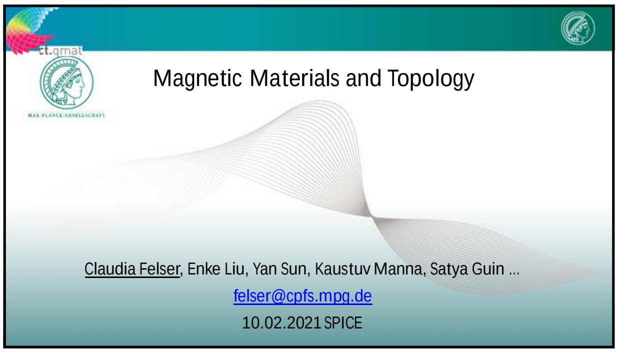
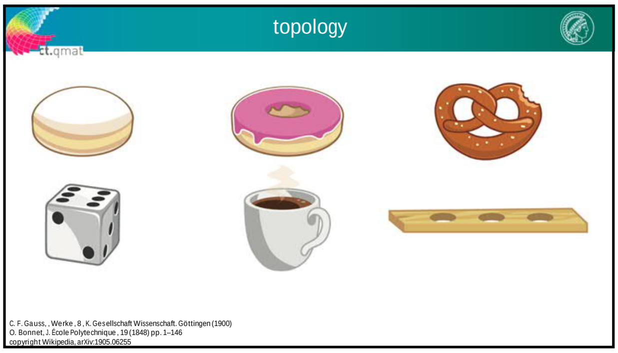
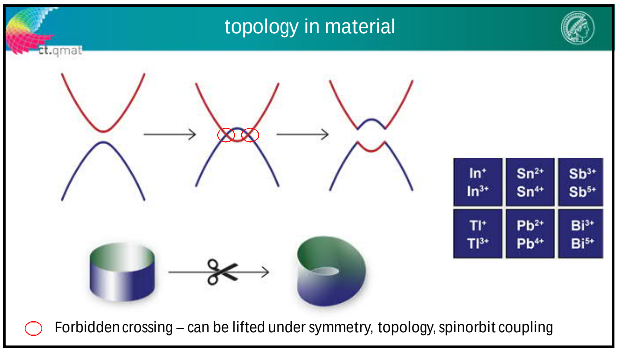
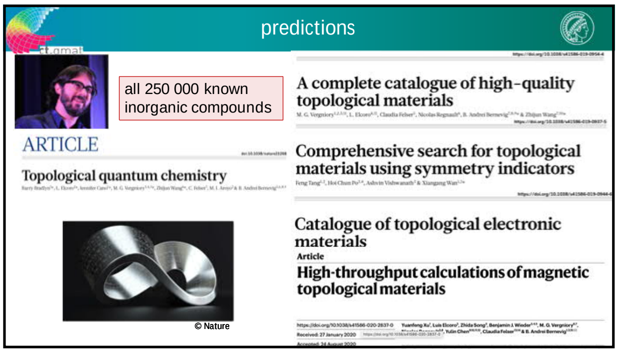
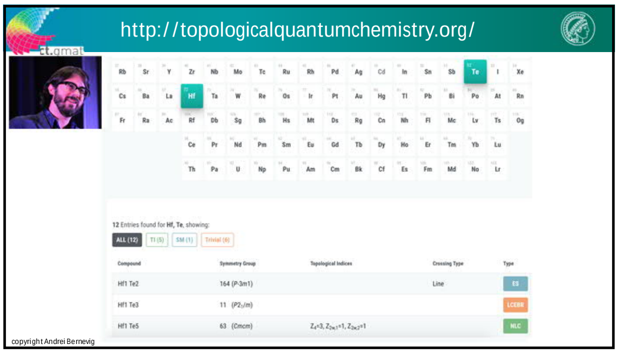
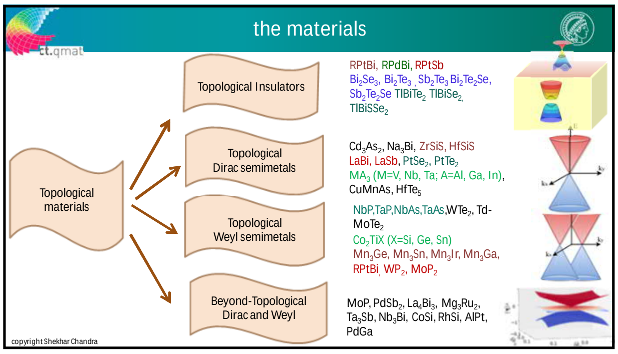

ct.qmat
Magnetic Materials and Topology
Claudia Felser, Enke Liu, Yan Sun, Kaustuv Manna, Satya Guin ...
felser@cpfs.mpg.de
10.02.2021 SPICE

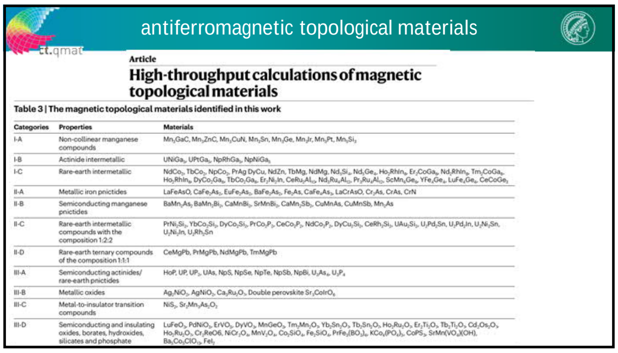

topology
ct.qmat
C. F. Gauss, , Werke , 8 , K. Gesellschaft Wissenschaft. Göttingen (1900)
O. Bonnet, J. École Polytechnique, 19 (1848) pp. 1–146
copyright Wikipedia, arXiv:1905.06255

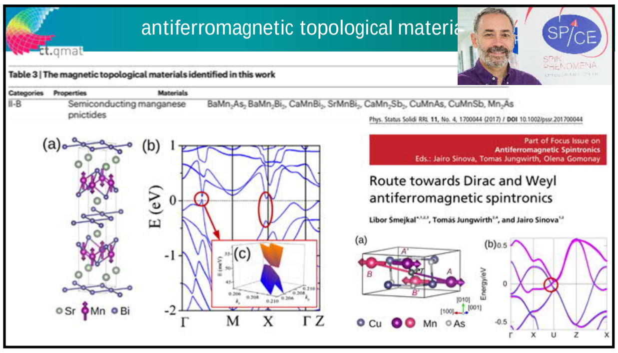

topology in material
ct.qmat
In⁺ In³⁺
Sn²⁺ Sn⁴⁺
Sb³⁺ Sb⁵⁺
Tl⁺ Tl³⁺
Pb²⁺ Pb⁴⁺
Bi³⁺ Bi⁵⁺
Forbidden crossing – can be lifted under symmetry, topology, spinorbit coupling

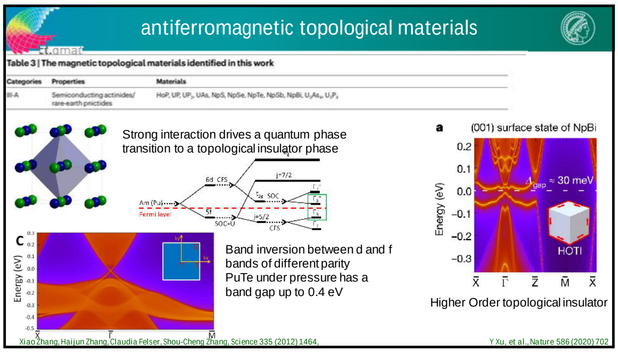

predictions
ct.qmat
all 250 000 known inorganic compounds
ARTICLE
Topological quantum chemistry
A complete catalogue of high-quality topological materials
Comprehensive search for topological materials using symmetry indicators
Catalogue of topological electronic materials
Article
High-throughput calculations of magnetic topological materials
© Nature
Received: 27 January 2020
Accepted: 24 August 2020


http://topologicalquantumchemistry.org/
ct.qmat
copyright Andrei Bernevig


the materials
ct.qmat
Topological materials
Topological Insulators
Topological Dirac semimetals
Topological Weyl semimetals
Beyond-Topological Dirac and Weyl
RPtBi, RPdBi, RPtSb
Bi2Se3, Bi2Te3 , Sb2Te3 Bi2Te2Se, Sb2Te2Se TlBiTe2, TlBiSe2, TlBiSSe2
Cd3As2, Na3Bi, ZrSiS, HfSiS
LaBi, LaSb, PtSe2, PtTe2
MA3 (M=V, Nb, Ta; A=Al, Ga, In),
CuMnAs, HfTe5
NbP,TaP,NbAs,TaAs,WTe2, Td-MoTe2
Co2TiX (X=Si, Ge, Sn)
Mn3Ge, Mn3Sn, Mn3Ir, Mn3Ga,
RPtBi, WP2, MoP2
MoP, PdSb2, La4Bi3, Mg3Ru2, Ta3Sb, Nb3Bi, CoSi, RhSi, AlPt, PdGa
copyright Shekhar Chandra


antiferromagnetic topological materials
ct.qmat
Article
High-throughput calculations of magnetic topological materials
Table 3 | The magnetic topological materials identified in this work
Categories | Properties | Materials
I-A | Non-collinear manganese compounds | Mn3GaC, Mn3ZnC, Mn3CuN, Mn3Sn, Mn3Ge, Mn3Ir, Mn3Pt, Mn5Si3
I-B | Actinide intermetallic | UNiGa5, UPtGa5, NpRhGa5, NpNiGa5
I-C | Rare-earth intermetallic | NdCo2, TbCo2, NpCo2, PrAg DyCu, NdZn, TbMg, NdMg, Nd5Si4, Nd5Ge4, Ho2RhIn8, Er2CoGa8, Nd2RhIn8, Tm2CoGa8, Ho2RhIn8, DyCo2Ga8, TbCo2Ga8, Er2Ni2In, CeRu2Al10, Nd3Ru4Al12, Pr3Ru4Al12, ScMn6Ge6, YFe6Ge6, LuFe6Ge6, CeCoGe3
II-A | Metallic iron pnictides | LaFeAsO, CaFe2As2, EuFe2As2, BaFe2As2, Fe2As, CaFe4As3, LaCrAsO, Cr2As, CrAs, CrN
II-B | Semiconducting manganese pnictides | BaMn2As2, BaMn2Bi2, CaMnBi2, SrMnBi2, CaMn2Sb2, CuMnAs, CuMnSb, Mn2As
II-C | Rare-earth intermetallic compounds with the composition 1:2:2 | PrNi2Si2, YbCo2Si2, DyCo2Si2, PrCo2P2, CeCo2P2, NdCo2P2, DyCu2Si2, CeRh2Si2, UAu2Si2, U2Pd2Sn, U2Pd2In, U2Ni2Sn, U2Ni2In, U2Rh2Sn
II-D | Rare-earth ternary compounds of the composition 1:1:1 | CeMgPb, PrMgPb, NdMgPb, TmMgPb
III-A | Semiconducting actinides/rare-earth pnictides | HoP, UP, UP2, UAs, NpS, NpSe, NpTe, NpSb, NpBi, U3As4, U3P4
III-B | Metallic oxides | Ag2NiO2, AgNiO2, Ca3Ru2O7, Double perovskite Sr2CoIrO6
III-C | Metal-to-insulator transition compounds | NiS2, Sr2Mn3As2O2
III-D | Semiconducting and insulating oxides, borates, hydroxides, silicates and phosphate | LuFeO3, PdNiO3, ErVO3, DyVO3, MnGeO3, Tm2Mn2O7, Yb2Sn2O7, Tb2Sn2O7, Ho2Ru2O7, Er2Ti2O7, Tb2Ti2O7, Cd2Os2O7, Ho2Ru2O7, Cr2ReO6, NiCr2O4, MnV2O4, Co2SiO4, Fe2SiO4, PrFe3(BO3)4, KCo4(PO4)3, CoPS3, SrMn(VO4)(OH), Ba3Co2ClO12, FeI2


antiferromagnetic topological materia
ct.qmat
SP/CE
SPIN PHENOMENA
Table 3 | The magnetic topological materials identified in this work
Categories | Properties | Materials
II-B | Semiconducting manganese pnictides | BaMn2As2, BaMn2Bi2, CaMnBi2, SrMnBi2, CaMn2Sb2, CuMnAs, CuMnSb, Mn2As
Phys. Status Solidi RRL 11, No. 4, 1700044 (2017) / DOI 10.1002/pssr.201700044
Part of Focus Issue on Antiferromagnetic Spintronics
Eds.: Jairo Sinova, Tomas Jungwirth, Olena Gomonay
Route towards Dirac and Weyl antiferromagnetic spintronics
Libor Šmejkal, Tomáš Jungwirth, and Jairo Sinova
(a)
(b)
(c)
E (eV)
Γ M X Γ Z
Sr Mn Bi
Cu Mn As
Energy/eV
Γ X U Z X


antiferromagnetic topological materials
ct.qmat
Table 3 | The magnetic topological materials identified in this work
Categories | Properties | Materials
III-A | Semiconducting actinides/rare-earth pnictides | HoP, UP, UP2, UAs, NpS, NpSe, NpTe, NpSb, NpBi, U3As4, U3P4
Strong interaction drives a quantum phase transition to a topological insulator phase
Fermi level
Band inversion between d and f bands of different parity
PuTe under pressure has a band gap up to 0.4 eV
a
(001) surface state of NpBi
Energy (eV)
≈ 30 meV
HOTI
Higher Order topological insulator
Xiao Zhang, Haijun Zhang, Claudia Felser, Shou-Cheng Zhang, Science 335 (2012) 1464,
Y Xu, et al., Nature 586 (2020) 702

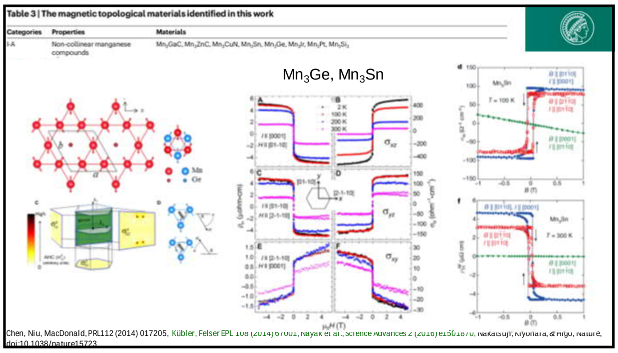
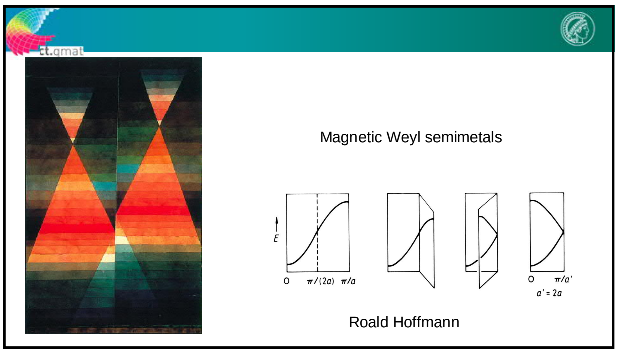
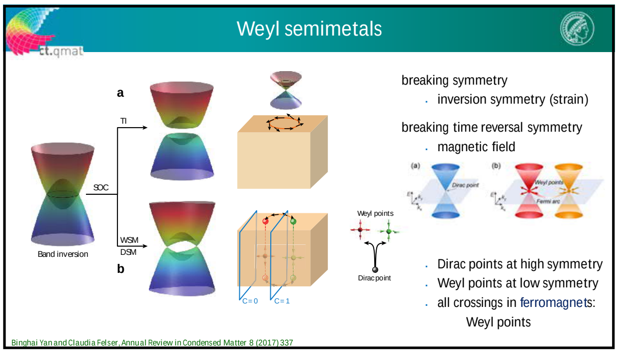
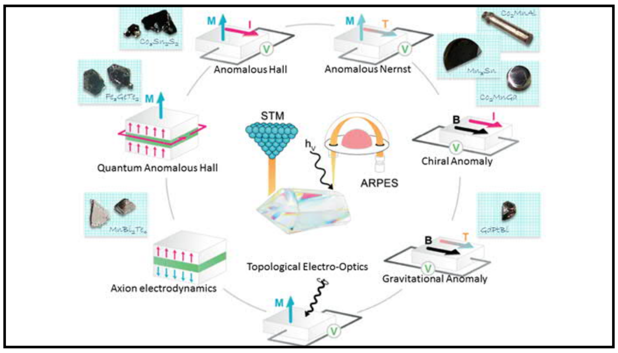
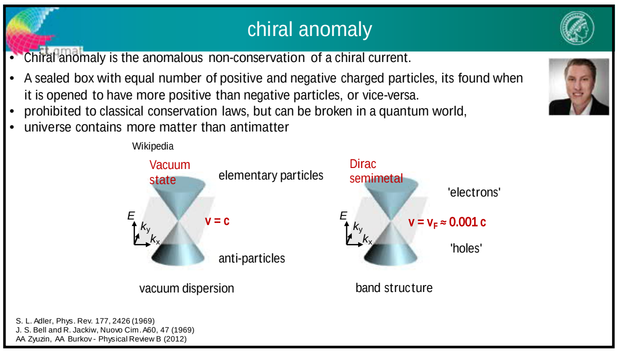


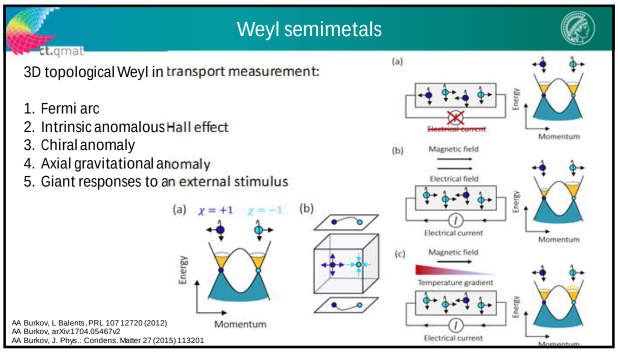
Table 3 | The magnetic topological materials identified in this work
Categories | Properties | Materials
I-A | Non-collinear manganese compounds | Mn3GaC, Mn3ZnC, Mn3CuN, Mn3Sn, Mn3Ge, Mn3Ir, Mn3Pt, Mn5Si3
Mn3Ge, Mn3Sn
Mn
Ge
2 K
100 K
200 K
300 K
Mn3Sn
T = 100 K
T = 300 K
B (T)
μ0H (T)
Chen, Niu, MacDonald, PRL112 (2014) 017205, Kübler, Felser EPL 108 (2014) 67001, Nayak et al., Science Advances 2 (2016) e1501870, Nakatsuji, Kiyohara, & Higo, Nature, doi:10.1038/nature15723

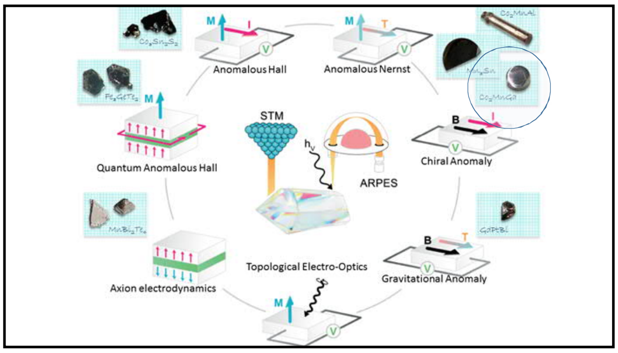

ct.qmat
Magnetic Weyl semimetals
E
0 π/(2a) π/a
0 π/a'
a' = 2a
Roald Hoffmann

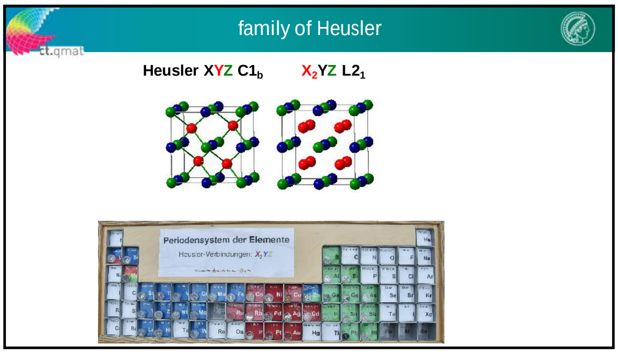

Weyl semimetals
ct.qmat
a
TI
SOC
Band inversion
WSM
DSM
b
C=0
C=1
Weyl points
Dirac point
breaking symmetry
inversion symmetry (strain)
breaking time reversal symmetry
magnetic field
(a)
(b)
Dirac point
Weyl points
Fermi arc
Dirac points at high symmetry
Weyl points at low symmetry
all crossings in ferromagnets: Weyl points
Binghai Yan and Claudia Felser, Annual Review in Condensed Matter 8 (2017) 337

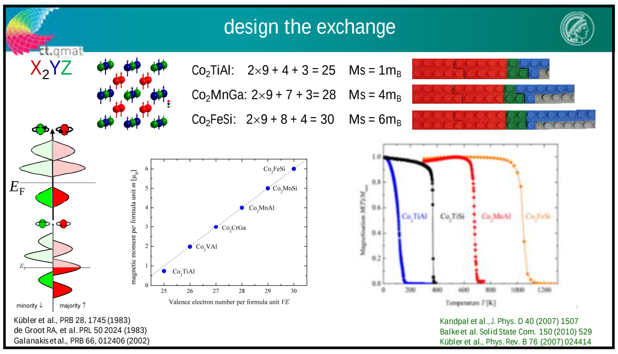

Anomalous Hall
Anomalous Nernst
STM
Quantum Anomalous Hall
Chiral Anomaly
ARPES
Topological Electro-Optics
Gravitational Anomaly
Axion electrodynamics

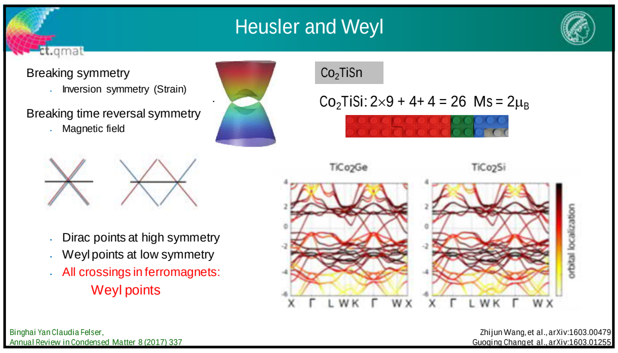

chiral anomaly
• Chiral anomaly is the anomalous non-conservation of a chiral current.
• A sealed box with equal number of positive and negative charged particles, its found when it is opened to have more positive than negative particles, or vice-versa.
• prohibited to classical conservation laws, but can be broken in a quantum world,
• universe contains more matter than antimatter
Wikipedia
Vacuum state
elementary particles
v = c
anti-particles
vacuum dispersion
Dirac semimetal
'electrons'
v = v_F ≈ 0.001 c
'holes'
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)

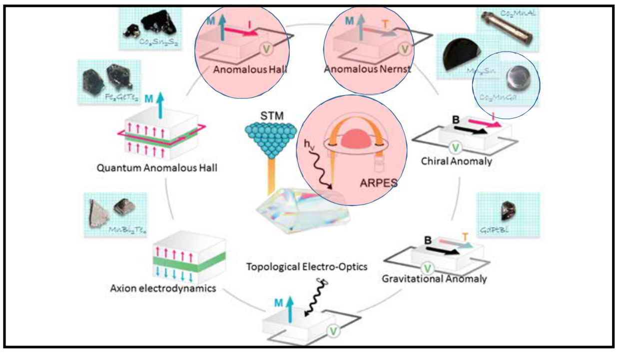

Weyl semimetals
3D topological Weyl in transport measurement:
1. Fermi arc
2. Intrinsic anomalous Hall effect
3. Chiral anomaly
4. Axial gravitational anomaly
5. Giant responses to an external stimulus
Magnetic field
Electrical field
Electrical current
Temperature gradient
Energy
Momentum
AA Burkov, L Balents, PRL 107 12720 (2012)
AA Burkov, arXiv:1704.05467v2
AA Burkov, J. Phys.: Condens. Matter 27 (2015) 113201

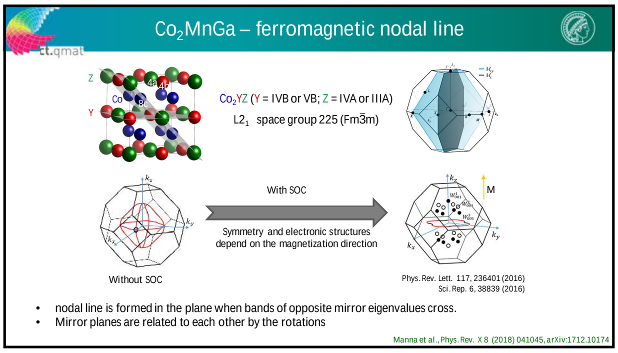

Anomalous Hall
Anomalous Nernst
STM
Quantum Anomalous Hall
Chiral Anomaly
ARPES
Topological Electro-Optics
Gravitational Anomaly
Axion electrodynamics

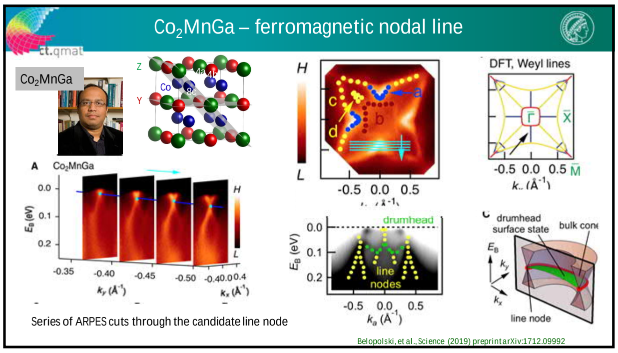

family of Heusler
Heusler XYZ C1b
X2YZ L21
Periodensystem der Elemente
Heusler-Verbindungen: X2YZ

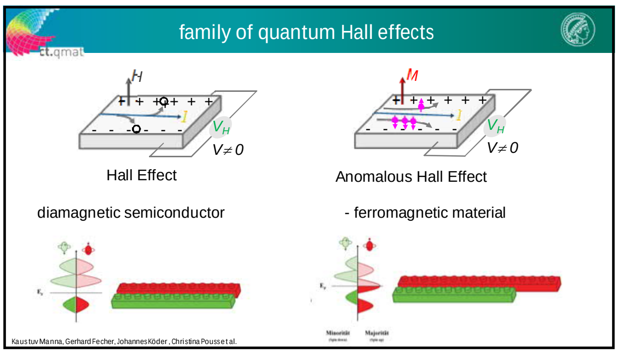

design the exchange
X2YZ
Co2TiAl: 2×9 + 4 + 3 = 25 Ms = 1mB
Co2MnGa: 2×9 + 7 + 3= 28 Ms = 4mB
Co2FeSi: 2×9 + 8 + 4 = 30 Ms = 6mB
EF
minority ↓
majority ↑
Valence electron number per formula unit FE
Temperature T [K]
Kübler et al., PRB 28, 1745 (1983)
de Groot RA, et al. PRL 50 2024 (1983)
Galanakis et 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

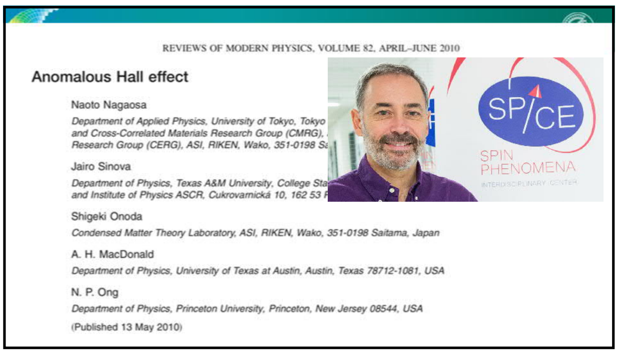

Heusler and Weyl
Breaking symmetry
Inversion symmetry (Strain)
Breaking time reversal symmetry
Magnetic field
Co2TiSn
Co2TiSi: 2×9 + 4+ 4 = 26 Ms = 2μB
TiCo2Ge
TiCo2Si
orbital localization
Dirac points at high symmetry
Weyl points at low symmetry
All crossings in ferromagnets:
Weyl points
Binghai Yan Claudia Felser,
Annual Review in Condensed Matter 8 (2017) 337
Zhijun Wang, et al., arXiv:1603.00479
Guoqing Chang et al., arXiv:1603.01255

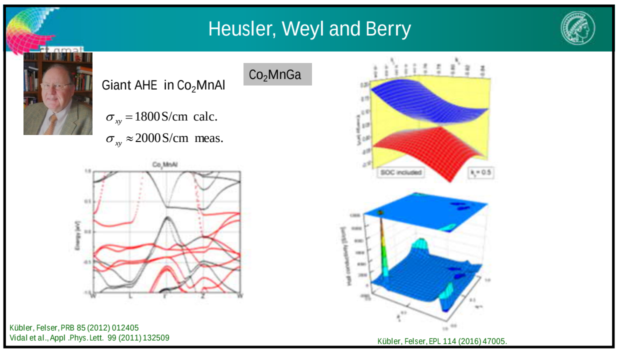

Anomalous Hall
Anomalous Nernst
Quantum Anomalous Hall
STM
ARPES
Chiral Anomaly
Topological Electro-Optics
Gravitational Anomaly
Axion electrodynamics

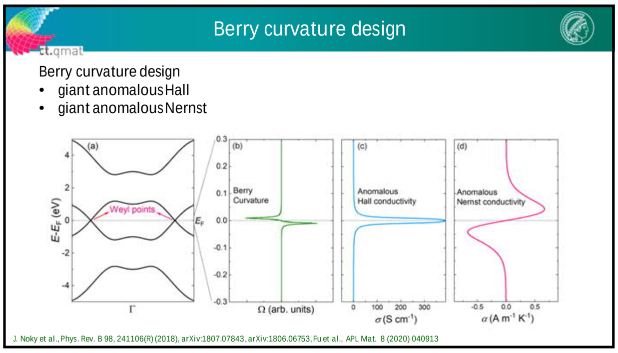

Co2MnGa – ferromagnetic nodal line
Co2YZ (Y = IVB or VB; Z = IVA or IIIA)
L21 space group 225 (Fm3m)
With SOC
Symmetry and electronic structures depend on the magnetization direction
Without SOC
Phys. Rev. Lett. 117, 236401 (2016)
Sci. Rep. 6, 38839 (2016)
nodal line is formed in the plane when bands 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

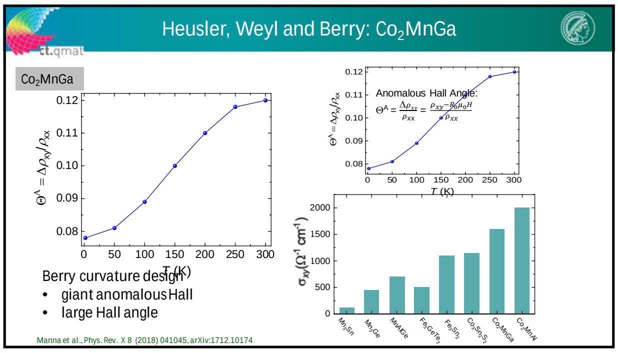

Co2MnGa – ferromagnetic nodal line
Co2MnGa
DFT, Weyl lines
drumhead
line nodes
drumhead surface state
bulk cone
line node
Series of ARPES cuts through the candidate line node
Belopolski, et al., Science (2019) preprint arXiv:1712.09992

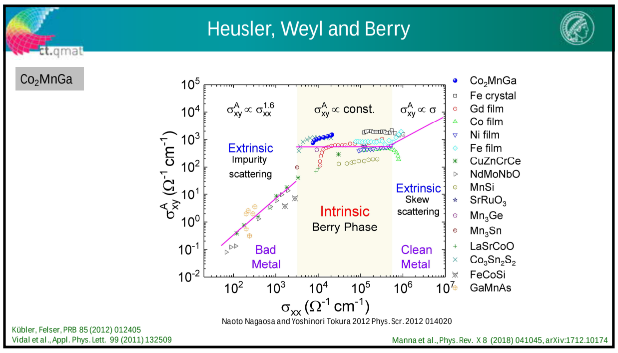

family of quantum Hall effects
Hall Effect
Anomalous Hall Effect
diamagnetic semiconductor
- ferromagnetic material
Kaustuv Manna, Gerhard Fecher, Johannes Köder, Christina Pousset al.

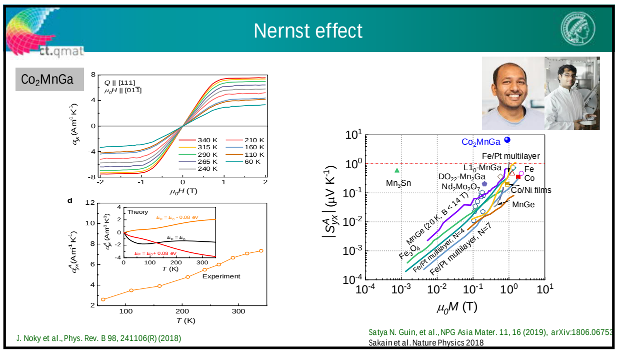

REVIEWS OF MODERN PHYSICS, VOLUME 82, APRIL–JUNE 2010
Anomalous Hall effect
Naoto Nagaosa
Jairo Sinova
Shigeki Onoda
Condensed Matter Theory Laboratory, ASI, RIKEN, Wako, 351-0198 Saitama, Japan
A. H. MacDonald
Department of Physics, University of Texas at Austin, Austin, Texas 78712-1081, USA
N. P. Ong
Department of Physics, Princeton University, Princeton, New Jersey 08544, USA
(Published 13 May 2010)
SP/CE
SPIN PHENOMENA

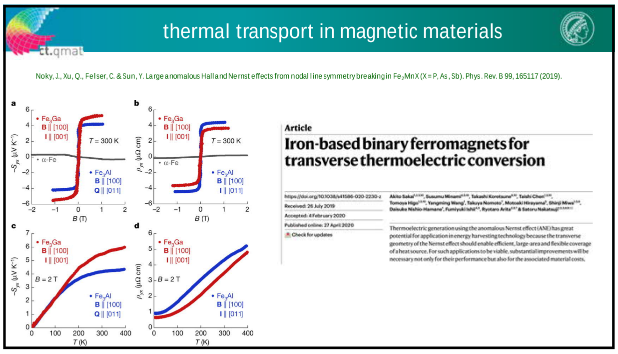

Heusler, Weyl and Berry
Giant AHE in Co_2MnAl
Co_2MnGa
$\sigma_{xy} = 1800$ S/cm calc.
$\sigma_{xy} \approx 2000$ S/cm meas.
Kübler, Felser, PRB 85 (2012) 012405
Vidal et al., Appl. Phys. Lett. 99 (2011) 132509
Kübler, Felser, EPL 114 (2016) 47005.

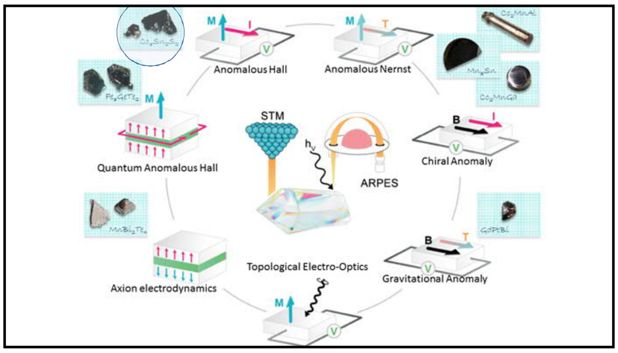

Berry curvature design
Berry curvature design
• giant anomalous Hall
• giant anomalous Nernst
Weyl points
Berry Curvature
Anomalous Hall conductivity
Anomalous Nernst conductivity
$E-E_F$ (eV)
Ω (arb. units)
σ (S cm⁻¹)
α (A m⁻¹ K⁻¹)
J. Noky et al., Phys. Rev. B 98, 241106(R) (2018), arXiv:1807.07843, arXiv:1806.06753, Fu et al., APL Mat. 8 (2020) 040913

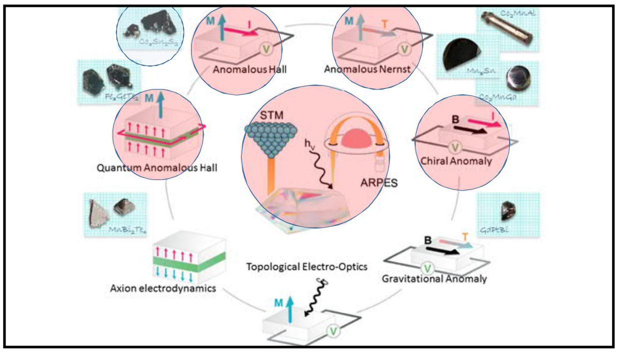

Heusler, Weyl and Berry: Co_2MnGa
Co_2MnGa
$\Theta^A = \Delta\rho_{xy}/\rho_{xx}$
T (K)
Anomalous Hall Angle:
Berry curvature design
• giant anomalous Hall
• large Hall angle
$\sigma_{xy}(\Omega^{-1}\,cm^{-1})$
Manna et al., Phys. Rev. X 8 (2018) 041045, arXiv:1712.10174

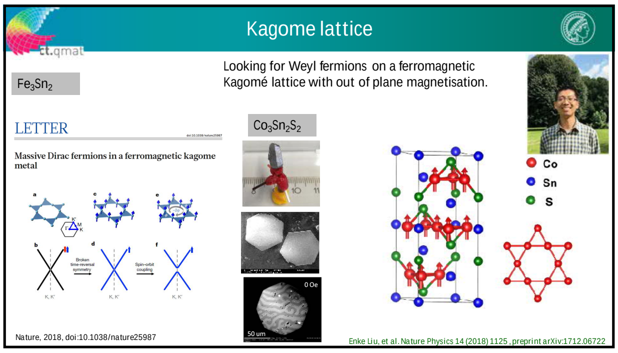

Heusler, Weyl and Berry
Co_2MnGa
$\sigma^A_{xy} \propto \sigma^{1.6}_{xx}$
$\sigma^A_{xy} \propto$ const.
$\sigma^A_{xy} \propto \sigma$
Extrinsic
Impurity scattering
Intrinsic
Berry Phase
Extrinsic
Skew scattering
Bad Metal
Clean Metal
σ_{xx} (Ω^{-1} cm^{-1})
Co_2MnGa
Fe crystal
Gd film
Co film
Ni film
Fe film
CuZnCrCe
NdMoNbO
MnSi
$SrRuO_3$
Mn_3Ge
Mn_3Sn
LaSrCoO
$Co_3Sn_2S_2$
FeCoSi
GaMnAs
Naoto Nagaosa and Yoshinori Tokura 2012 Phys. Scr. 2012 014020
Kübler, Felser, PRB 85 (2012) 012405
Vidal et al., Appl. Phys. Lett. 99 (2011) 132509
Manna et al., Phys. Rev. X 8 (2018) 041045, arXiv:1712.10174

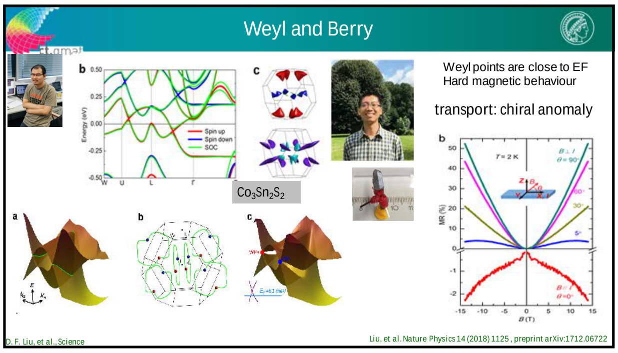

Nernst effect
Co_2MnGa
$\mu_0 H$ (T)
T (K)
Theory
Experiment
Co_2MnGa
Fe/Pt multilayer
Mn_3Sn
Co/Ni films
MnGe
$\mu_0 M$ (T)
J. Noky et al., Phys. Rev. B 98, 241106(R) (2018)
Satya N. Guin, et al., NPG Asia Mater. 11, 16 (2019), arXiv:1806.06753
Sakai et al. Nature Physics 2018

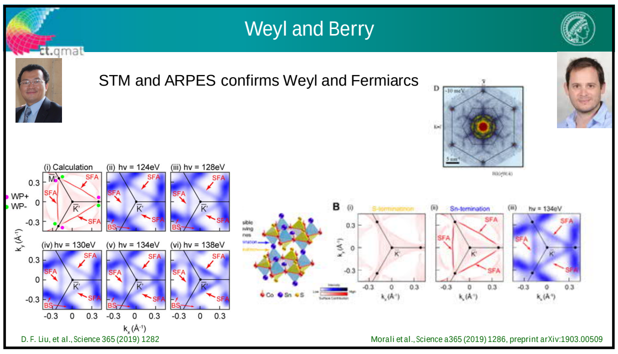

thermal transport in magnetic materials
Noky, J., Xu, Q., Felser, C. & Sun, Y. Large anomalous Hall and Nernst effects from nodal line symmetry breaking in Fe_2MnX (X = P, As, Sb). Phys. Rev. B 99, 165117 (2019).
Article
Iron-based binary ferromagnets for transverse thermoelectric conversion

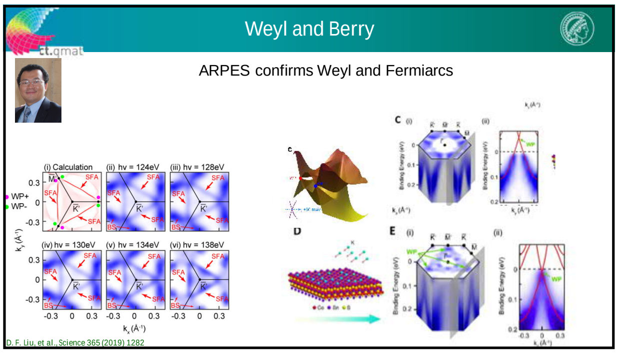

Anomalous Hall
Anomalous Nernst
STM
ARPES
Chiral Anomaly
Quantum Anomalous Hall
Topological Electro-Optics
Gravitational Anomaly
Axion electrodynamics

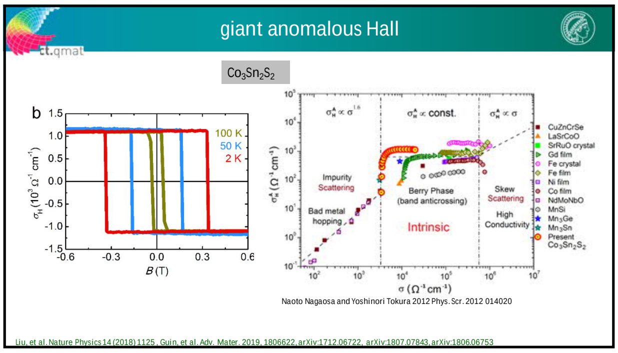

Anomalous Hall
Anomalous Nernst
STM
ARPES
Chiral Anomaly
Quantum Anomalous Hall
Topological Electro-Optics
Gravitational Anomaly
Axion electrodynamics

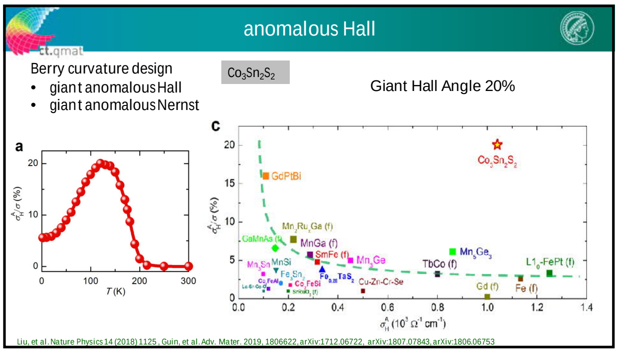

Kagome lattice
Fe_3Sn_2
LETTER
Massive Dirac fermions in a ferromagnetic kagome metal
Looking for Weyl fermions on a ferromagnetic Kagomé lattice with out of plane magnetisation.
$Co_3Sn_2S_2$
Co
Sn
S
Nature, 2018, doi:10.1038/nature25987
Enke Liu, et al. Nature Physics 14 (2018) 1125, preprint arXiv:1712.06722

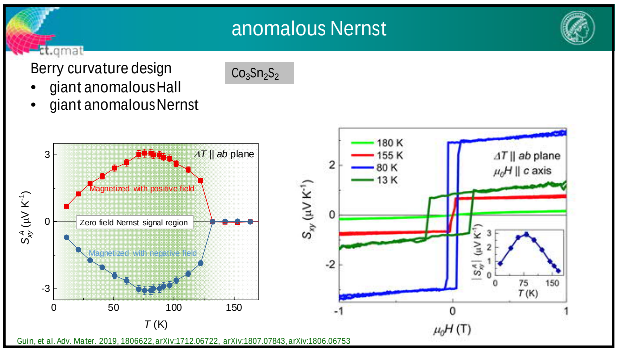

Weyl and Berry
Weyl points are close to EF
Hard magnetic behaviour
transport: chiral anomaly
$Co_3Sn_2S_2$
Spin up
Spin down
SOC
D. F. Liu, et al., Science
Liu, et al. Nature Physics 14 (2018) 1125, preprint arXiv:1712.06722

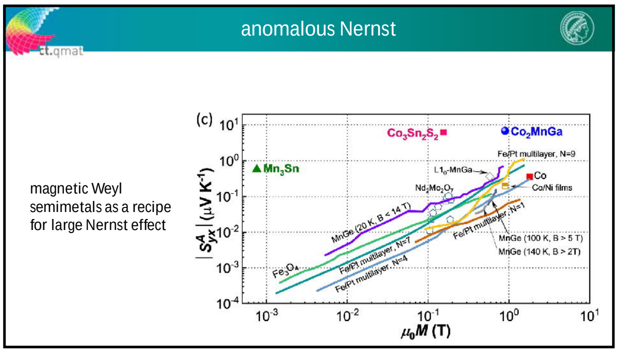

Weyl and Berry
STM and ARPES confirms Weyl and Fermiarcs
(i) Calculation
(ii) hv = 124eV
(iii) hv = 128eV
(iv) hv = 130eV
(v) hv = 134eV
(vi) hv = 138eV
WP+
WP-
SFA
S-termination
Sn-termination
D. F. Liu, et al., Science 365 (2019) 1282
Morali et al., Science a365 (2019) 1286, preprint arXiv:1903.00509

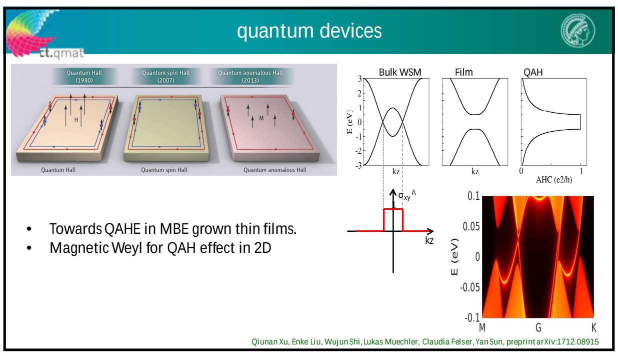

Weyl and Berry
ARPES confirms Weyl and Fermiarcs
(i) Calculation
(ii) hv = 124eV
(iii) hv = 128eV
(iv) hv = 130eV
(v) hv = 134eV
(vi) hv = 138eV
WP+
WP-
SFA
D. F. Liu, et al., Science 365 (2019) 1282

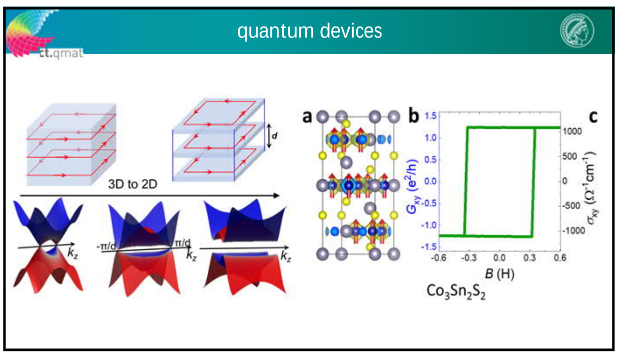

giant anomalous Hall
$Co_3Sn_2S_2$
100 K
50 K
2 K
B (T)
Impurity Scattering
Bad metal hopping
Berry Phase (band anticrossing)
Intrinsic
Skew Scattering
High Conductivity
Naoto Nagaosa and Yoshinori Tokura 2012 Phys. Scr. 2012 014020
Liu, et al. Nature Physics 14 (2018) 1125, Guin, et al. Adv. Mater. 2019, 1806622, arXiv:1712.06722, arXiv:1807.07843, arXiv:1806.06753

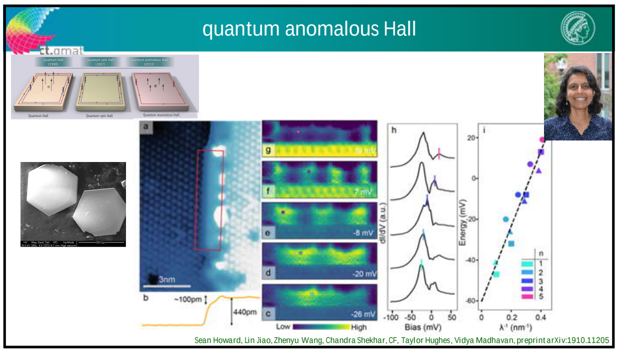

anomalous Hall
Berry curvature design
• giant anomalous Hall
• giant anomalous Nernst
$Co_3Sn_2S_2$
Giant Hall Angle 20%
T (K)
Liu, et al. Nature Physics 14 (2018) 1125, Guin, et al. Adv. Mater. 2019, 1806622, arXiv:1712.06722, arXiv:1807.07843, arXiv:1806.06753

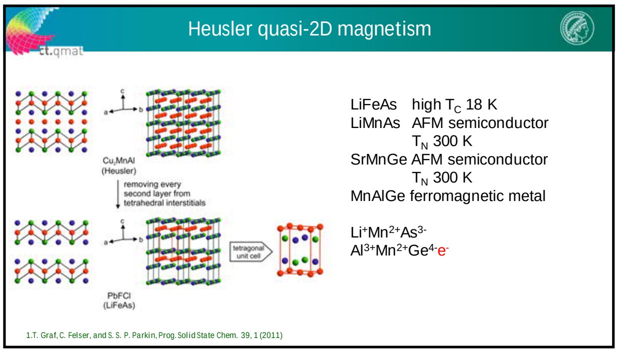

anomalous Nernst
Berry curvature design
• giant anomalous Hall
• giant anomalous Nernst
$Co_3Sn_2S_2$
Magnetized with positive field
Zero field Nernst signal region
Magnetized with negative field
T (K)
180 K
155 K
80 K
13 K
Guin, et al. Adv. Mater. 2019, 1806622, arXiv:1712.06722, arXiv:1807.07843, arXiv:1806.06753

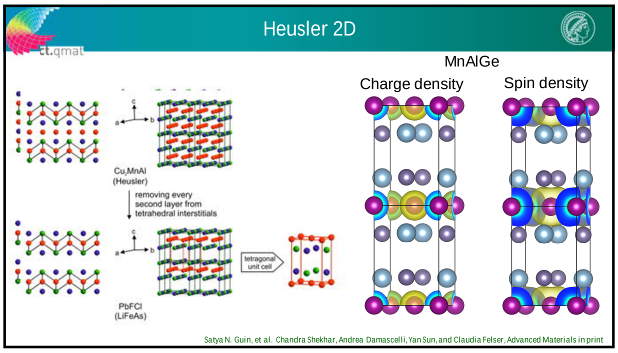

anomalous Nernst
magnetic Weyl semimetals as a recipe for large Nernst effect
$Co_3Sn_2S_2$
Co_2MnGa
Mn_3Sn
μ_0M (T)

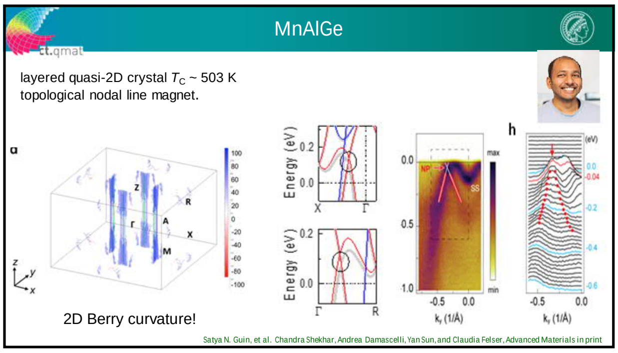

quantum devices
Bulk WSM
Film
QAH
• Towards QAHE in MBE grown thin films.
• Magnetic Weyl for QAH effect in 2D
Qiunan Xu, Enke Liu, Wujun Shi, Lukas Muechler, Claudia Felser, Yan Sun, preprint arXiv:1712.08915

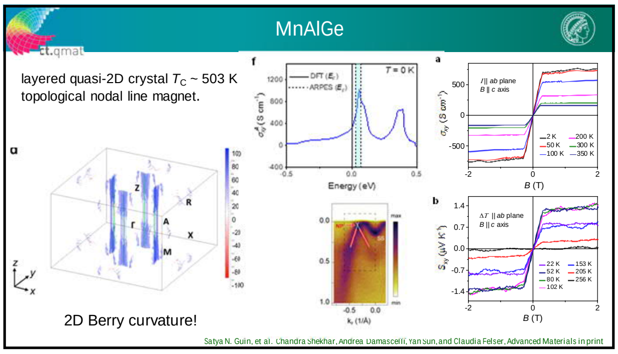

quantum devices
3D to 2D
B (H)
$Co_3Sn_2S_2$

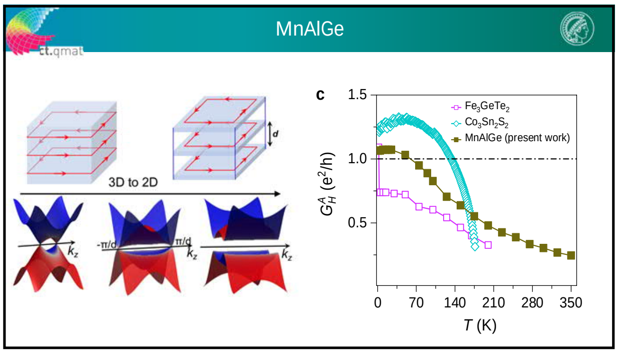

quantum anomalous Hall
Sean Howard, Lin Jiao, Zhenyu Wang, Chandra Shekhar, CF, Taylor Hughes, Vidya Madhavan, preprint arXiv:1910.11205


Heusler quasi-2D magnetism
Cu2MnAl (Heusler)
removing every second layer from tetrahedral interstitials
PbFCl (LiFeAs)
tetragonal unit cell
LiFeAs high TC 18 K
LiMnAs AFM semiconductor TN 300 K
SrMnGe AFM semiconductor TN 300 K
MnAlGe ferromagnetic metal
Li+Mn2+As3-
Al3+Mn2+Ge4-e-
1.T. Graf, C. Felser, and S. S. P. Parkin, Prog. Solid State Chem. 39, 1 (2011)


Heusler 2D
MnAlGe
Charge density
Spin density
Cu2MnAl (Heusler)
removing every second layer from tetrahedral interstitials
PbFCl (LiFeAs)
tetragonal unit cell
Satya N. Guin, et al. Chandra Shekhar, Andrea Damascelli, Yan Sun, and Claudia Felser, Advanced Materials in print


MnAlGe
layered quasi-2D crystal TC ~ 503 K
topological nodal line magnet.
2D Berry curvature!
Satya N. Guin, et al. Chandra Shekhar, Andrea Damascelli, Yan Sun, and Claudia Felser, Advanced Materials in print

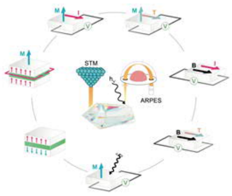

MnAlGe
layered quasi-2D crystal TC ~ 503 K
topological nodal line magnet.
2D Berry curvature!
Energy (eV)
B (T)
Satya N. Guin, et al. Chandra Shekhar, Andrea Damascelli, Yan Sun, and Claudia Felser, Advanced Materials in print


MnAlGe
3D to 2D
Fe3GeTe2
Co3Sn2S2
MnAlGe (present work)
T (K)

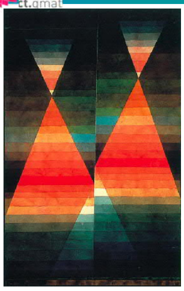
vision

new physics
- Antiferromagnetic topological materials – more to come
- Berry phase design of magnetic materials for energy conversion and Hall sensors
- more ferromagnetic Weyl semimetals – oxides ...
- Quantum anomalous Hall effect at room temperature
- from 2D to 3D quantum effects
- light – magnetic Weyl interaction

potential applications
- energy conversion
- quantum computing
- spintronics



thank you for your attention



Thank you for your attention!