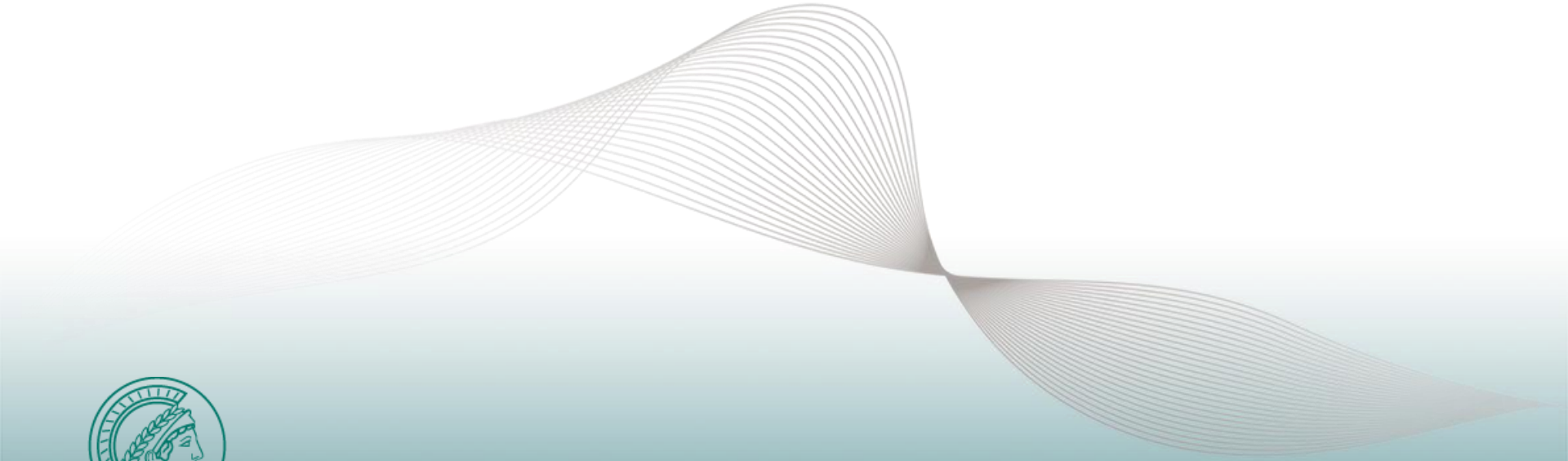
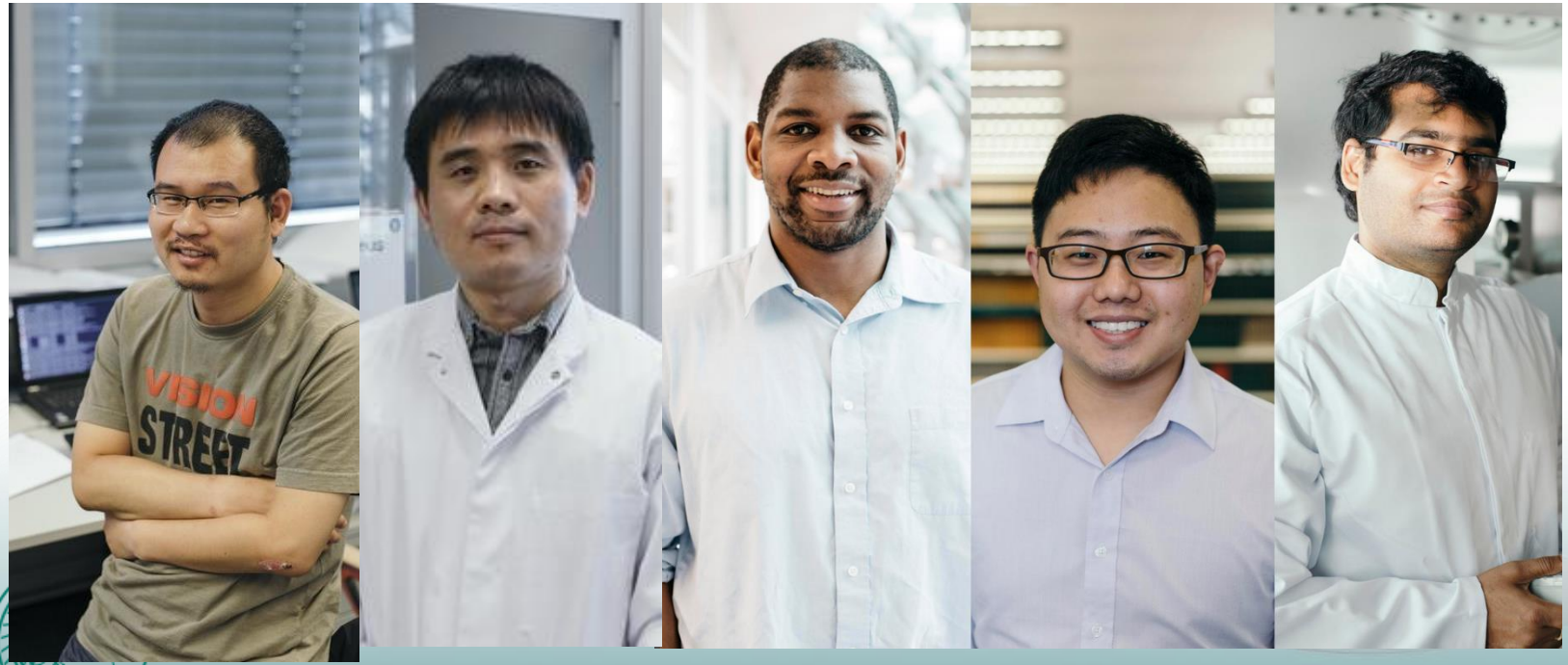
Topology, Magnetism and Chirality



Claudia Felser

MAX-PLANCK-GESELLSCHAFT



Claudia Felser

MAX-PLANCK-GESELLSCHAFT


$\hat{H} = \hat{T} + \hat{V}$
$i\hbar\gamma^a\partial_a\psi - mc\psi = 0$

Topological quantum chemistry

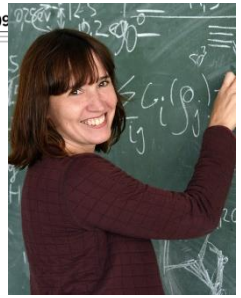
from all 250,000 known inorganic compounds 25% are topological!

ARTICLE

https://doi.org/10.1038/s41586-019-09

A complete catalogue of high-quality topological materials

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



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

Topological quantum chemistry

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

Comprehensive search for topological materials using symmetry indicators

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

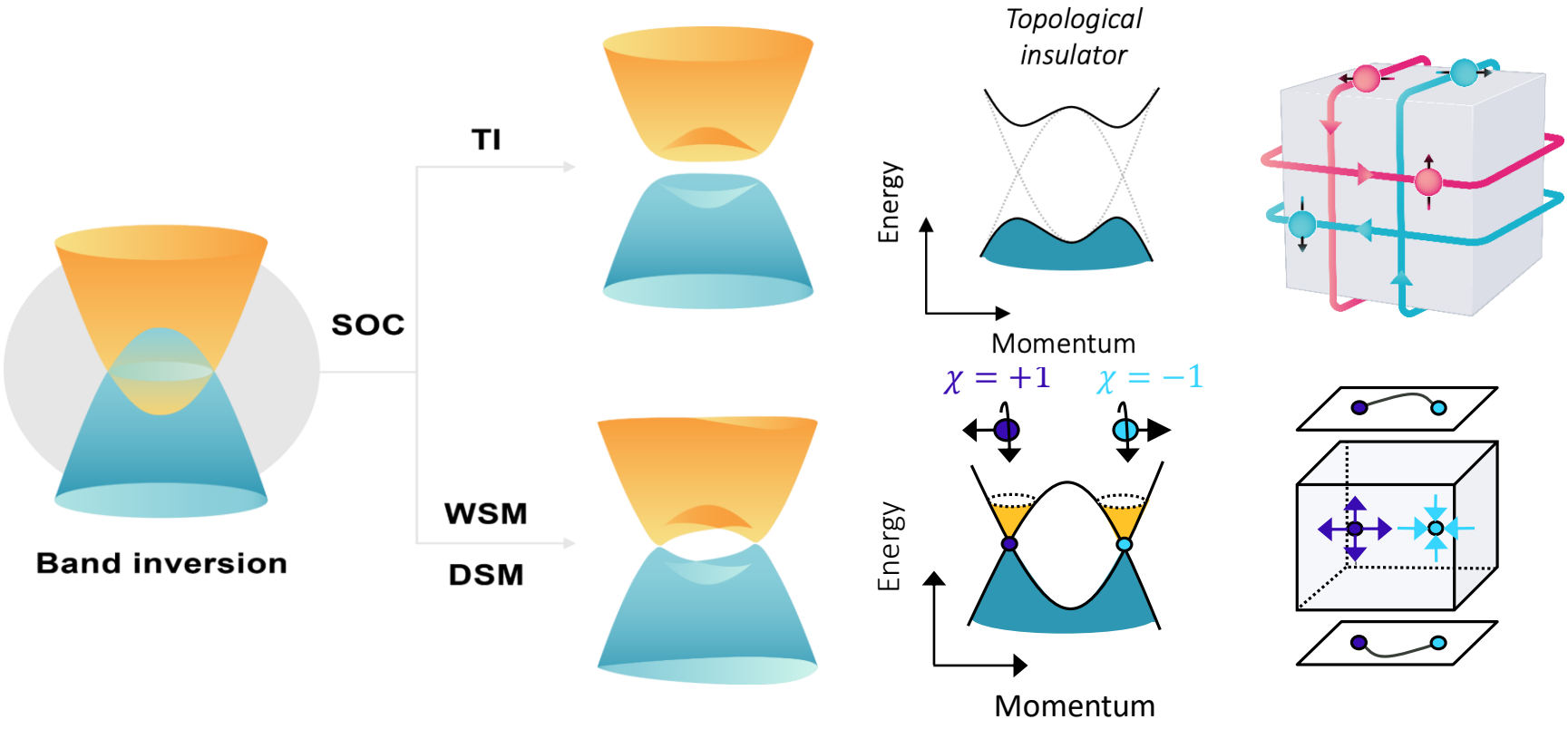
High-throughput calculations of magnetic topological materials

https://doi.org/10.1038/s41586-020-2837-0
Received: 27 January 2020
Accepted: 24 August 2020

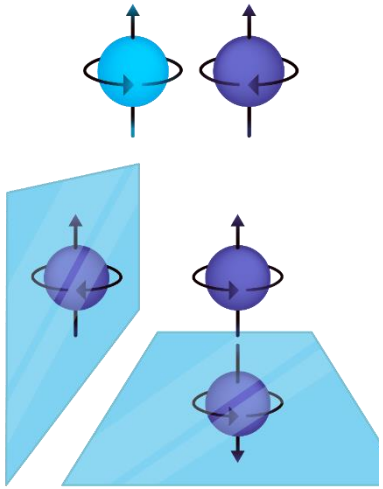
Yuanfeng Xu[1], Luis Elcoro[2], Zhida Song[3], Benjamin J. Wieder[3,4,5], M. G. Vergniory[6,7], [illegible], Yulin Chen[9,10,11,12], Claudia Felser[13,14] & B. Andrei Bernevig[1,3,15]

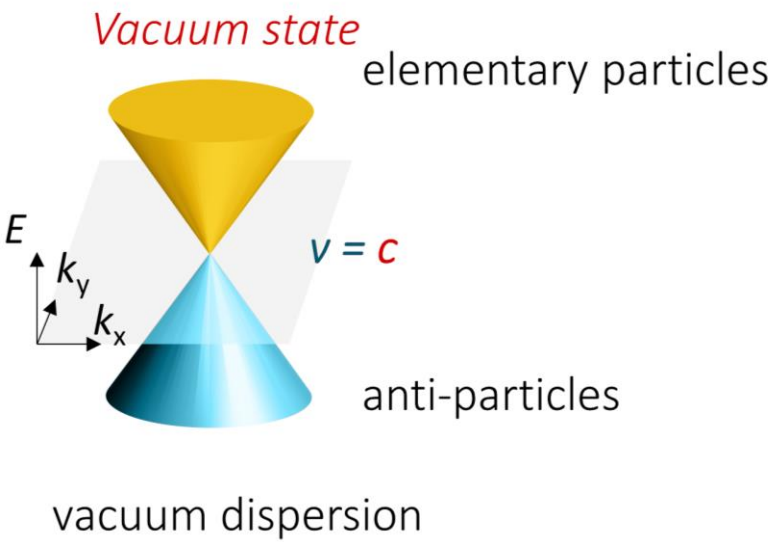
https://doi.org/10.1038/s41586-020-2837-0

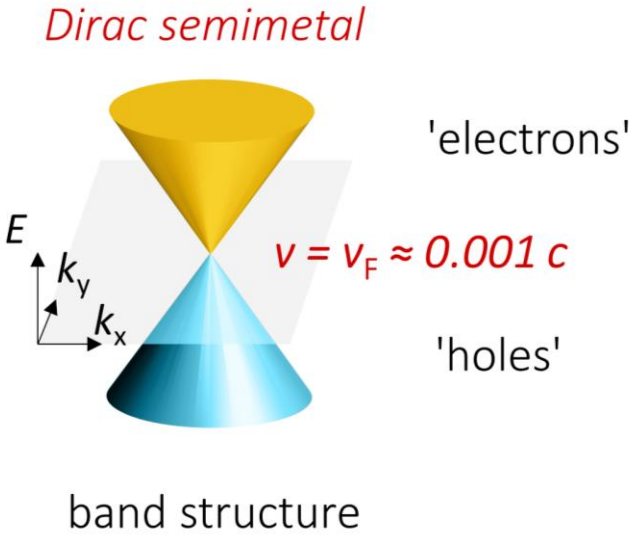
Topological quantum chemistry



Chiral electrons







Chiral anomaly is the **anomalous non-conservation** of a chiral current.

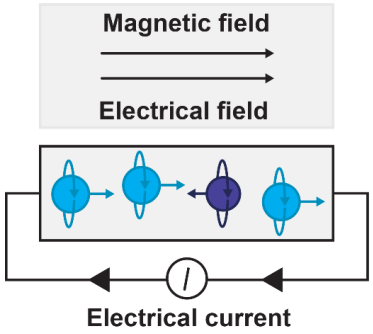
A sealed box with equal numbers of positive and negative charged particles is found when it is opened to have more positive than negative particles, or vice-versa.
Prohibited from classical conservation laws, but can be **broken in a quantum world**.
Universe contains more matter than antimatter

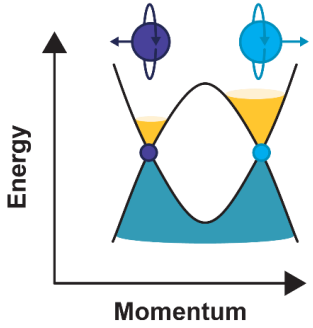
Wikipedia

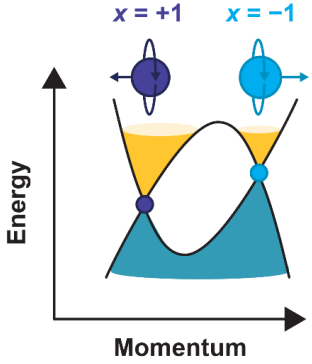
Chiral electrons

Chiral anomaly: broken parity – one explanation for the asymmetry of matter and antimatter
Axial gravitational anomaly

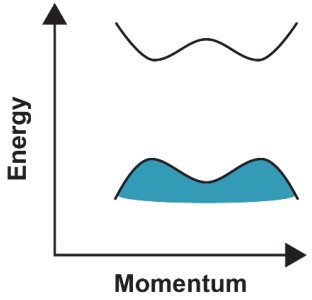
NbP



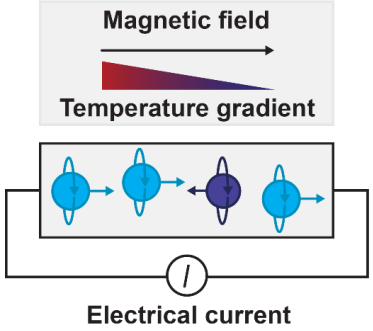


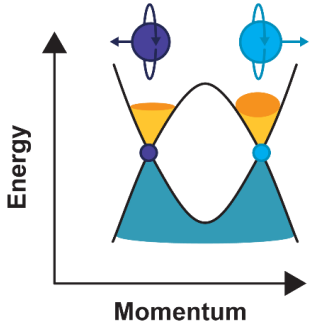


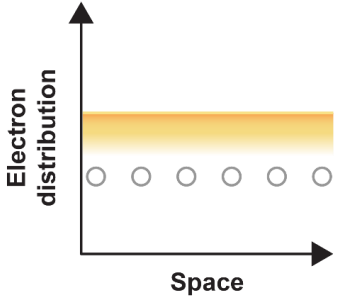
Axion phason

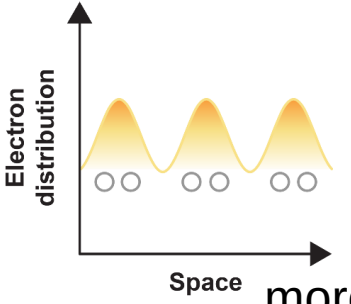


Ta_2Se_8I





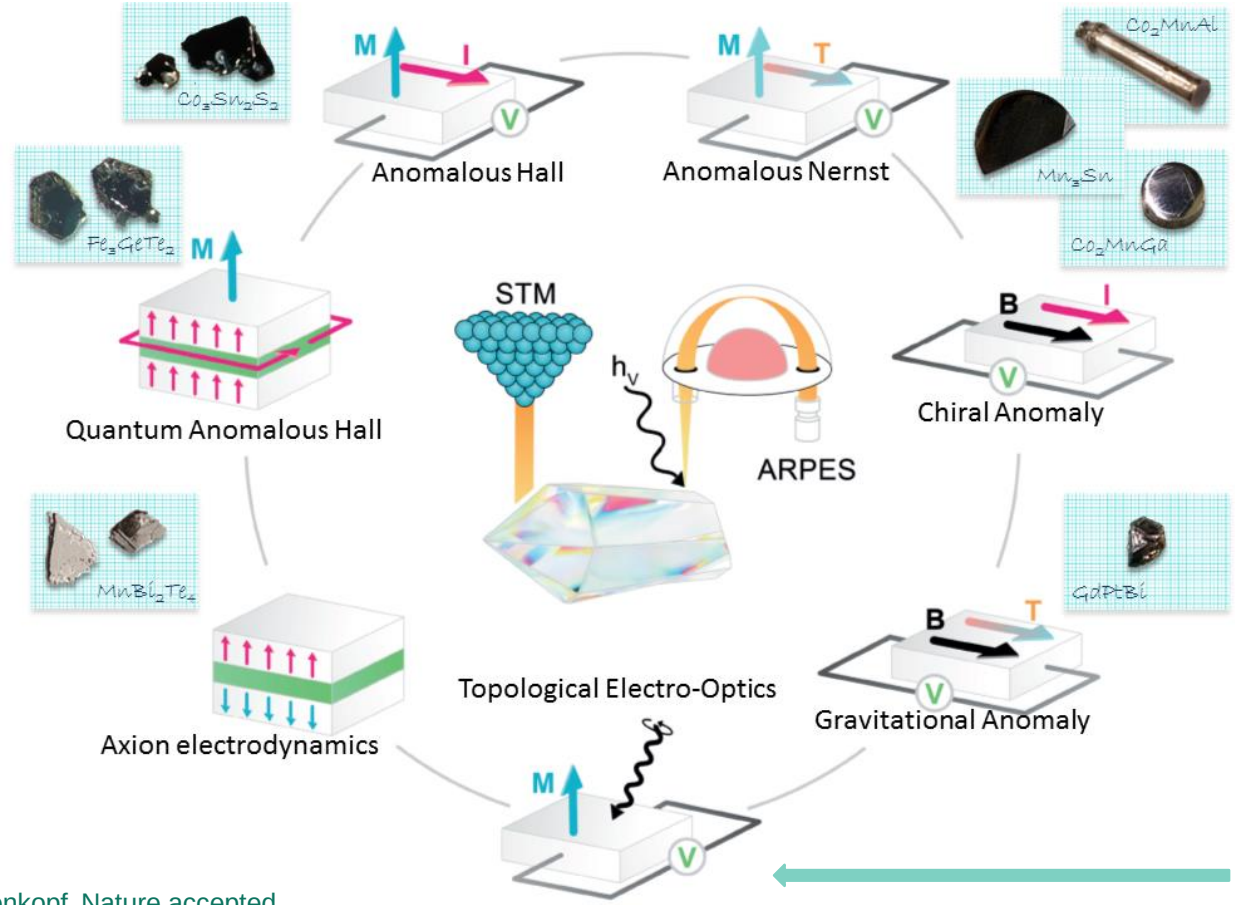




…more to come

Johannes Gooth et al., Nature 547 (2017) 324, Gooth et al. Nature 575 (2019) 315, Shi, et al., Nature Physics 17 (2021) 284

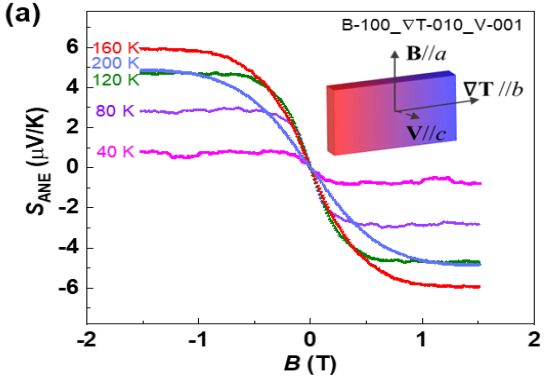
Magnetic Weyl Semimetals

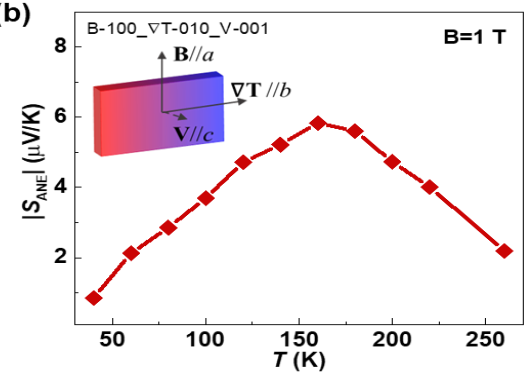


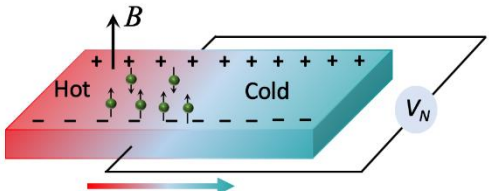
Bernevig, Felser and Beidenkopf, Nature accepted

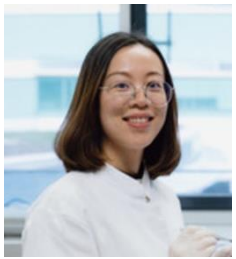
Non collinear Weyl semimetals

Giant Nernst effect with magnetic moment

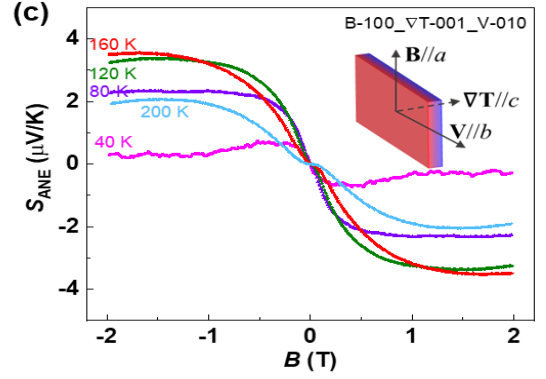


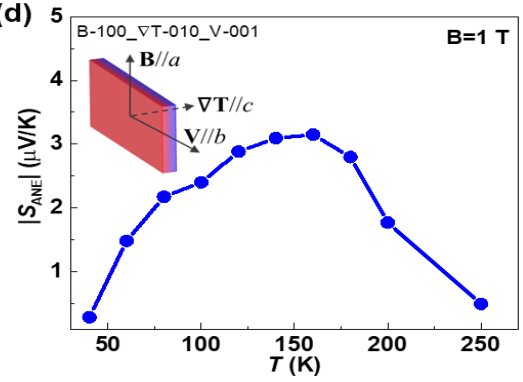


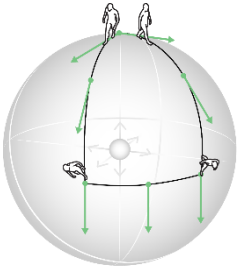




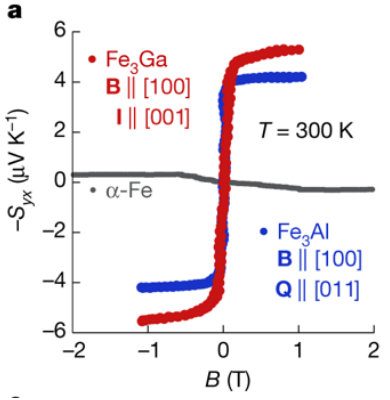
YbMnBi$_2$







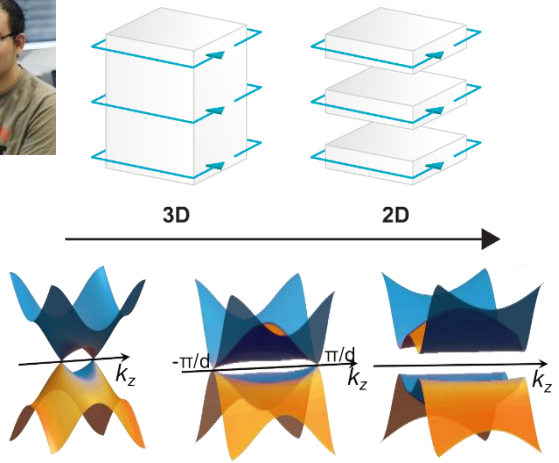
Berry phase

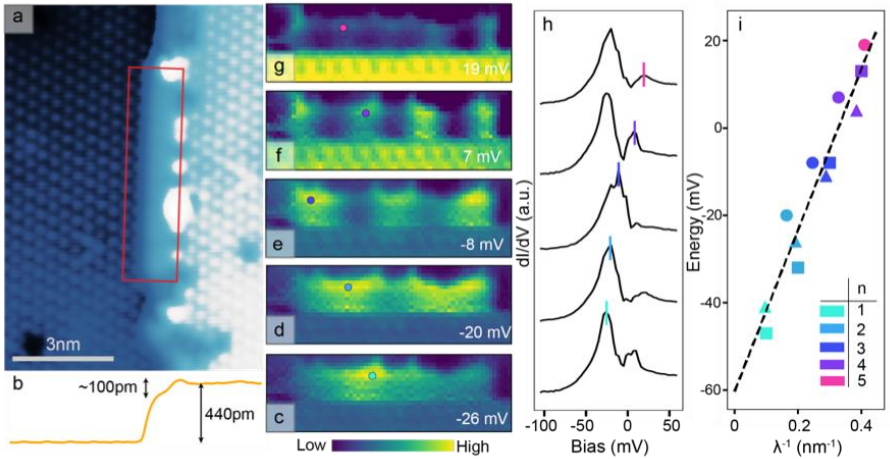


Pan et al., Nature Materials, accepted, JP Heremans, S Watzman, N Trivedi, T Mccormick, C Felser, US Patent App. 16/157,522

Sakai et al. Nature 2020

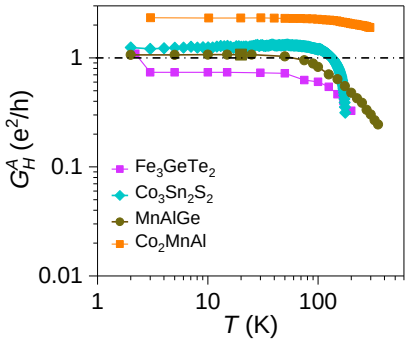
2D-Magnetic Weyl semimetals

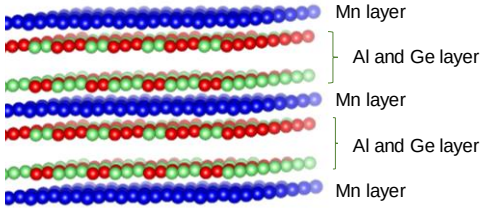




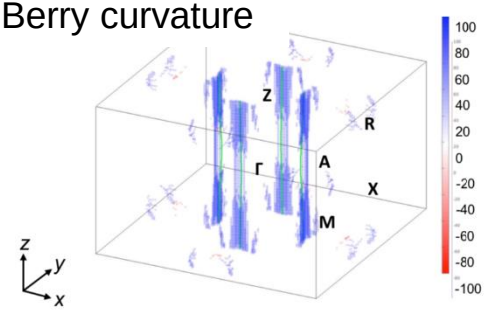
Sean Howard, *et al.*, Nature Communications **12** (2021) 4269

$Co_2Sn_3S_2$

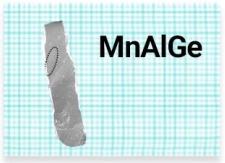




Berry curvature

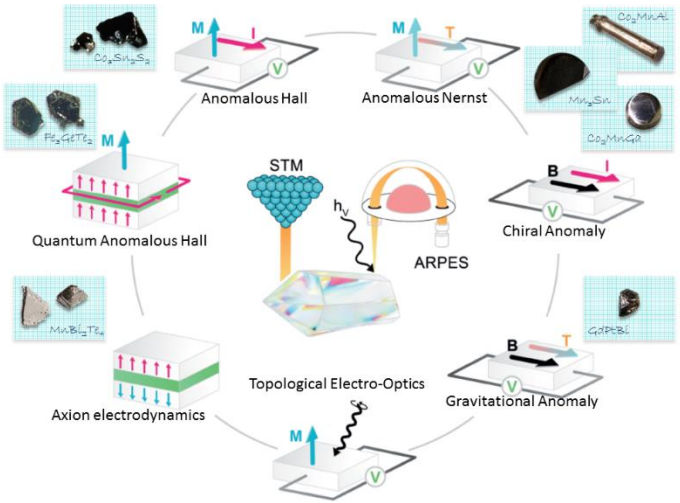


MnAlGe



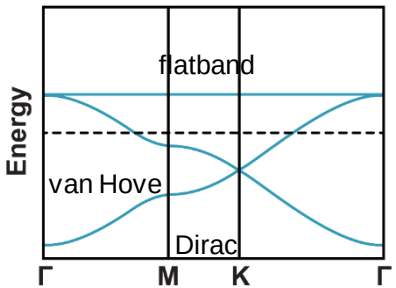
Satya N. Guin, *et al.*, Advanced Materials **33** (2021) 2006301

More kagome Weyl semimetals

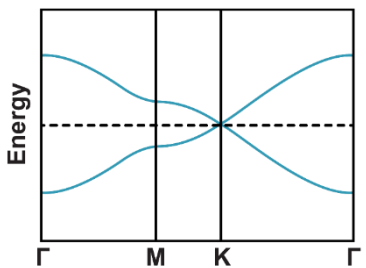


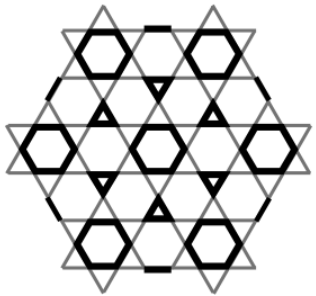
non collinear AFM: Mn_3Sn, Mn_3Ge
ferromagnet: $Co_3Sn_2S_2$
superconductor: $Cs(K)V_3Sb_5$
new compounds already grown
YMn_6X_6 …

kagome

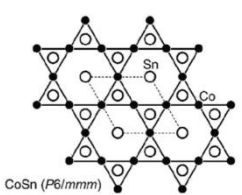


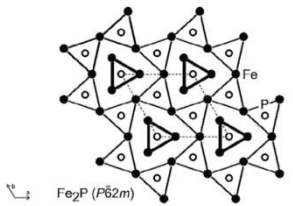
honeycomb

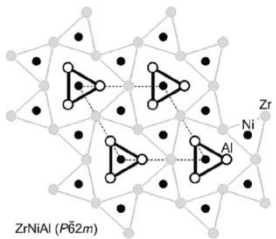


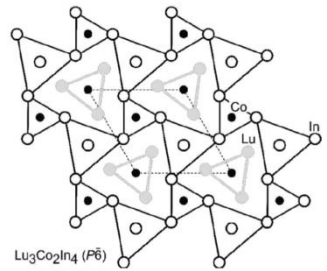


distorted kagome









Pöttgen, Z. Anorg. Allg. Chem. 640 (2014) 869

New Fermions

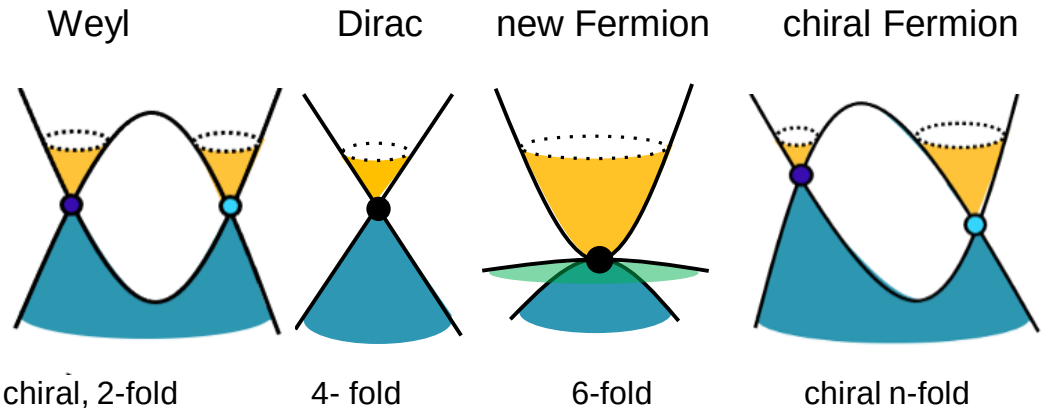
RESEARCH

RESEARCH ARTICLE SUMMARY

TOPOLOGICAL MATTER

Beyond Dirac and Weyl fermions: Unconventional quasiparticles in conventional crystals

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

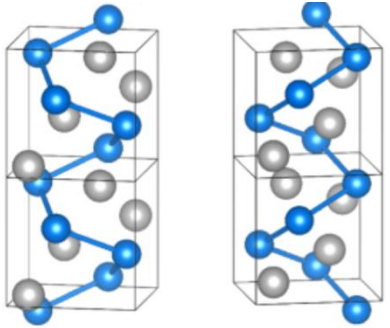


Free fermionic excitations in solid-state systems that have **no high-energy counterparts.**

Some of these new Fermions are even chiral

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

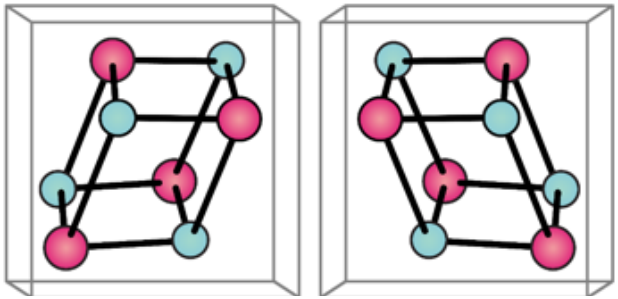
Enantiomer A and enantiomer B
Crystal structure

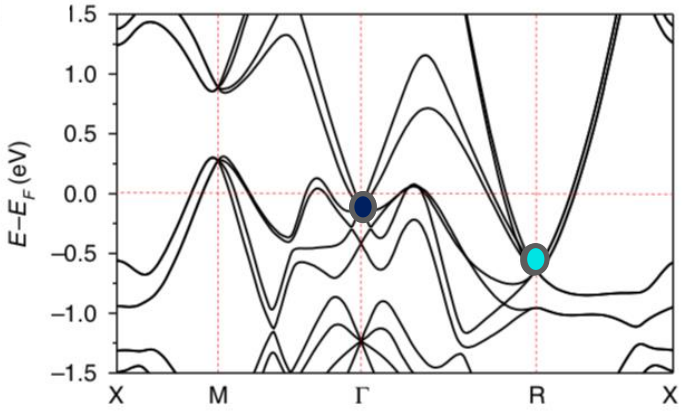


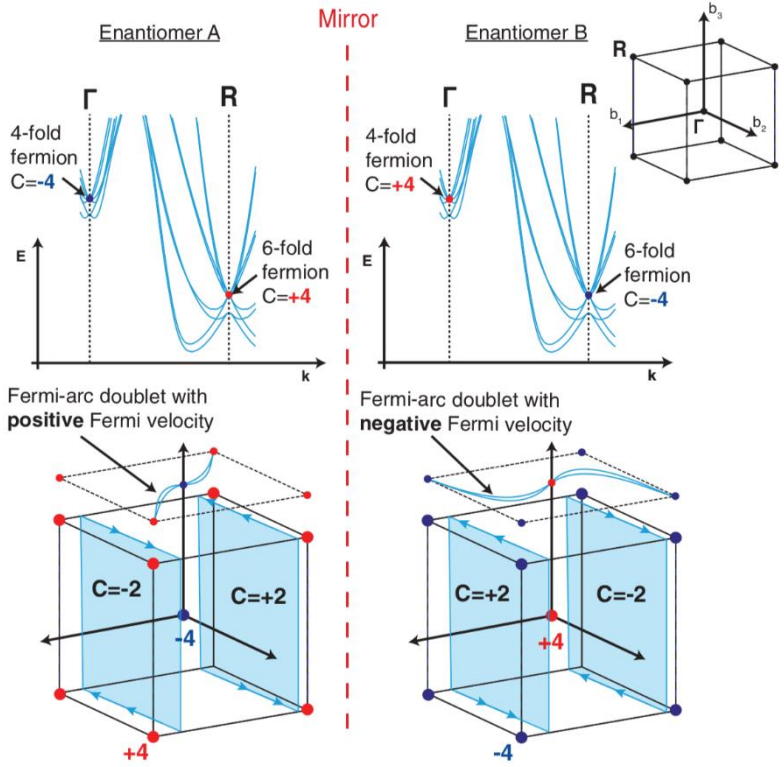
Bradlyn et al. Science 353, (2016) 6299

Chiral Fermions

The structure is **chiral** but the band structure is achiral





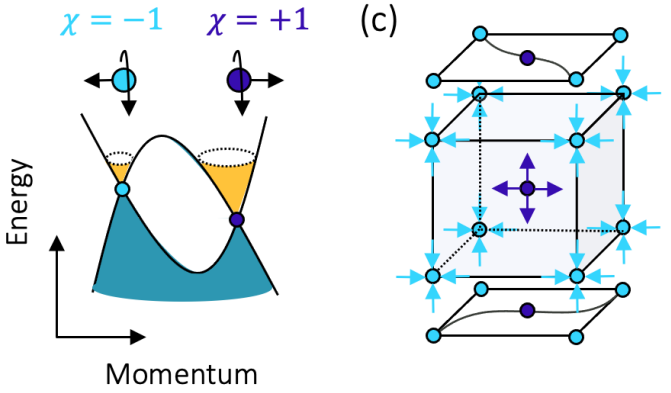


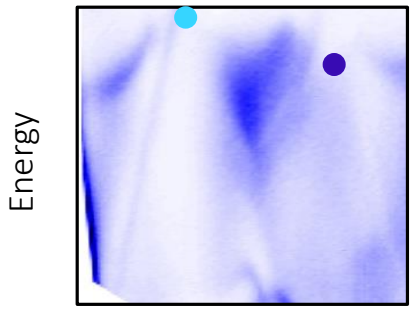
PdGa

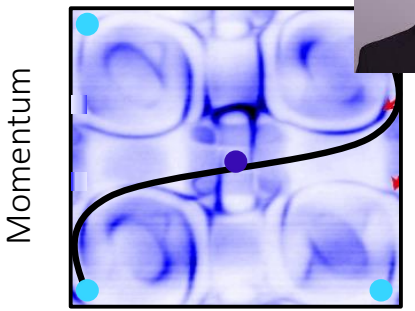
Schröter et al., Nature Physics 2019, Schröder et al., Science 369 (2020) 179, Sanchez et al. Nature Nature 567 (2019) 500

Chiral Fermions

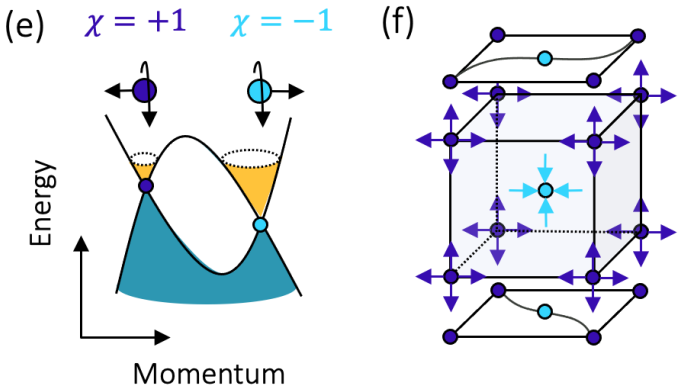
The Weyl electrons and the Fermi arc **chiral**

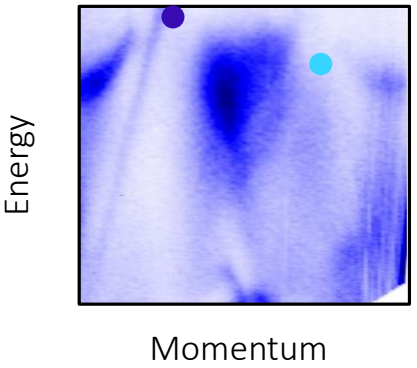


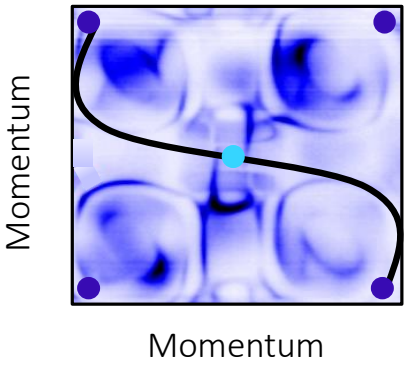




PdGa



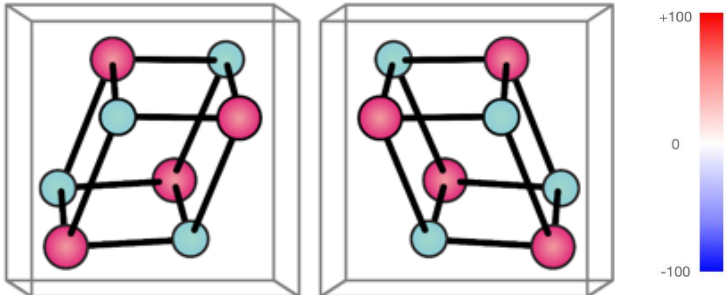


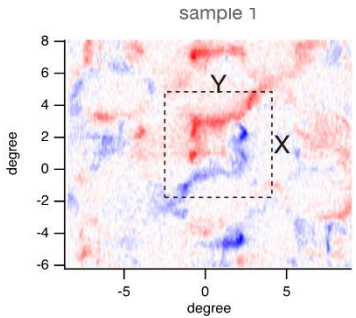


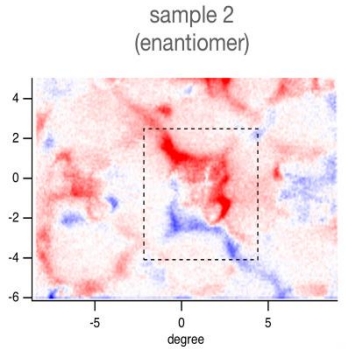
Schröter et al., Nature Physics 2019, Schröder et al., Science 369 (2020) 179, Sanchez et al. Nature Nature 567 (2019) 500

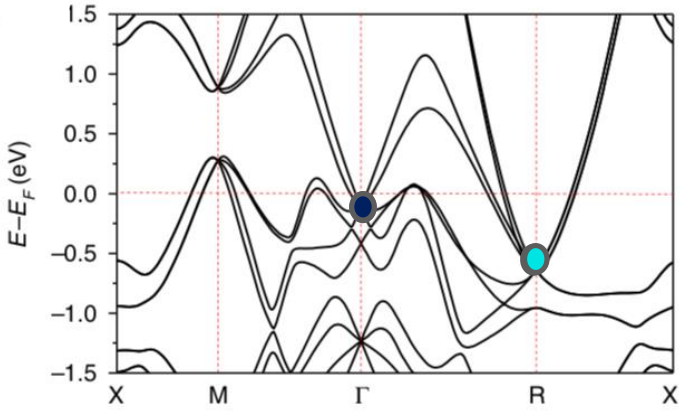
Chiral Fermions

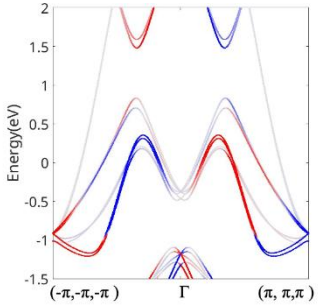
With circular polarized light we can visualize the difference in the band structure

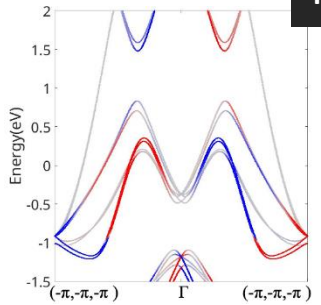






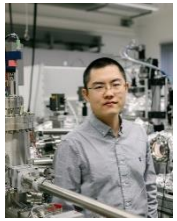






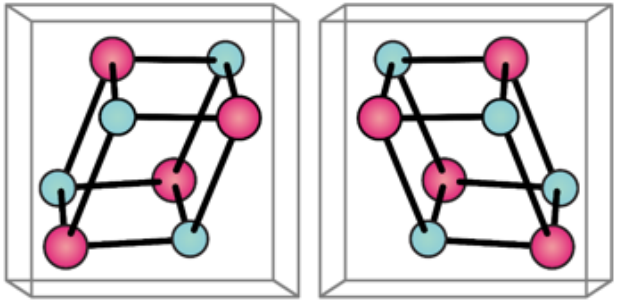
PdGa

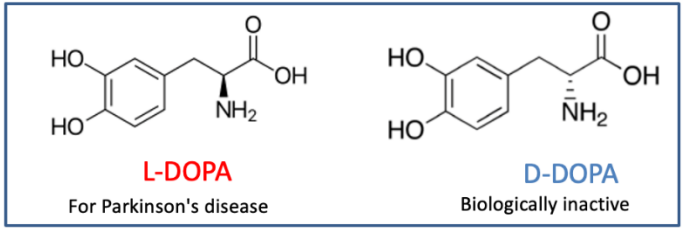
Orbital angular momentum, <111>

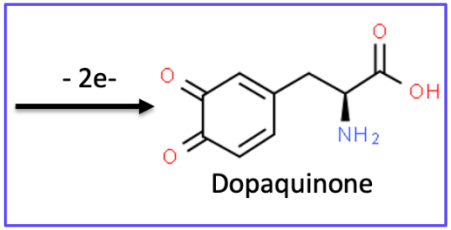


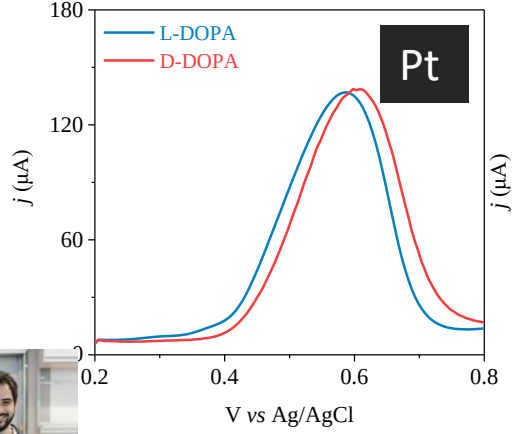
Mengyu Yao et al., to be published

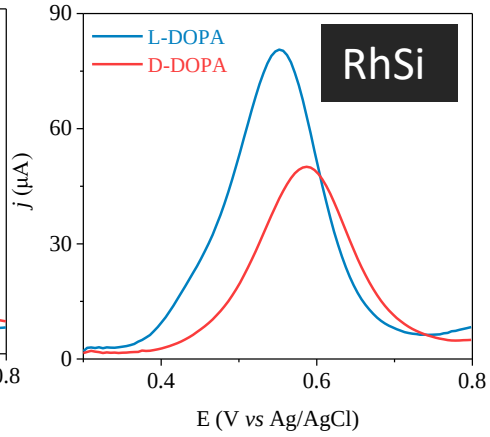
Chiral Fermions and catalysis

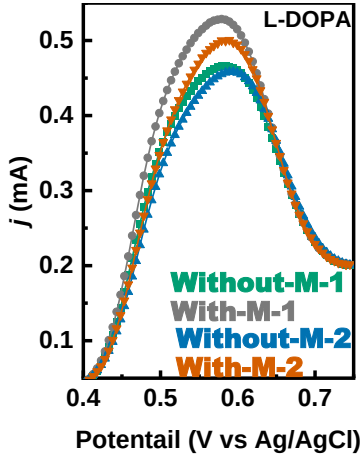


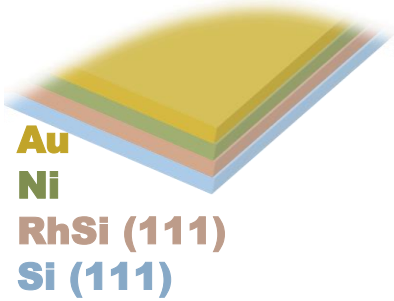


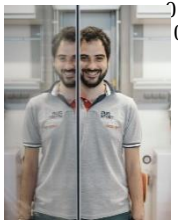








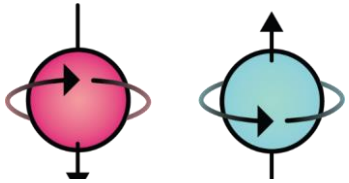


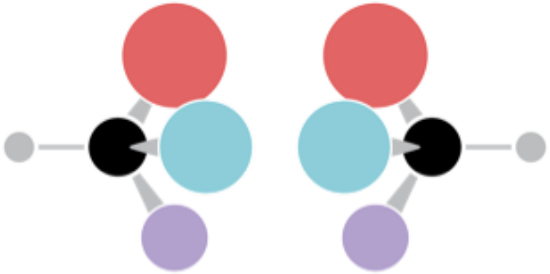


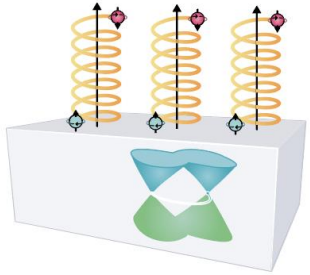
RhSi thin films, B20 structure (only one chirality available so far), with only (111) surface we can see clearly the different oxidation behaviors for D- and L-DOPA.

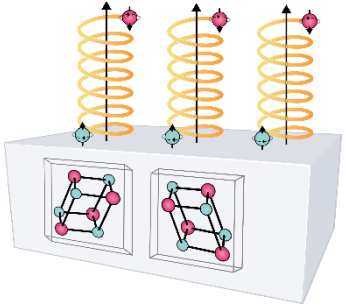
Open question: (1) chiral structure/surface, (2) chiral surface state, (3) orbital angular momentum

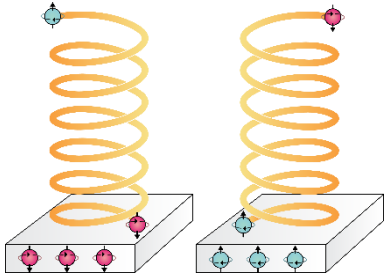
Chiral electrons – molecules, surfaces and crystals

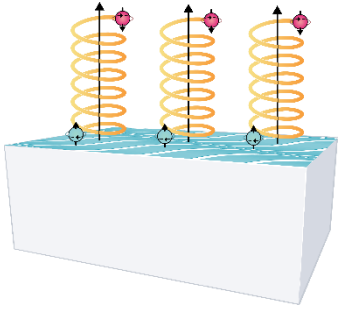






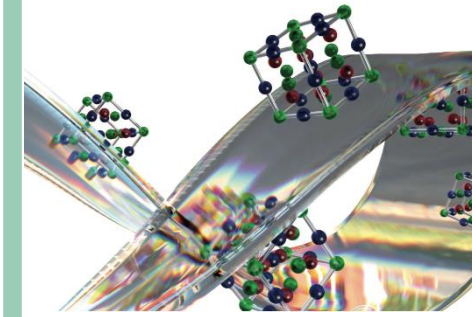






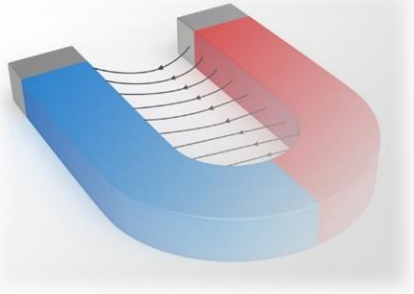
Summary

Topological chemistry



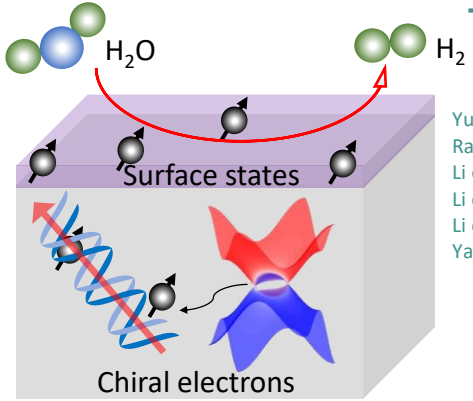
Xu et al., Nature 586 (2020) 702
Kumar et al, Chem. Rev. 2020
Bradlyn, et al, Nature 547 (2017) 298
Vergniory et al, Nature 566 (2019) 480

Topological magnets



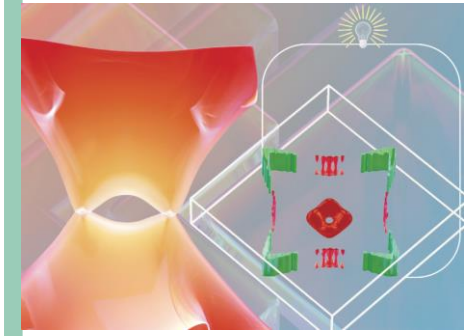
He et al.,, Nat. Com. 12, 4576 (2021).
Xu et al., Nature 586 (2020) 702
He et al, Adv. Mat. 32 (2020), 2004331
Liu, et al. Nature Physics 14 (2018) 1125
Liu, et al., Science 365 (2019) 1282
Morali et al., Science a365 (2019) 1286,
Manna et al., Nat. Mat. Rev. 2018

Topological catalysis



Yu et al, Angew. Chemie 60 (2021) 1
Rajamathi et al, Dalton Trans. (2020) 3398
Li et al, Science Adv. 5 (2019) eaaw9867
Li et al, Angew. Chemie 58 (2019) 13107
Li et al, APL 116 (2020) 070501
Yang et al, Adv. Mat. 32 (2020) 1908518

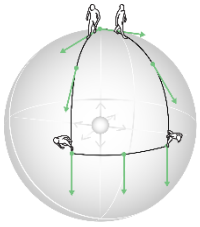
Topological thermoelectrics

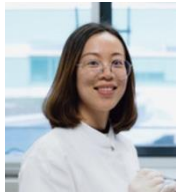


Pan et al. Nature Mater. in press
Guin et al, Adv. Mat. 33 (2021),
Pan et al, Adv. Mat. 33 (2021), 2003168
Guin et al, Adv. Mat. 31 (2019) 1806622
Guin et al, npg materials asia 11 (2019) 11
Liu et al., Adv. Mat. 30 (2018) 1800881
Fu et al., Energy & Envir. Science 2018

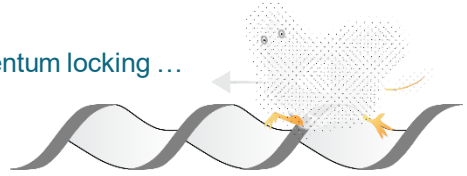
Vision

- Berry curvature design of large responses
  - in ferromagnetic Weyl semimetals
  - non collinear antiferromagnets
  - high temperature Nernst measurements

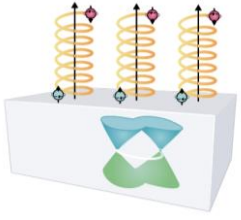


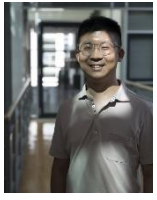


- Crystal growth of both enantiomers of topological chiral compounds
  - interfaces, grain boundaries, chiral phonons, magnons, …
  - the interplay between chiral structure, chiral surface state, orbital momentum, spin momentum locking …
  - strain and magnetic field



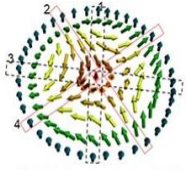
- Chiral electrons, chiral Fermions, chiral surfaces and **catalysis**
  - enhanced light matter interaction and magnetic field





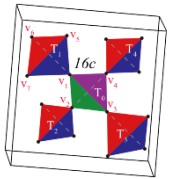
- Non local transport in chiral crystals
  - spin polarized currents

- Chirality plus magnetism, superconductivity, correlations …
  - Skyrmions, Antiskyrmions …

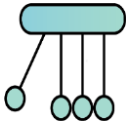


Vision

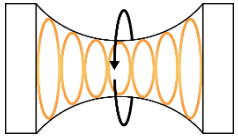
- Quantum chemistry beyond topology:
  - filling enforced obstructed surface states …
  - interfaces, grain boundaries



- More kagome compounds – magnetic and nonmagnetic
- Flatbands beyond kagome … pyrochlore, Lieb lattices



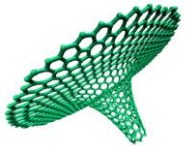
- Beyond the **single particle picture** – topology in correlated materials such as oxides

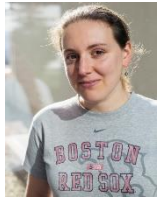


- Light topological matter interaction

Collaboration:

- New quantum effects such as quantum anomalous Nernst effect …
- Twist, bend …
- Experiments and understanding of **3D quantum Hall** effects
- More crystals for quantum simulation of high energy and astrophysics



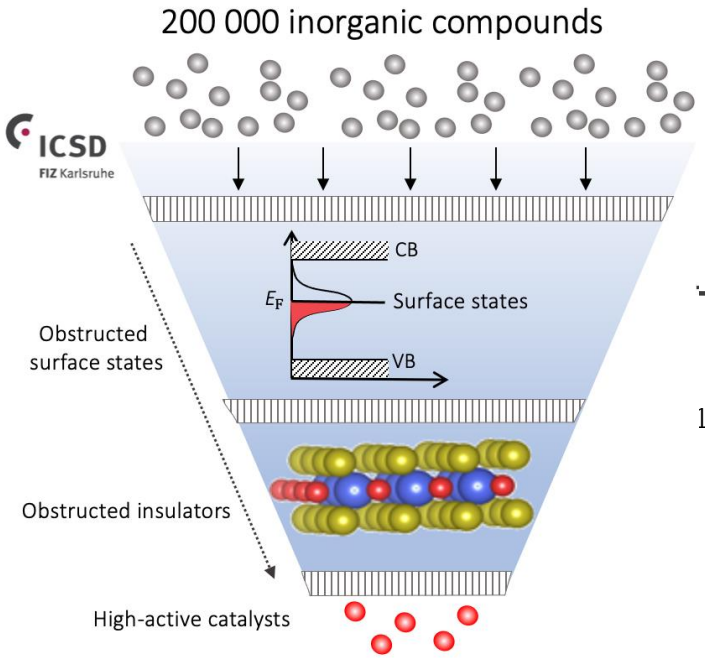


Thank you for your attention

Yulin Chen
Stuart Parkin
and teams

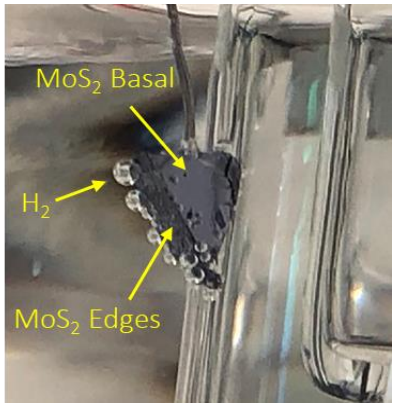
Andrei
Bernevig
Haim
Beidenkopf

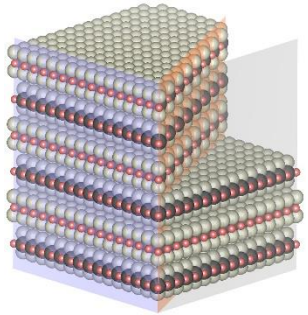
Quantum chemistry beyond topology

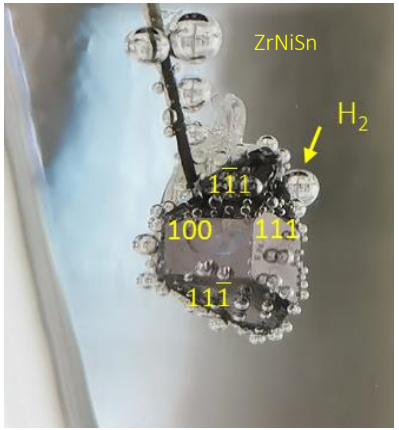


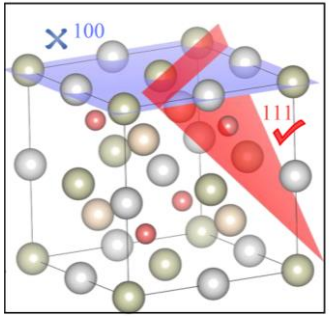
surface states
electronic structure
real space

surface states
edges of MoS_2
111 surface of Heusler
…





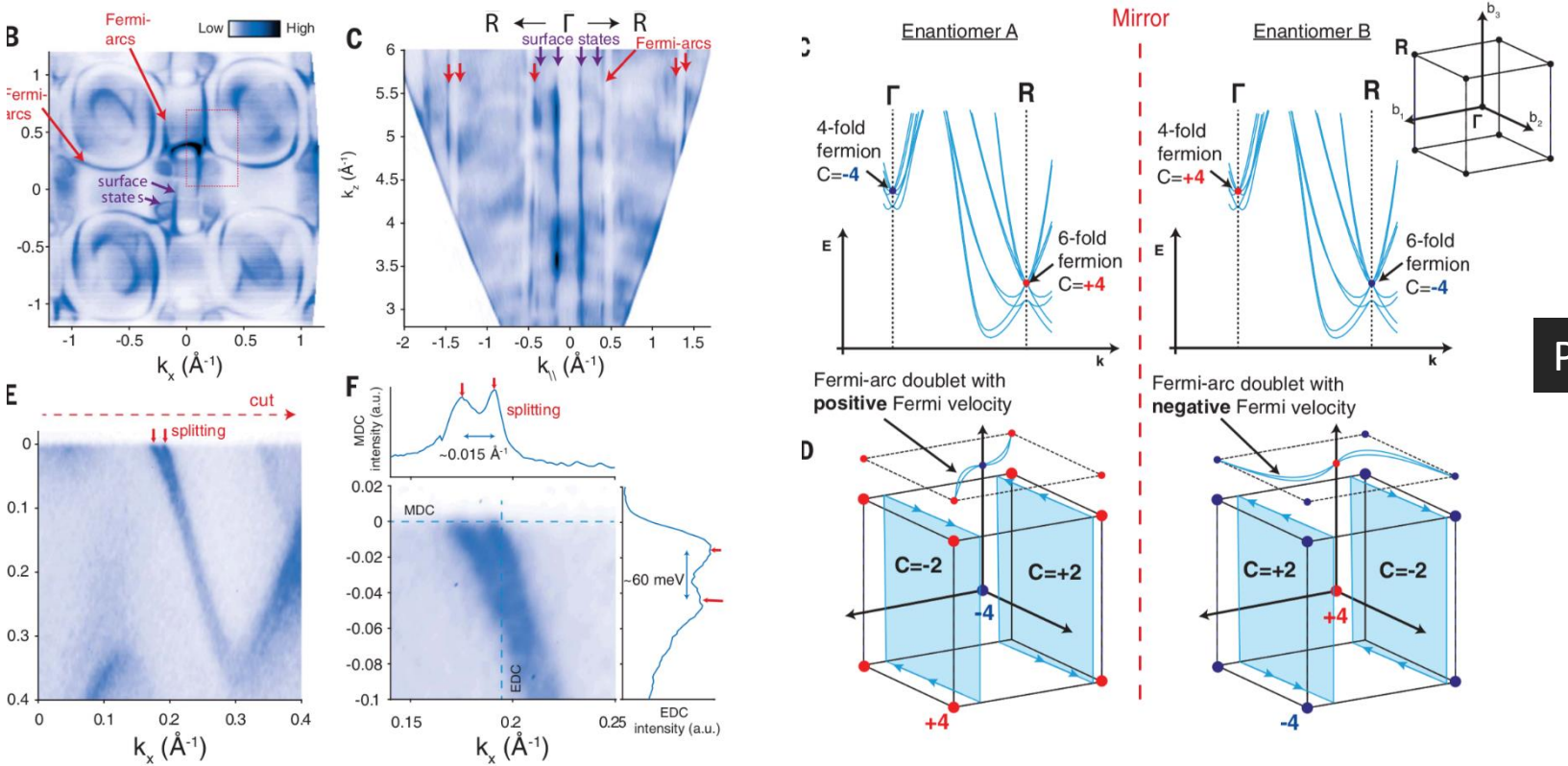




Guowei Li et. al., submitted

Chiral Fermions

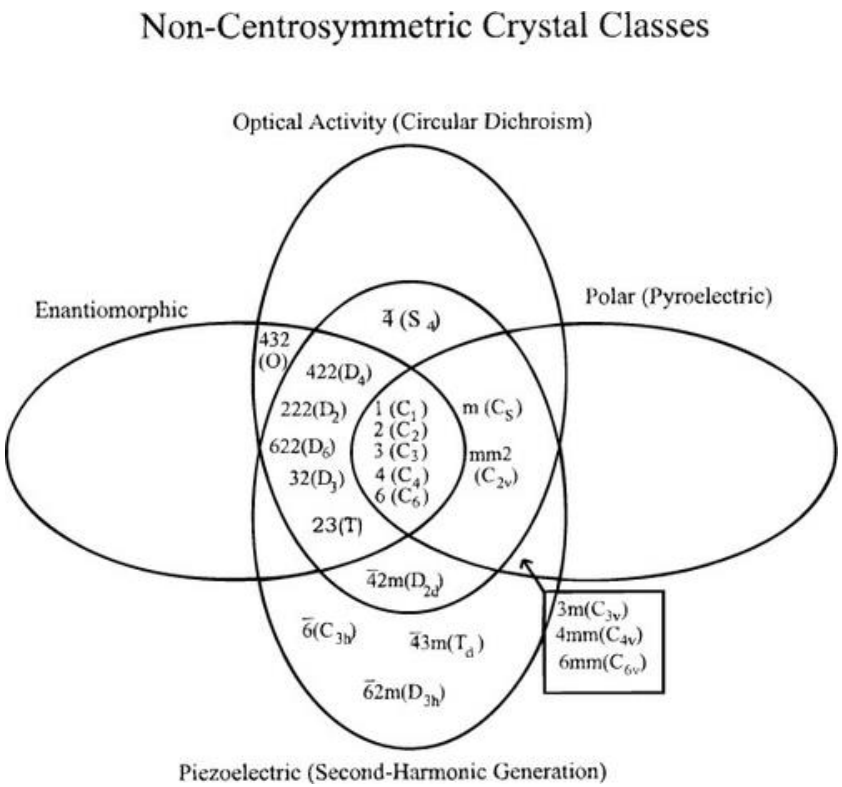
The Fermi-arc doublets visualize the Chern number = 4



PdGa

Schröter et al., Nature Physics 2019, Schröder et al., Science 369 (2020) 179, Sanchez et al. Nature Nature 567 (2019) 500

Chiral oxides and chalcogenides



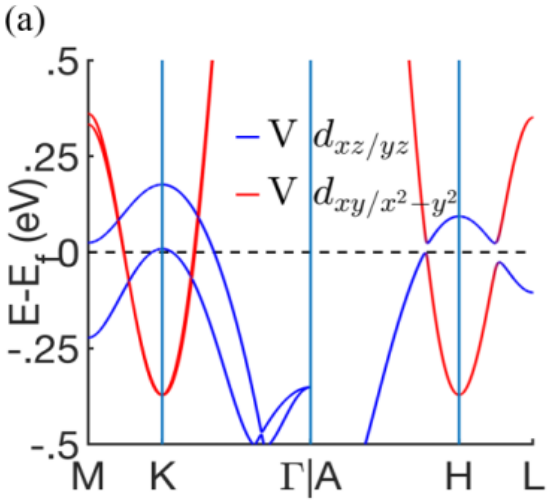
cubic Manganites

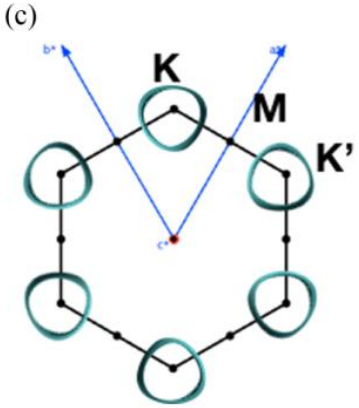
hexagonal Manganited (*P*6$_3$*cm* space group)

YXO_3, X = V- Co

Double perovskite

e.g. Sr_2FeMoO_6





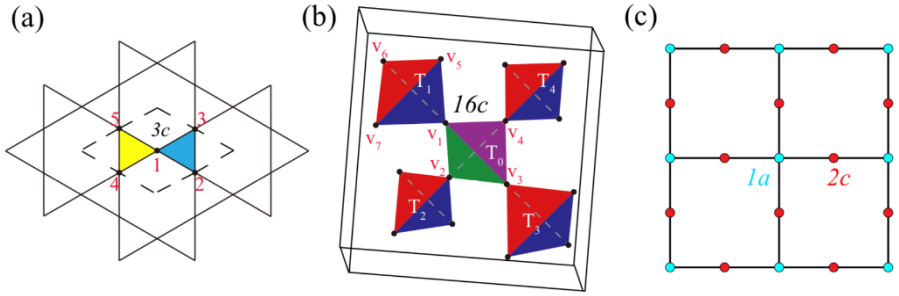
S. Halasyamani and K. R. Poeppelmeier, Chem. Mater. 10 (1998) 2753-2769

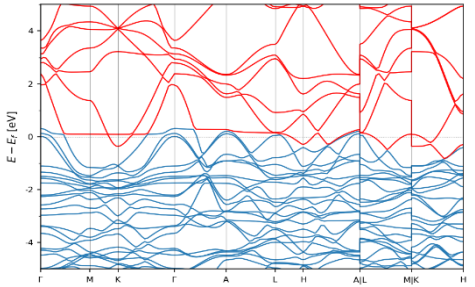
flatbands

Catalogue of Flat Band Stoichiometric Materials

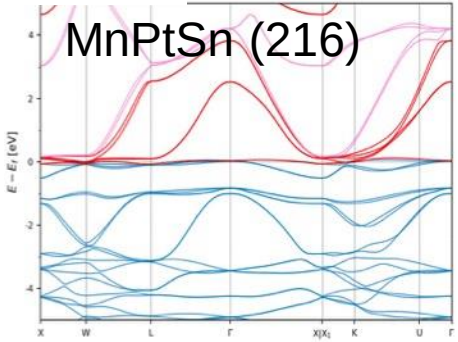
Nicolas Regnault,[1,2,*] Yuanfeng Xu,[3,*] Ming-Rui Li,[4,*] Da-Shuai Ma,[5,*] Milena Jovanovic,[6] Ali Yazdani,[1] Stuart S. P. Parkin,[3] Claudia Felser,[7] Leslie M. Schoop,[6] N. Phuan Ong,[1] Robert J. Cava,[6] Luis Elcoro,[8,*] Zhi-Da Song,[1,*] and B. Andrei Bernevig[1,9,10,†]

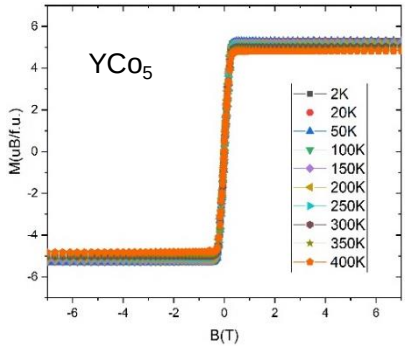
[1] *Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*



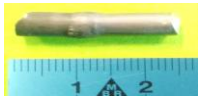


Kagome, pyrochlore and Lieb lattices



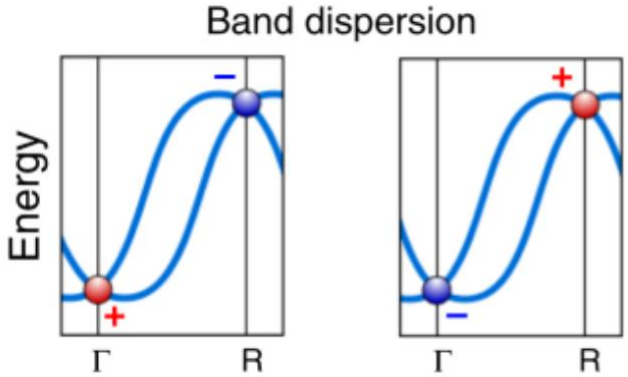


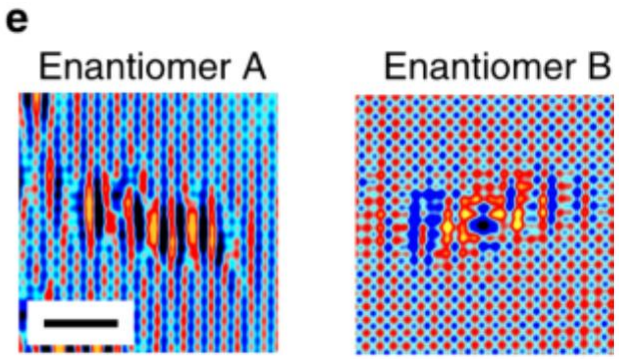
YNi$_5$



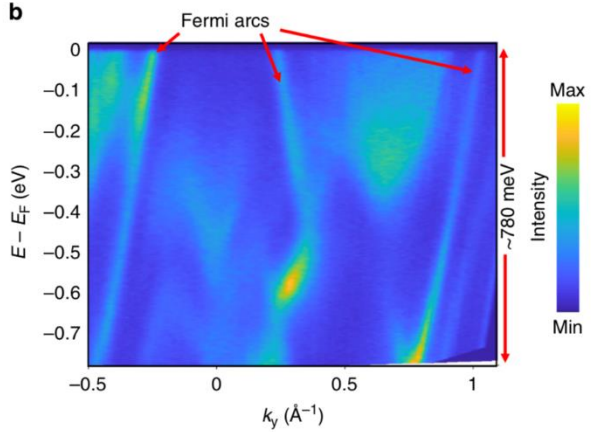
Flat-band compound from various space groups: 87, 221, 216, 225 ….many more

chiral surface states with STM

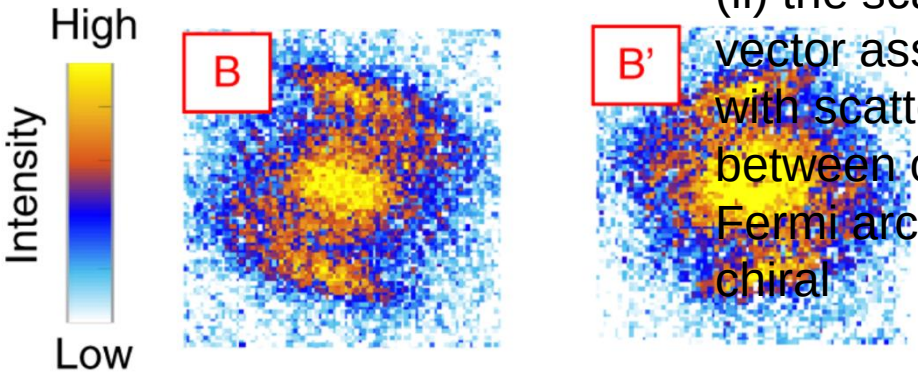




From STM investigations:
(i) the perturbation developing around native defects is chiral
(ii) the scattering vector associated with scattering events between opposite Fermi arcs is also chiral



Quasiparticle interference of two PdGa(001) enantiomer



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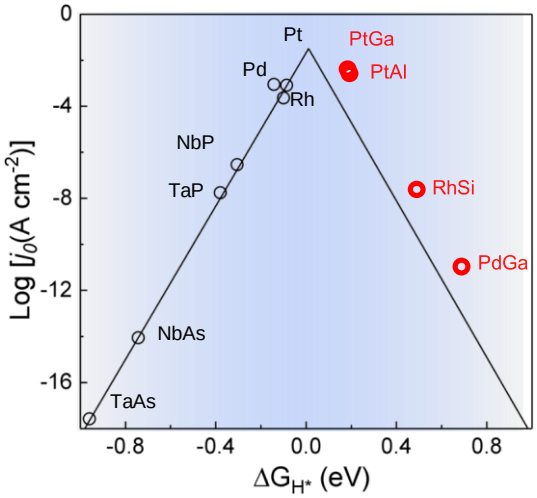
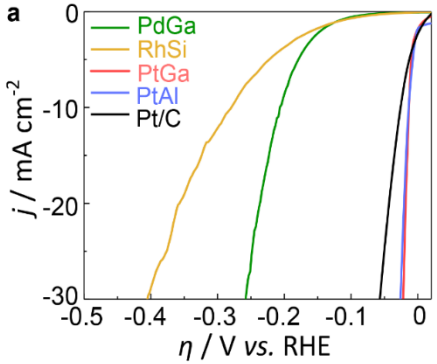
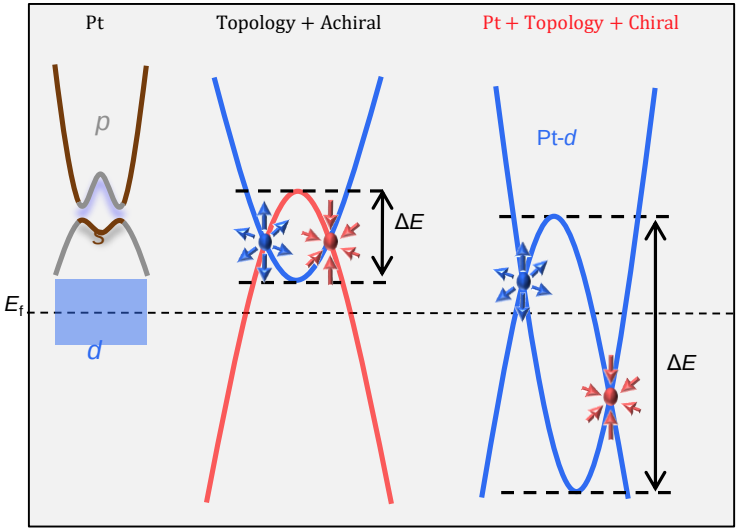
Quasiparticle interference of two PdGa(001) enantiome

new catalysist with chiral surface states





better than Pt for hydrogen evolution reaction (HER) and IrO_2 (OER, oxygen evolution reaction), Pt and IrO2 are topological relativistic effects and spin orbit coupling



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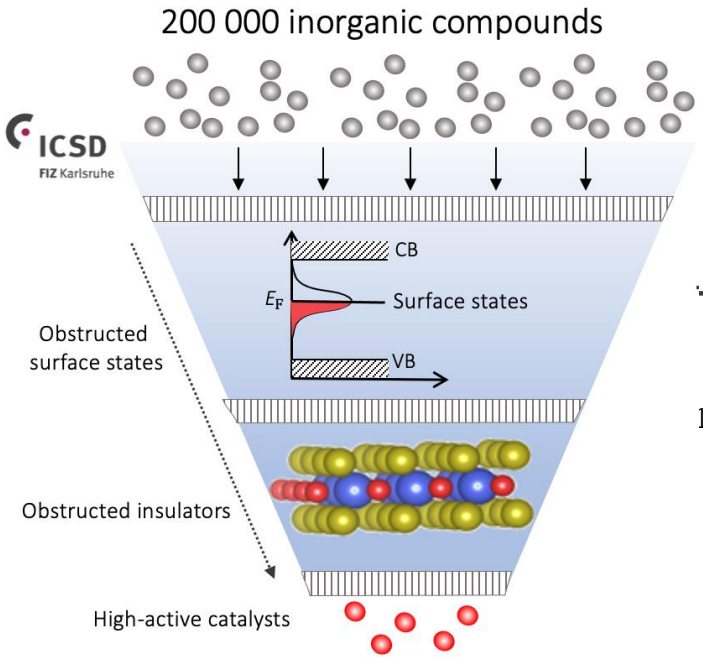
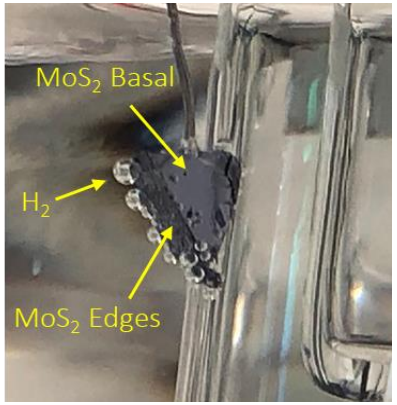
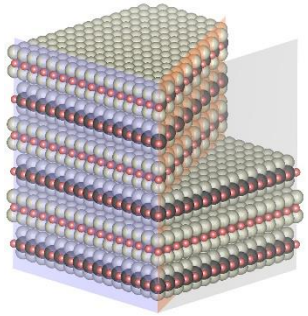
Quantum chemistry beyond topology

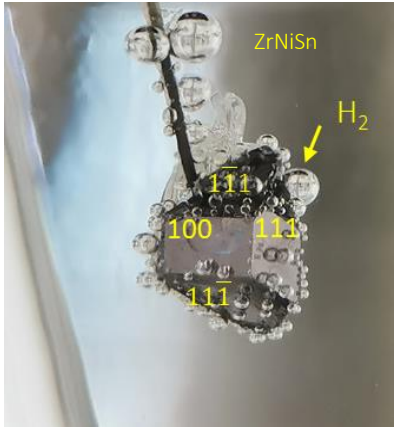


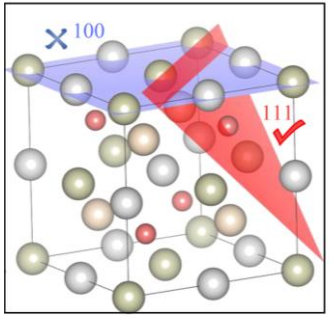
surface states
electronic structure
real space

surface states
edges of MoS_2
111 surface of Heusler
…

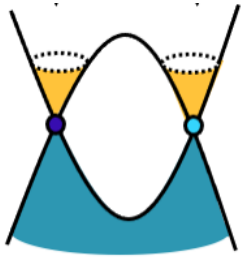






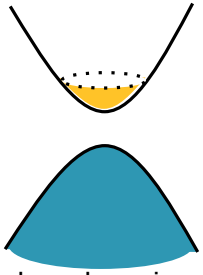


Light on the band structure

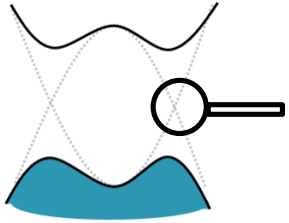


Weyl fermion

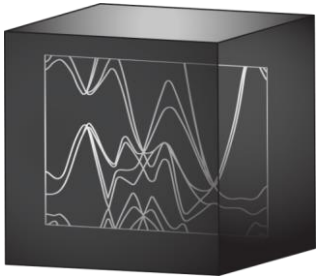
flatbands

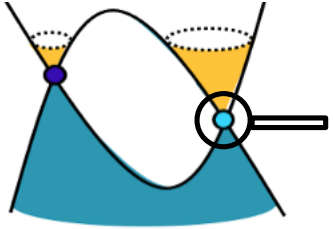


doped semiconductors



surface state

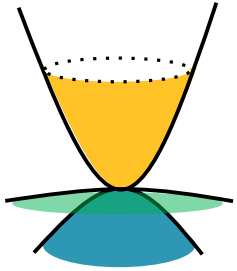




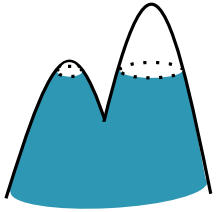
phase

chiral Fermion

nodal line



new Fermion



van Hove Singularity