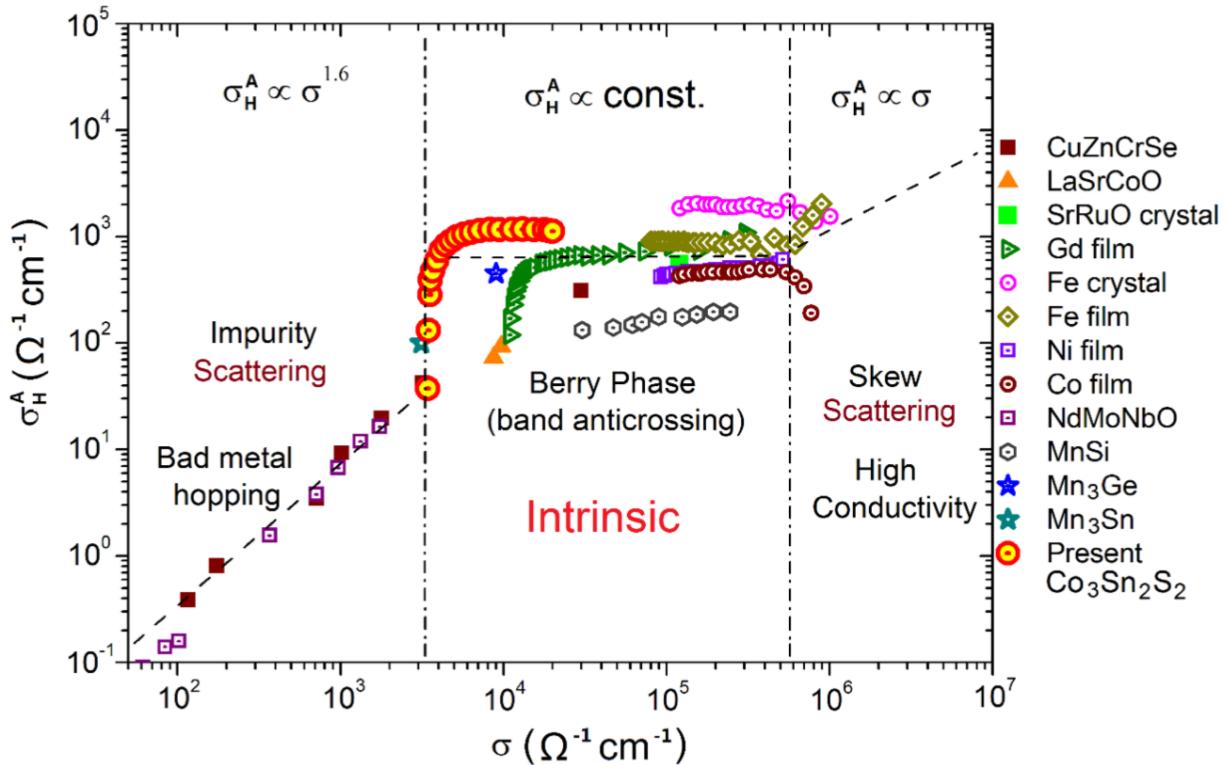
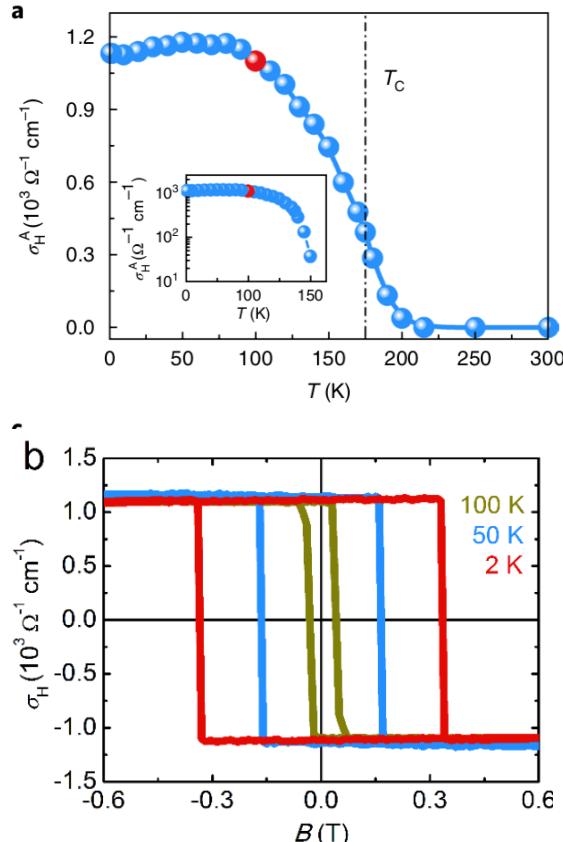


E





new transport properties

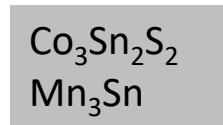
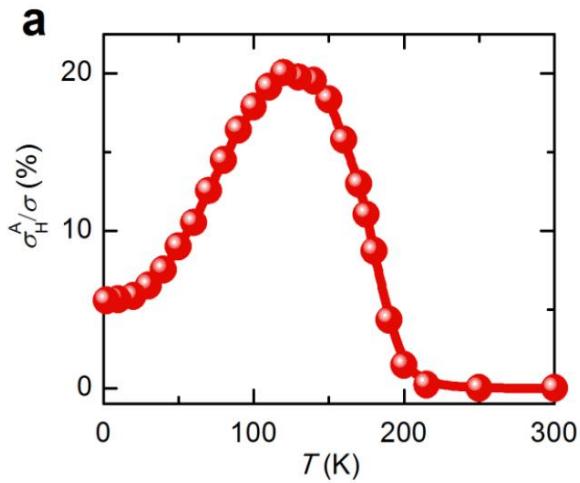




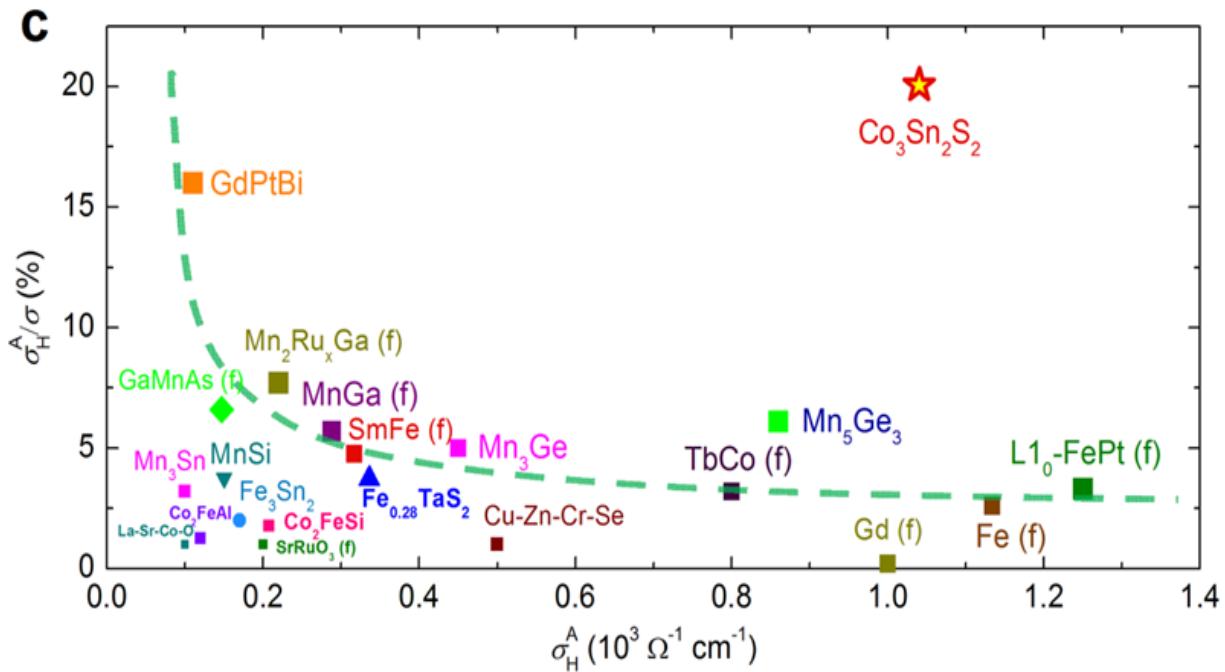
new transport properties

Berry curvature design

- giant anomalous Hall
- giant anomalous Nernst



Giant Hall Angle 20%



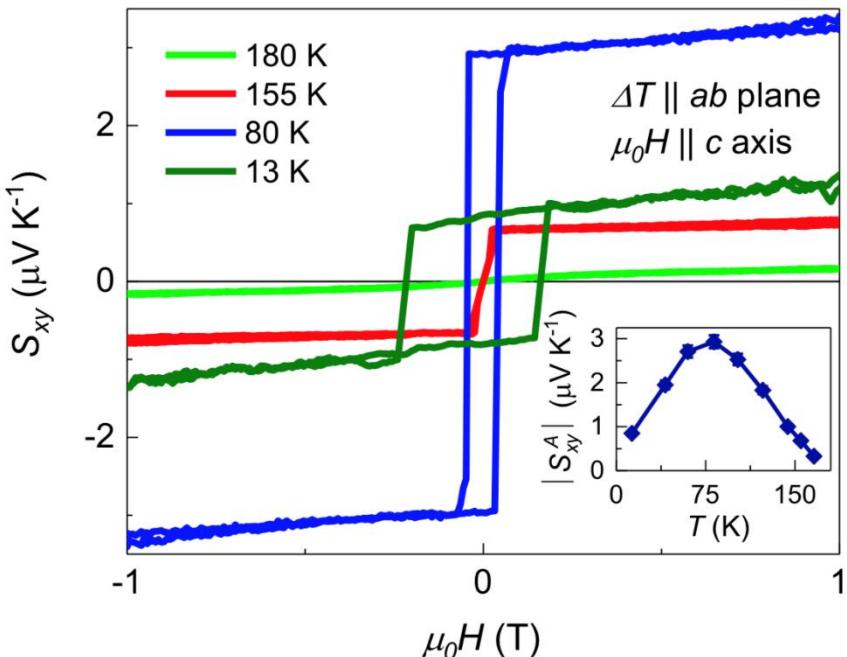
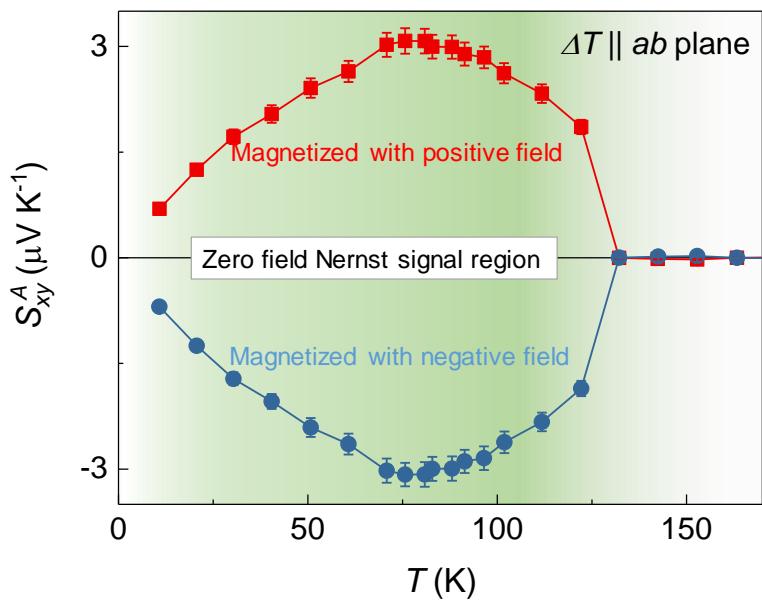


new transport properties

Berry curvature design

- giant anomalous Hall
- giant anomalous Nernst

Co₂MnGa
Co₃Sn₂S₂
Mn₃Sn



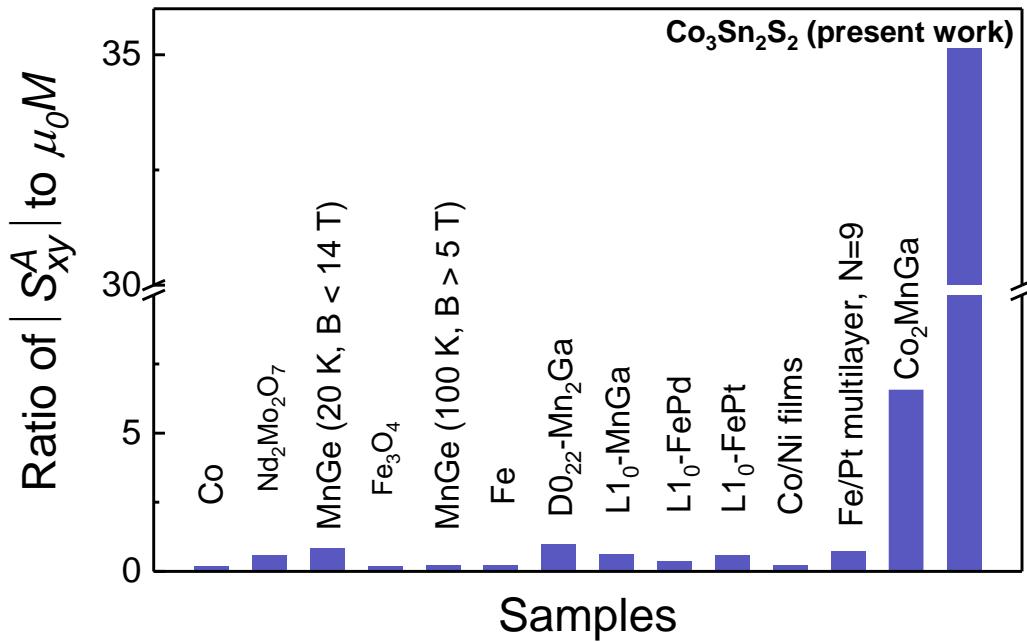
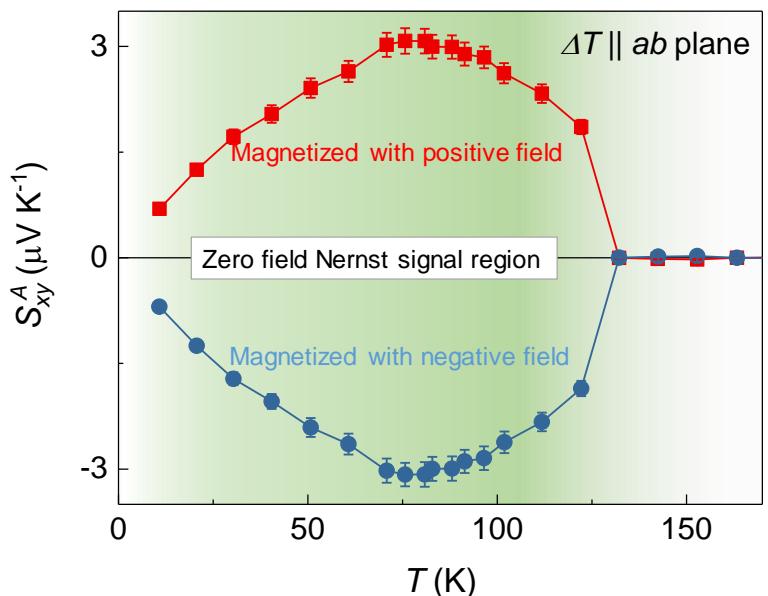


new transport properties

Berry curvature design

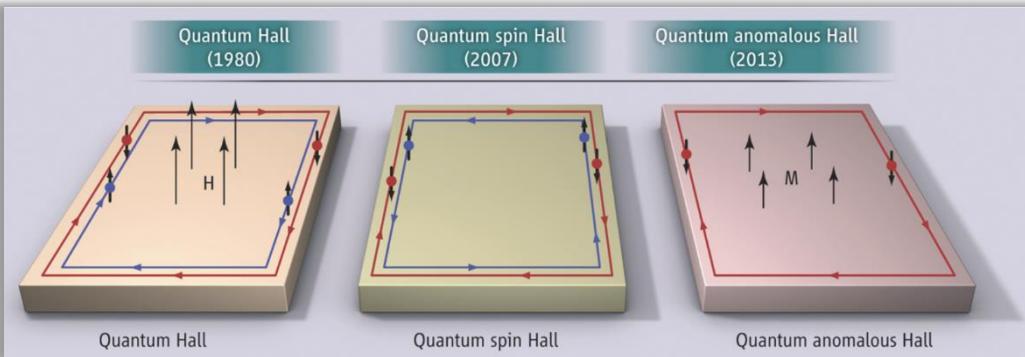
- giant anomalous Hall
- giant anomalous Nernst

Co_2MnGa
 $\text{Co}_3\text{Sn}_2\text{S}_2$
 Mn_3Sn

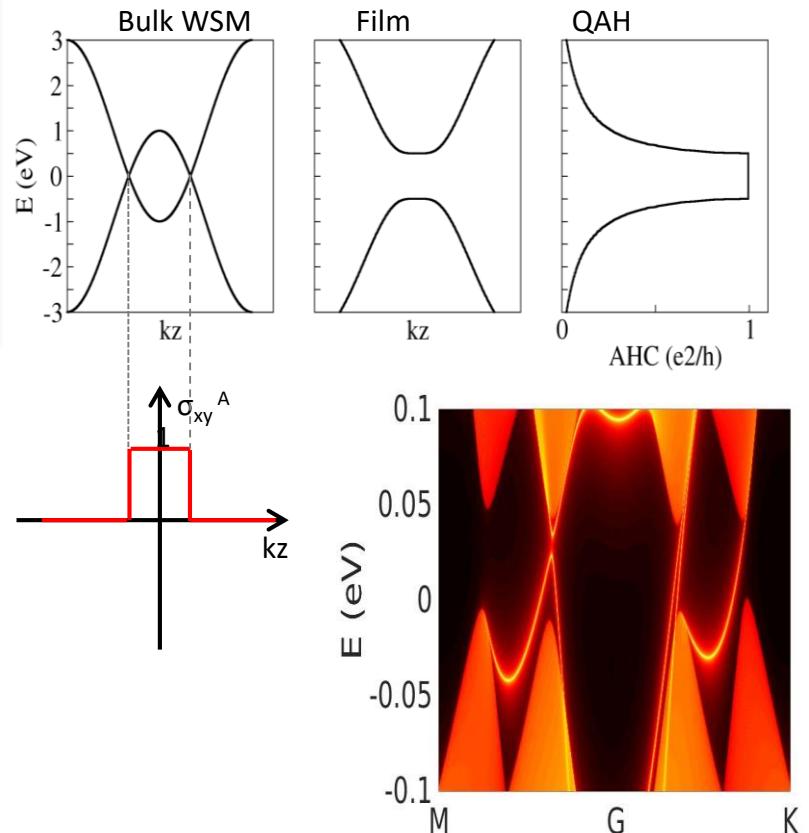




quantum devices

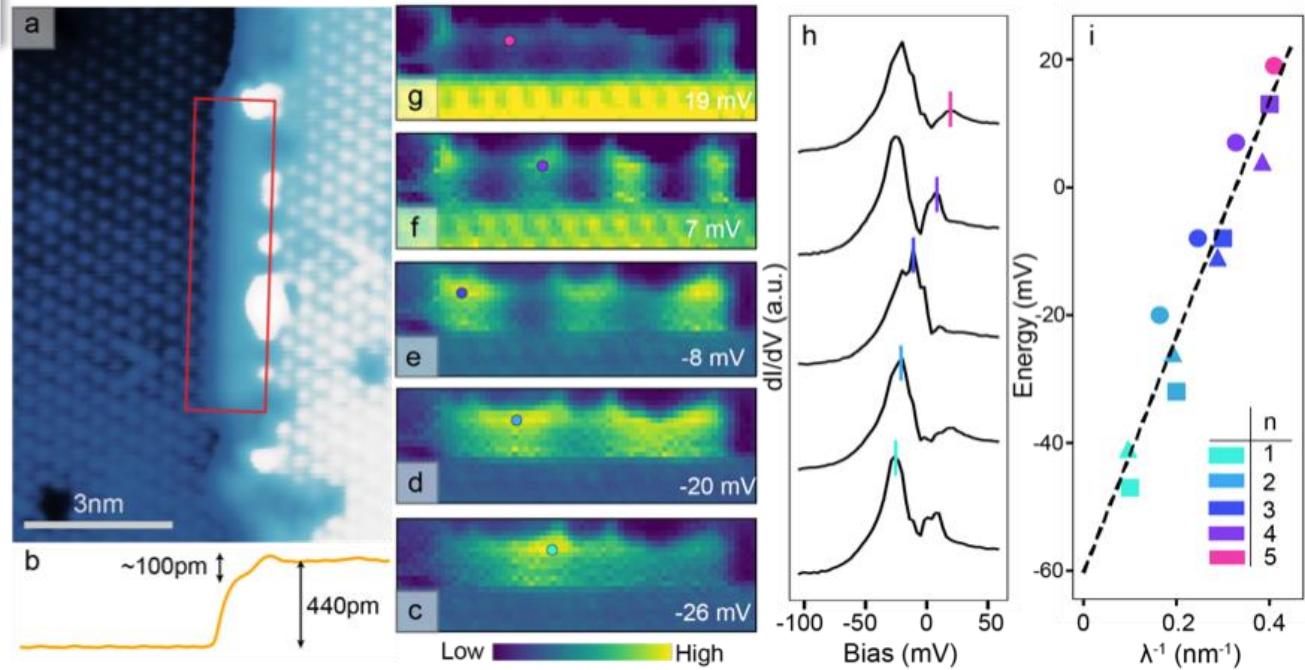
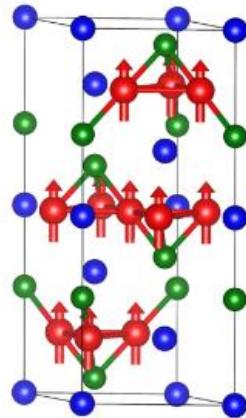
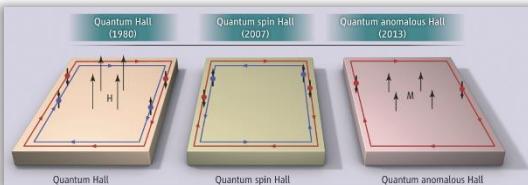


- Towards QAHE in MBE grown thin films.
- Magnetic Weyl for QAH effect in 2D





quantum anomalous Hall





new physics

- Berry phase design of materials for energy conversion and Hall sensors
- Quantum anomalous Hall effect at room temperature
- Berry curvature design in real and reciprocal space
- devices made of thin films and crystals

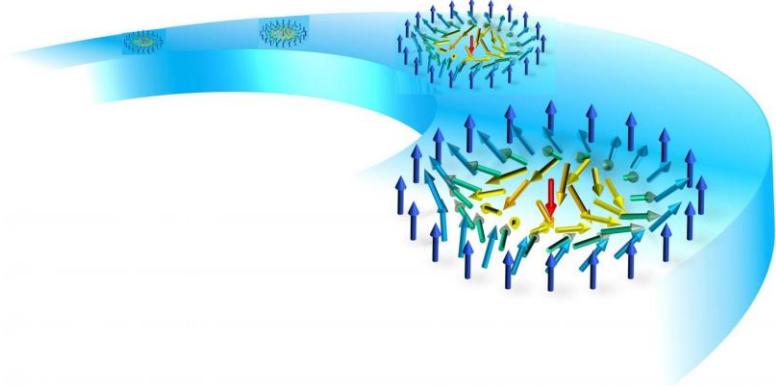
- potential applications

- spintronics

- Racetrack memory
- Majorana fermions
- Spin Hall based MRAM
- antiferromagnetic Spintronics
- Spincaloritronics

- quantum computing

- energy conversion



thank you for your attention



Yulin Chen
Stuart Parkin
and teams



Andrei
Bernevig
and Zahid
Hasan

