

Topology, Magnetism und Chirality



Claudia Felser, MPI CPfS <u>felser@cpfs.mpg.de</u>

Claudia Felser, Johannes Gooth, Topology and Chirality, arXiv:2205.05809

topology



J. Kroder, et al., Chemie in unserer Zeit 56 (2022) 12–20

topology



from molecule to solid



Roald Hoffmann Angewandte. Chem. 26 (1987) 846

from benzen to graphene



electronic structure





topological insulators







from all 250 000 known inorganic compounds 25% are topological

A complete catalogue of high-quality topological materials

^{8,9}* & Zhijun Wang^{7,}

RESEARCH

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

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

opological

indicators

ectronic

1g^{1,4}, Hongming Weng^{1,5,6,7,8}* &

sofmagnetic

RESEARCH ARTICLE SUMMARY

Topological TOPOLOGICAL MATTER

Barry Bradlyn¹*, L. Elcoro²*, Jennifer

All topological bands of all nonmagnetic stoichiometric materials

Maia G. Vergniory*+, Benjamin J. Wieder*+, Luis Elcoro, Stuart S. P. Parkin, Claudia Felser, B. Andrei Bernevig, Nicolas Regnault*



topological materials

Yuanfeng Xu¹, Luis Elcoro², Zhida Song³, Benjamin J. Wieder^{3,4,5}, M. G. Vergniory^{6,7}, https://doi.org/10.1038/s41586-020-2837-0 Nicolog Boggood 143.8, Yulin Chen^{910,11,12}, Claudia Felser^{13,14} & B. Andrei Bernevig^{1,3,15} https://doi.org/10.1038/s41586-020-2837-0 Received: 27 January 2020

Accepted: 24 August 2020





topologicalquantumchemistry.org

³⁷ Rb	³⁸ Sr	³⁹ Y	40 Zr	41 Nb	42 Mo	⁴³ Tc	44 Ru	45 Rh	⁴⁶ Pd	47 Ag	48 Cd	49 In	⁵⁰ Sn	⁵¹ Sb	⁵² Te	53	⁵⁴ Xe
55 Cs	⁵⁶ Ba	57 La	72 Hf	⁷³ Ta	⁷⁴ W	75 Re	⁷⁶ 0s	77 Ir	⁷⁸ Pt	⁷⁹ Au	80 Hg	⁸¹ TI	⁸² Pb	⁸³ Bi	84 Po	⁸⁵ At	86 Rn
⁸⁷ Fr	88 Ra	89 Ac	¹⁰⁴ Rf	105 Db	106 Sg	107 Bh	¹⁰⁸ Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 FI	115 Mc	116 Lv	117 Ts	118 Og
			58 Ce	⁵⁹ Pr	60 Nd	61 Pm	62 Sm	63 Eu	⁶⁴ Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
			90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

12 Entries found for Hf, Te, showing:



Compound	Symmetry Group	Topological Indices	Crossing Type	Туре
Hf1 Te2	164 (<i>P</i> -3 <i>m</i> 1)		Line	ES
Hf1 Te3	11 (P2 ₁ /m)			LCEBR
Hf1 Te5	63 (Cmcm)	Z ₄ =3, Z _{2w,1} =1, Z _{2w,2} =1		NLC

chemistry <u>magic electron number of π -electrons</u>

Hückel:

- 4n+2 aromatic
- 4n antiaromatic

Möbius:4n aromatic4n+2 antiaromatic

topology in chemistry



Magic electron numbers

Hückel:		Möbius:	
4n+2	aromatic	4n	aromatic
4n	antiaromatic	4n+2	antiaromatic

Aromatics with a twist

Rainer Herges

The properties of flat aromatic molecules are well known to chemists, but some non-planar aromatics remain a mystery. A molecule that can twist into a Möbius band on command might shed light on their features.



Figure 2 | **A molecular topological switch.** Latos-Grażyński and colleagues¹ have made a compound that is antiaromatic in nonpolar solvents, but not in polar solvents. **a**, In nonpolar solvents, the two benzene rings (purple) in the molecule are parallel, and the molecule is a two-sided, non-twisted band. **b**, In polar solvents, the upper benzene ring twists by 90°, so that the molecule becomes a one-sided, Möbius structure. This conformational change alters the aromaticity of the molecule.



graphene – the twist



TREND

AB

Bilayer Graphene's Wicked, Twisted Road

Superconductivity, magnetism, and other forms of interacting electron behavior—bilayers of graphene seem to have it all. Researchers are now using this pristine material to unlock the secrets of interacting-electron phenomena with unprecedented control and tunability.





Unconventional superconductivity in magic-angle ..., Y Cao, , et al., Nature 556 (2018), 43-50, Spectroscopy of Twisted Bilayer Graphene ..., Dumitru Călugăru et al., arXiv:2110.15300



graphene – the twist

Physics

TREND

Bilayer Graphene's Wicked, Twisted Road

Superconductivity, magnetism, and other forms of interacting electron behavior—bilayers of graphene seem to have it all. Researchers are now using this pristine material to unlock the secrets of interacting-electron phenomena with unprecedented control and tunability.



AA π -elektrons localised AB π -electrons delocalised



Spectroscopy with STM

AB

AA



Unconventional superconductivity in magic-angle ..., Y Cao, , et al., Nature 556 (2018), 43-50, Spectroscopy of Twisted Bilayer Graphene ..., Dumitru Călugăru et al., arXiv:2110.15300



graphene – the twist

VIP Nanographenes Very Important Paper

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

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

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



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

twisted graphene – aromatic – antiaromatic ???

Unconventional superconductivity in magic-angle ..., Y Cao, , et al., Nature 556 (2018), 43-50, Spectroscopy of Twisted Bilayer Graphene ..., Dumitru Călugăru et al., arXiv:2110.15300

topological insulators



semiconductor







XYZ

ternary semiconductor



half Heusler compounds are ternary semiconductors

XYZ





average nuclear charge Z

J. Kroder, G. Fecher, C. Felser, , Chem. Unserer Zeit 56 (2022) 12–20 S Chadov, et al., Nature materials 9 (2010) 541-545

gold: a topological metal



measurements



Hall-measurements of semiconductors



quantum Hall effect





Klaus von Klitzing ©mpg

quantum Hall effect:

- exotic effect
- in complex layer systems of semiconductors
- precisely adjusted charge carrier concentration
- high magnetic fields
- low temperature



B



quantum Hall effect in a crystal



J. Gooth et al., Nature Communications 12 (2021) 3197, Fangdong Tang, et al., Nature 569 (2019) 537



quantum anomalous Hall – quantum spin Hall



VOLUME 61, NUMBER 18 P

PHYSICAL REVIEW LETTERS

31 October 1988

Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"

F. D. M. Haldane Department of Physics, University of California, San Diego, La Jolla, California 92093 (Precived 16 Sentember 1987)



Topological Quantum Matter

Nobel Lecture, December 8, 2016

Z₂ Topological Order and the Quantum Spin Hall Effe

C. L. Kane and E. J. Mele and Astronomy University of Pennsylvania Philadelphia F

Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA (Received 22 June 2005; published 28 September 2005)



Prediction of the quantum anomalous Hall effect without magnetic fieldPrediction of the quantum spin Hall effectSolution: Magnetic materialsSolution: materials with large spin orbit coupling

Haldane, PRL 61, 2015 (1988)



topological insulators – quantum spin Hall

Heavy insulating elements?

\mathbb{Z}_2 Topological Order and the Quantum Spin Hall Effect

C.L. Kane and E.J. Mele Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA



Strained α -Sn and Bi-bilayer



Prediction of the quantum spin Hall effect Solution: materials with large spin orbit coupling

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

Kane and Mele, PRL 95, 146802 (2005)



Element Bismuth Bi-Sb alloys Bi₂Se₃ and related structures



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

topological insulators

Se

Bi









measurements

- protected surface states
- quantized effects
- large effects in response to
 - the magnetic field, ...







topologic or trivial



from insulator to semimetal



Binghai Yan and Claudia Felser, Annual Review Condensed Matter Physics 8 (2017) 337, Prineha Narang, Christina A. C. Garcia and Claudia Felser, Nature Materials 20 (2021) 293

semimetals are common



Roald Hoffmann Angewandte. Chem. 26 (1987) 846



chirality







Nobel Symposium 167 on Chiral matter June 28 – July 1, 2021 Lidingö, Sweden



NOBEL SYMPOSIA

synthesis



M. Scheffler et al., Nature 604 (2022) 635–642
chiral anomaly



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

Adler, Phys. Rev. **177**, 2426 (1969) Bell and. Jackiw, Nuovo Cim. **A60**, 47 (1969) Zyuzin, Burkov - Physical Review B (2012) Burkov, Balents, PRL **107**, 12720 (2012) Burkov, J. Phys.: Condens. Matter **27**, 113201 (2015) Volovik, The Universe in a Helium Droplet (International Series of Monographs on Physics, Band 117) ISBN: 9780199564842

Wikipedia

3D topological Weyl - transport measurements:

(a) $\chi = +1$ $\chi = -1$

- 1. Giant responses to an external stimuli
- 2. Fermi arc
- 3. Chiral anomaly
- 4. Axial gravitational anomaly

Energy

Momentum



(b)



Burkov, Balents, PRL **107** 12720 (20..., Burkov, arXiv:1704.05467v2 Burkov, J. Phys.: Condens. Matter **27** (2015) 113201

chiral anomaly



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)



Metal Monophosphides

Phys. Rev. X 5, 011029 – Published 17 March 2015

Weyl semimetals

NbP, NbAs, TaP, TaAs

а

ARTICLE

Received 24 Nov 2014 | Accepted 30 Apr 2015 | Published 12 Jun 2015

DOI: 10.1038/ncomms8373

OPEN

-0.5

0.5

A Weyl Fermion semimetal with surface Fermi arcs in the transition metal monopnictide TaAs class

Shin-Ming Huang^{1,2,*}, Su-Yang Xu^{3,4,*}, Ilya Belopolski^{3,4,*}, Chi-Cheng Lee^{1,2}, Guoqing Chang^{1,2}, BaoKai Wang^{1,2,5}, Nasser Alidoust^{3,4}, Guang Bian³, Madhab Neupane^{3,4,6}, Chenglong Zhang⁷, Shuang Jia^{7,8}, Arun Bansil⁵, Hsin Lin^{1,2} & M. Zahid Hasan^{3,4,9}

2

0

-0.5

0

 $k_x(2\pi/a)$

а

 k_z (2 π /c)



Hongming Weng, Chen Fang, Zhong Fang, B. Andrei Bernevig, and Xi Dai

Weyl Semimetal Phase in Noncentrosymmetric Transition-

x = +1

x = -1

S.-Y. Xu, et al., Science 349 (2015) 613



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



Weng, et al. Phys. Rev. X 5, 11029 (2015) Huang et al. preprint arXiv:1501.00755 Shekhar, et al. , Nature Physics 11 (2015) 645 Frank Arnold, et al. Nature Communication 7 (2016) 11615



giant magnetoresistance

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

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



giant mobility

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

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

chiral anomaly



Jensen, et al. Thermodynamics, gravitational anomalies and cones. Journal of High Energy Physics 2013, 88 (2013).

chirale Anomalie



Landsteiner K., et al. Gravitational anomaly and transport phenomena. Phys. Rev. Lett. **107**, 021601 (2011). URL Jensen, et al. Thermodynamics, gravitational anomalies and cones. Journal of High Energy Physics **2013**, 88 (2013).

chiral anomaly



axial gravitional anomaly



Jensen, et al. Thermodynamics, gravitational anomalies and cones. Journal of High Energy Physics 2013, 88 (2013).

axial gravitional anomaly



J. Gooth, J. Kübler, C. Felser, Physik Journal 20 (2021) 29.



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

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

chiral and axial gravitational anomaly





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

Lucas, A., Davison, R. A. & Sachdev, S. PNAS **113**, 9463–9468 (2016).

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

Landsteiner K., et al. Gravitational anomaly and transport phenomena. Phys. Rev. Lett. 107, 021601 (2011). URL Jensen, et al. Thermodynamics, gravitational anomalies and cones. Journal of High Energy Physics 2013, 88 (2013).



chiral and axial gravitational anomaly



the universe in a crystal



The New Hork Times https://nyti.ms/2vCMCGi

SCIENCE

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

By KENNETH CHANG JULY 19, 2017

magnetic Weyl



antiferromagnetic topological materials

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	Mn_3GaC , Mn_3ZnC , Mn_3CuN , Mn_3Sn , Mn_3Ge , Mn_3Ir , Mn_3Pt , Mn_5Si_3
I-B	Actinide intermetallic	UNiGa5, UPtGa5, NpRhGa5, NpNiGa5
I-C	Rare-earth intermetallic	NdCo ₂ , TbCo ₂ , NpCo ₂ , PrAg DyCu, NdZn, TbMg, NdMg, Nd ₅ Si ₄ , Nd ₅ Ge ₄ , Ho ₂ RhIn ₈ , Er ₂ CoGa ₈ , Nd ₂ RhIn ₈ , Tm ₂ CoGa ₈ , Ho ₂ RhIn ₈ , DyCo ₂ Ga ₈ , TbCo ₂ Ga ₈ , Er ₂ Ni ₂ In, CeRu ₂ Al ₁₀ , Nd ₃ Ru ₄ Al ₁₂ , Pr ₃ Ru ₄ Al ₁₂ , ScMn ₆ Ge ₆ , YFe ₄ Ge ₄ , LuFe ₄ Ge ₄ , CeCoGe ₃
II-A	Metallic iron pnictides	LaFeAsO, CaFe ₂ As ₂ , EuFe ₂ As ₂ , BaFe ₂ As ₂ , Fe ₂ As, CaFe ₄ As ₃ , LaCrAsO, Cr ₂ As, CrAs, CrN
II-B	Semiconducting manganese pnictides	BaMn ₂ As ₂ BaMn ₂ Bi ₂ , CaMnBi ₂ , SrMnBi ₂ , CaMn ₂ Sb ₂ , CuMnAs, CuMnSb, Mn ₂ As
II-C	Rare-earth intermetallic compounds with the composition 1:2:2	PrNi ₂ Si ₂ , YbCo ₂ Si ₂ , DyCo ₂ Si ₂ , PrCo ₂ P ₂ , CeCo ₂ P ₂ , NdCo ₂ P ₂ , DyCu ₂ Si ₂ , CeRh ₂ Si ₂ , UAu ₂ Si ₂ , U ₂ Pd ₂ Sn, U ₂ Pd ₂ In, U ₂ Ni ₂ Sn, U ₂ Ni ₂ In, U ₂ Ni ₂ In, U ₂ Rh ₂ Sn
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, UP ₂ , UAs, NpS, NpSe, NpTe, NpSb, NpBi, U ₃ As ₄ , U ₃ P ₄
III-B	Metallic oxides	Ag ₂ NiO ₂ , AgNiO ₂ , Ca ₃ Ru ₂ O ₇ , Double perovskite Sr ₃ ColrO ₆
III-C	Metal-to-insulator transition compounds	NiS ₂ , Sr ₂ Mn ₃ As ₂ O ₂
III-D	Semiconducting and insulating oxides, borates, hydroxides, silicates and phosphate	LuFeO ₃ , PdNiO ₃ , ErVO ₃ , DyVO ₃ , MnGeO ₃ , Tm ₂ Mn ₂ O ₇ , Yb ₂ Sn ₂ O ₇ , Tb ₂ Sn ₂ O ₇ , Ho ₂ Ru ₂ O ₇ , Er ₂ Ti ₂ O ₇ , Tb ₂ Ti ₂ O ₇ , Cd ₂ Os ₂ O ₇ , Ho ₂ Ru ₂ O ₇ , Cr ₂ ReO6, NiCr ₂ O ₄ , MnV ₂ O ₄ , Co ₂ SiO ₄ , Fe ₂ SiO ₄ , PrFe ₃ (BO ₃) ₄ , KCo ₄ (PO ₄) ₃ , CoPS ₃ , SrMn(VO ₄)(OH), Ba ₅ Co ₅ ClO ₁₃ , Fel ₂

antiferromagnetic topological materials

Semiconducting actinides/ rare-earth pnictides

III-A

HoP, UP, UP₂, UAs, NpS, NpSe, NpTe, NpSb, NpBi, U₃As₄, U₃P₄

Strong interaction drives a quantum



phase transition to a topological insulator phase e_g Gd CFSf = 7/2f = 7/2



Band inversion between d and f bands of different parity PuTe under pressure has a band gap up to 0.4 eV



Higher Order topological insulator

Heusler Verbindungen



Heusler compounds



topological Heusler compounds





magnetic Weyl semimetals

Weyl points at low symmetry points

breaking time reversal symmetry

- magnetic field
- all crossings in the band structure in

ferromagnets are Weyl points

















Heusler compounds



Heusler X₂YZ L2₁



T. Graf, C. Felser, and S. S. P. Parkin, Prog. Solid State Chem. 39, 1 (2011)

Heusler Verbindungen



Heusler X₂YZ L2₁



Heusler compounds



magnetic Heusler



half metallic Heusler

$$Co_2TiAl:$$
 $2 \times 9 + 4 + 3 = 25$ $Ms = 1m_B$ $Co_2MnGa:$ $2 \times 9 + 7 + 3 = 28$ $Ms = 4m_B$ $Co_2FeSi:$ $2 \times 9 + 8 + 4 = 30$ $Ms = 6m_B$





 X_2YZ



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

Tunneling magnetoresistance effect in Heusler



Read-Head Fabrication w/Heusler alloy

HITACHI Inspire the Next





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



Kübler, Felser, EPL 114 (2016) 47005.

0.0

1.0

Berry curvature and anomalous Nernst



Jonathan Noky, Claudia Felser, and Yan Sun, Physical Review B 99 (2019) 165117

Berry curvature design





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


Article Observation of a linked-loop quantum state in a topological magnet

(6)

(7)

-0.4 0 0.4 -0.4 0 0.4

 k_z (Å⁻¹)

 k_v (Å⁻¹)

Co2MnGa



Belopolski, et al., Nature | Vol604 | 28April2022 | 647



Hall effect



T. Graf, C. Felser, and S. S. P. Parkin, Prog. Solid State Chem. 39, 1 (2011)

Anomalous Hall



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

Anomalous Hall



Naoto Nagaosa and Yoshinori Tokura 2012 Phys. Scr. 2012 014020

anomalous Nernst Effect









Satya N. Guin, et al., NPG Asia Mater. 11, 16 (2019), arXiv:1806.06753 Sakain et al. Nature Physics 2018

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

Nernst Effect of iron compounds

Noky, J., Xu, Q., Felser, C. & Sun, Y. Large anomalous Hall and Nernst effects from nodal line symmetry breaking in Fe₂MnX (X = P, As, Sb). Phys. Rev. B 99, 165117 (2019).



Article Iron-based binary ferromagnets for transverse thermoelectric conversion

ttps://doi.org/10.1038/s41586-020-2230-z
eceived: 26 July 2019
accepted: 4 February 2020
ublished online: 27 April 2020
D Check for updates

Akito Sakai^{1,2,3,0}, Susumu Minami^{4,5,10}, Takashi Koretsune^{6,10}, Taishi Chen^{1,3,10}, Tomoya Higo^{1,3,10}, Yangming Wang¹, Takuya Nomoto⁷, Motoaki Hirayama⁵, Shinji Miwa^{1,3,8}, Daisuke Nishio-Hamane¹, Fumiyuki Ishii^{4,5}, Ryotaro Arita^{3,5,7} & Satoru Nakatsuji^{1,2,3,8,9}

Thermoelectric generation using the anomalous Nernst effect (ANE) has great potential for application in energy harvesting technology because the transverse geometry of the Nernst effect should enable efficient, large-area and flexible coverage of a heat source. For such applications to be viable, substantial improvements will be necessary not only for their performance but also for the associated material costs,

Heusler compounds



topological Heusler compounds

Heusler compounds with crystalline anisotropy



Mn₃Ga Mn₃Ge Mn₃Sn

Heusler compounds for STT MRAM

- Materials with low magnetic damping
- Materials with low magnetic moments
- Materials with high perpendicular anisotrop



Mn₂Ga





Stuart S. P. Parkin, et al.: *Magnetic Domain-Wall Racetrack Memory, Science* 320 (2008) 190–194



Skyrmions on the track

Albert Fert, Vincent Cros and João Sampaio



A. K. Nayak, et al., Nature 548 (2017) 561

Heusler compounds







- Dirac cone,
- flat band, and
- van Hove singularity

Mn₃Ga, Mn₃Ge, Mn₃Sn

antiferromagnetic topological materials

Table 3 | The magnetic topological materials identified in this work

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I-A	Non-collinear manganese compounds	Mn_3GaC , Mn_3ZnC , Mn_3CuN , Mn_3Sn , Mn_3Ge , Mn_3Ir , Mn_3Pt , Mn_5Si_3
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I-C	Rare-earth intermetallic	NdCo ₂ , TbCo ₂ , NpCo ₂ , PrAg DyCu, NdZn, TbMg, NdMg, Nd ₅ Si ₄ , Nd ₅ Ge ₄ , Ho ₂ RhIn ₈ , Er ₂ CoGa ₈ , Nd ₂ RhIn ₈ , Tm ₂ CoGa ₈ , Ho ₂ RhIn ₈ , DyCo ₂ Ga ₈ , TbCo ₂ Ga ₈ , Er ₂ Ni ₂ In, CeRu ₂ Al ₁₀ , Nd ₃ Ru ₄ Al ₁₂ , Pr ₃ Ru ₄ Al ₁₂ , ScMn ₆ Ge ₆ , YFe ₄ Ge ₄ , LuFe ₄ Ge ₄ , CeCoGe ₃
II-A	Metallic iron pnictides	LaFeAsO, CaFe2As2, EuFe2As2, BaFe2As2, Fe2As, CaFe4As3, LaCrAsO, Cr2As, CrAs, CrN
II-B	Semiconducting manganese pnictides	BaMn ₂ As ₂ BaMn ₂ Bi ₂ , CaMnBi ₂ , SrMnBi ₂ , CaMn ₂ Sb ₂ , CuMnAs, CuMnSb, Mn ₂ As
II-C	Rare-earth intermetallic compounds with the composition 1:2:2	PrNi ₂ Si ₂ , YbCo ₂ Si ₂ , DyCo ₂ Si ₂ , PrCo ₂ P ₂ , CeCo ₂ P ₂ , NdCo ₂ P ₂ , DyCu ₂ Si ₂ , CeRh ₂ Si ₂ , UAu ₂ Si ₂ , U ₂ Pd ₂ Sn, U ₂ Pd ₂ In, U ₂ Ni ₂ Sn, U ₂ Ni ₂ In, U ₂ Ni ₂ In, U ₂ Rh ₂ Sn
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, UP ₂ , UAs, NpS, NpSe, NpTe, NpSb, NpBi, U ₃ As ₄ , U ₃ P ₄
III-B	Metallic oxides	Ag ₂ NiO ₂ , AgNiO ₂ , Ca ₃ Ru ₂ O ₇ , Double perovskite Sr ₃ CoIrO ₆
III-C	Metal-to-insulator transition compounds	NiS ₂ , Sr ₂ Mn ₃ As ₂ O ₂
III-D	Semiconducting and insulating oxides, borates, hydroxides, silicates and phosphate	LuFeO ₃ , PdNiO ₃ , ErVO ₃ , DyVO ₃ , MnGeO ₃ , Tm ₂ Mn ₂ O ₇ , Yb ₂ Sn ₂ O ₇ , Tb ₂ Sn ₂ O ₇ , Ho ₂ Ru ₂ O ₇ , Er ₂ Ti ₂ O ₇ , Tb ₂ Ti ₂ O ₇ , Cd ₂ Os ₂ O ₇ , Ho ₂ Ru ₂ O ₇ , Cr ₂ ReO6, NiCr ₂ O ₄ , MnV ₂ O ₄ , Co ₂ SiO ₄ , Fe ₂ SiO ₄ , PrFe ₃ (BO ₃) ₄ , KCo ₄ (PO ₄) ₃ , CoPS ₃ , SrMn(VO ₄)(OH), Ba ₅ Co ₅ ClO ₁₃ , Fel ₂

antiferromagnetic materials





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

The anomalous Hall conductivity in an antiferromagnetic metal is zero

Manna et al., Phys. Rev. X 8 (2018) 041045, arXiv:1712.10174 Manna et al., Nature Review Materials, 3 (2018) 244 arXiv:1802.02838v1

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

Anomalous Hall effect

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N. P. Ong

Department of Physics, Princeton University, Princeton, New Jersey 08544, USA (Published 13 May 2010)

start end



Berry curvature

antiferromagnetic topological materials

Table 3 | The magnetic topological materials identified in this work



Chen, Niu, MacDonald, PRL112 (2014) 017205, Kübler, Felser EPL 108 (2014) 67001, Nayak et al., Science Advances 2 (2016) e1501870, Nakatsuji, et al., Nature, doi:10.1038/nature15723

Giant anomalous Nernst effect

TERS







doi:10.1038/nature25987

Massive Dirac fermions in a ferromagnetic kagome metal











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

















Τ.



 $Co_3Sn_2S_2$





D. F. Liu, et al., Science 365 (2019) 1282





STM and ARPES confirms Weyl and Fermiarcs















D. F. Liu, et al., Science 365 (2019) 1282

Giant anomalous Hall effect



Naoto Nagaosa and Yoshinori Tokura 2012 Phys. Scr. 2012 014020

Giant anomalous Nernst effect



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

Giant anomalous Nernst effect



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

from 3D to 2D quantum effects



Quantum anomalous Hall effect?



Berry curvature design



Satya N. Guin, et al. Chandra Shekhar, Andrea Damascelli, Yan Sun, and Claudia Felser, Advanced Materials DOI: 10.1002/adma.202006301



3D

2D

Energie

(b)

(d)

(c)

Energie

Nernst Leitfähigkeit

Co₃Sn₂S₂





Magnetfeld

antiferromagnetic topological materials

Table 3 | The magnetic topological materials identified in this work

Categories	Properties	Materials
I-A	Non-collinear manganese compounds	Mn_3GaC , Mn_3ZnC , Mn_3CuN , Mn_3Sn , Mn_3Ge , Mn_3Ir , Mn_3Pt , Mn_5Si_3
I-B	Actinide intermetallic	UNiGa5, UPtGa5, NpRhGa5, NpNiGa5
I-C	Rare-earth intermetallic	NdCo ₂ , TbCo ₂ , NpCo ₂ , PrAg DyCu, NdZn, TbMg, NdMg, Nd ₅ Si ₄ , Nd ₅ Ge ₄ , Ho ₂ RhIn ₈ , Er ₂ CoGa ₈ , Nd ₂ RhIn ₈ , Tm ₂ CoGa ₈ , Ho ₂ RhIn ₈ , DyCo ₂ Ga ₈ , TbCo ₂ Ga ₈ , Er ₂ Ni ₂ In, CeRu ₂ Al ₁₀ , Nd ₃ Ru ₄ Al ₁₂ , Pr ₃ Ru ₄ Al ₁₂ , ScMn ₆ Ge ₆ , YFe ₄ Ge ₄ , LuFe ₄ Ge ₄ , CeCoGe ₃
II-A	Metallic iron pnictides	LaFeAsO, CaFe2As2, EuFe2As2, BaFe2As2, Fe2As, CaFe4As3, LaCrAsO, Cr2As, CrAs, CrN
II-B	Semiconducting manganese opictides	BaMn ₂ As ₂ BaMn ₂ Bi ₂ , CaMnBi ₂ , SrMnBi ₂ , CaMn ₂ Sb ₂ , CuMnAs, CuMnSb, Mn ₂ As
II-C	Rare-earth intermetallic compounds with the composition 1:2:2	PrNi ₂ Si ₂ , YbCo ₂ Si ₂ , DyCo ₂ Si ₂ , PrCo ₂ P ₂ , CeCo ₂ P ₂ , NdCo ₂ P ₂ , DyCu ₂ Si ₂ , CeRh ₂ Si ₂ , UAu ₂ Si ₂ , U ₂ Pd ₂ Sn, U ₂ Pd ₂ In, U ₂ Ni ₂ Sn, U ₂ Ni ₂ In, U ₂ Ni ₂ In, U ₂ Ni ₂ In, U ₂ Rh ₂ Sn
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, UP ₂ , UAs, NpS, NpSe, NpTe, NpSb, NpBi, U ₃ As ₄ , U ₃ P ₄
III-B	Metallic oxides	Ag ₂ NiO ₂ , AgNiO ₂ , Ca ₃ Ru ₂ O ₇ , Double perovskite Sr ₃ CoIrO ₆
III-C	Metal-to-insulator transition compounds	NiS ₂ , Sr ₂ Mn ₃ As ₂ O ₂
III-D	Semiconducting and insulating oxides, borates, hydroxides, silicates and phosphate	LuFeO ₃ , PdNiO ₃ , ErVO ₃ , DyVO ₃ , MnGeO ₃ , Tm ₂ Mn ₂ O ₇ , Yb ₂ Sn ₂ O ₇ , Tb ₂ Sn ₂ O ₇ , Ho ₂ Ru ₂ O ₇ , Er ₂ Ti ₂ O ₇ , Tb ₂ Ti ₂ O ₇ , Cd ₂ Os ₂ O ₇ , Ho ₂ Ru ₂ O ₇ , Cr ₂ ReO6, NiCr ₂ O ₄ , MnV ₂ O ₄ , Co ₂ SiO ₄ , Fe ₂ SiO ₄ , PrFe ₃ (BO ₃) ₄ , KCo ₄ (PO ₄) ₃ , CoPS ₃ , SrMn(VO ₄)(OH), Ba ₅ Co ₅ ClO ₁₃ , Fel ₂

canting and anomalous Hall



Congcong Le, Claudia Felser, and Yan Sun, Phys. Rev. B 104, 125145



Sergey Borisenkoet al., Nature Communications 10 (2019) 3424

non-collinear antiferromagnet YbMnBi₂



non-collinear antiferromagnet YbMnBi₂



Pan et al., Nature Materials 21, 203–209 (2022), JP Heremans, S Watzman, N Trivedi, T Mccormick, C Felser, US Patent App. 16/157,522

chirality





new fermions

RESEARCH

Dirac new Fermion Weyl **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, chiral, 2-fold. 4- fold 6-fold R. J. Cava, B. Andrei Bernevig⁺ Enantiomer A Enantiomer B free fermionic excitations in solid-state systems that have Crystal structure no high-energy counterparts. Some of these new Fermions are even chiral

- Chiral Crystals
 - B20, Skyrmions, CoSi, MnSi, PdGa, RhSi
- **Superconductors**
 - A15 superconductors: Nb₃Sn, Li₂Pd₃B



chiral Fermion

chiral n-fold



chiral fermions

ARTICLES https://doi.org/10.1038/s41563-018-0169-3



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†

C SiCo (SG 198) C SiCo

Topological quantum properties of chiral crystals

Guoqing Chang[®]^{1,2,3,4,12}, Benjamin J. Wieder[®]^{5,6,7,12}, Frank Schindler^{8,12}, Daniel S. Sanchez¹, Ilya Belopolski¹, Shin-Ming Huang[®]⁹, Bahadur Singh[®]^{2,3}, Di Wu^{2,3}, Tay-Rong Chang¹⁰, Titus Neupert[®]⁸, Su-Yang Xu^{1*}, Hsin Lin^{2,3,4*} and M. Zahid Hasan[®]^{1,11*}



Unconventional Chiral Fermions and Large Topological Fermi Arcs in RhSi

Guoqing Chang, Su-Yang Xu, Benjamin J. Wieder, Daniel S. Sanchez, Shin-Ming Huang, Ilya Belopolski, Tay-Rong Chang, Songtian Zhang, Arun Bansil, Hsin Lin, and M. Zahid Hasan Phys. Rev. Lett. **119**, 206401 – Published 17 November 2017
Bringing order to the expanding fermion zoo Carlo Beenakker Commentary

Heisenberg (1930): We observe space as a continuum, but we might entertain the thought that there is an underlying lattice and that space is actually a crystal. Which particles would inhabit such a lattice world? Werner Heisenberg *Gitterwelt* (lattice world) **hosted electrons that could morph into protons, photons that were not massless,** and more peculiarities that compelled him to abandon "this completely crazy idea"

chirality and topology

chiral crystals optical activity

topological crystals unusual surface states large photogalvanic effect



new Fermions

largest Fermi arc Quantized circular photogalvanic effect

...

...

chirality and chiral anomaly





J. Gooth et al., Nature 547 (2017) 324 arXiv:1703.10682. J. Gooth, J. Kübler, C. Felser, Physik Journal 20 (2021) 29.



chirality in chemistry

Lord Kelvin: An object or a system is *chiral* if it is distinguishable from its <u>mirror image</u>; that is, it cannot be <u>superposed</u> onto it.

Molecules with different chiralities have different optical and catalytic properties In terms of <u>point groups</u>, all chiral molecules lack an improper axis of rotation (S_n)







Molecules with different chiralities have different optical and catalytic properties

chirality in chemistry

Chiral space groups contain symmetry operations of the first kind (rotation). There are 11 pairs of enantiomorphic space groups (e.g. P61 and P65) which are chiral. 43 achiral space groups can host a chiral crystal structure.





synthesis



Nitesh Kumar, Satya N. Guin, Kaustuv Manna, Chandra Shekhar, and Claudia Felser, Chem. Rev. 121 (2021) 2780.

chiral crystals which host new fermions



Fermions: more examples include CoSi, RhSi, PtAl, CoGe, RhGe, PtGa, PtAl and magnetic MnSi and FeGe



homochiral crystals

Compounds with the B20 structure

Enantiomer A and Enantiomer B Crystal structure







Absolute Structure from Scanning Electron Microscopy

Ulrich Burkhardt^{1*}, Horst Borrmann¹, Philip Moll^{1,2}, Marcus Schmidt¹, Yuri Grin¹ & Aimo Winkelmann^{3,4}

- X- ray (volume sensitive)
- electron backscatter diffraction (EBSD) (surface sensitive)







Fermions: more examples include CoSi, RhSi, PtAl, CoGe, RhGe, PtGa, PtAl and magnetic MnSi and FeGe













The crystal structure is chiral, the electronic structure is identical, however, the Weyl points and the Fermi arcs are chiral



The crystal structure is chiral, the electronic structure is identical, however, the Weyl points and the Fermi arcs are chiral

chiral Fermions





R

RH-a

1.2

PdGa











Energy (eV)

Energy (eV)

-1

-1

new fermions with chiral surface states $E_B = 0 meV$ 25meV 50meV 100meV 75meV 0.8-CoSi RhSi 0.5 $\underbrace{ \left(\begin{array}{c} 0.25 \\ -4 \end{array} \right) }_{A_{-0.25}} 0.25$ -0.5 -0.8 nar 0.4 0.8 0.4 0.8 0.4 0.8 0 0.4 0.8 0.4 0.8 0 0 0 0 RhSi k_x (A⁻¹) RhSi, giant topological Fermi arcs 0.8 RhSi (001) surface = Fermi Surface (CoSi) $C_2^{\text{R}} = -$ M $k_{y}(\pi/a)$ CoSi Fermi arc 0 6 High 5 \overline{X}_1 4 3 Fermi arc 2 Low 0 -0.8 0.8 -0.80 R Х Х Μ Г $k_x(\pi/a)$ M \overline{X}_2 M

S. Sanchez, K. Manna et al. Nature 567, 500 (2019).

quantum oscillations of PtGa



chiral surface states with STM





Enantiomer B

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) enantiomers

PdGa





Quasiparticle interference of two PdGa(001) enantiomers

chiral electrons in the bulk

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







PdGa

Yao et. al., to be published



Quantized circular photogalvanic effect

E (eV)

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

DOI: 10.1038/ncomms15995 OPEN

Quantized circular photogalvanic effect in Weyl semimetals

Fernando de Juan^{1,2,3}, Adolfo G. Grushin¹, Takahiro Morimoto¹ & Joel E. Moore^{1,4}

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

The rate of change of the difference in photocurrent generated by left-circularly and right-circularly polarized light, dj/dt, is quantized to the **Chern number**

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







Quantized circular photogalvanic effect

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

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Quasi-symmetry-protected topology



chiral surface states in CoSi

RhSi and CoSi: with multiple helicoid arc saddle points: type-I and type-II van Hove singularities.

CoSi

Charge instability of topological Fermi arcs in chiral crystal CoSi

Zhicheng Rao^{1,2,†}, Quanxin Hu^{1,2,†}, Shangjie Tian^{3,†}, Shunye Gao^{1,2}, Zhenyu Yuan^{1,2}, Cenyao Tang^{1,2}, Wenhui Fan^{1,2}, Jierui Huang^{1,2}, Yaobo Huang⁴, Li Wang⁵, Lu Zhang^{1,2}, Fangsen Li⁵, Huaixin Yang^{1,2,6}, Hongming Weng^{1,2,6}, Tian Qian^{1,2,6}, Jinpeng Xu^{1,2,7*}, Kun Jiang^{1,2}, Hechang Lei^{3*}, Yu-Jie Sun^{8,1*} and Hong Ding^{1,6,7}

Chirality locking charge density waves in a chiral crystal

Geng Li^{1,2,3,4#}, Haitao Yang^{1,2#}, Peijie Jiang^{1,2#}, Cong Wang^{5#}, Qiuzhen Cheng^{1,2}, Shangjie Tian⁵, Guangyuan Han^{1,2}, Chengmin Shen^{1,2}, Xiao Lin^{1,2}, Hechang Lei^{5*}, Wei Ji^{5*}, Ziqiang Wang^{6*}, Hong-Jun Gao^{1,2,3,4*}



chiral surface states in CoSi and RhSi

RhSi and CoSi: with multiple helicoid arc saddle points: type-I and type-II van Hove singularities.





Tunable topologically driven Fermi arc Van Hove singularities

Daniel S. Sanchez *,^{1,2} Tyler A. Cochran *,¹ Ilya Belopolski,^{1,3} Zi-Jia Cheng,¹ Xian P. Yang,¹ Yiyuan Liu,⁴ Tao Hou,⁵ Xitong Xu,⁴ Kaustuv Manna,^{6,7} Chandra Shekhar,⁶ Jia-Xin Yin,¹ Horst Borrmann,⁶ Alla Chikina,⁸ Jonathan D. Denlinger,⁹ Vladimir N. Strocov,⁸ Weiwei Xie,¹⁰ Claudia Felser,⁶ Shuang Jia,⁴ Guoqing Chang ^{†,5} and M. Zahid Hasan ^{†1,11,12}





new catalysist with chiral surface states



Surface State of Platinum B. Yan, et al. Nat. Commun. 2015, 6, 10167.



Nodal line in IrO₂

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





Q. Yang, et al, Adv. Mater., 2020, 32,1908518.

Chiral crystals for Water electrolysis and fuel cells, European patent, 19211719.0, submission 27.11.2019

new catalysist with chiral surface states





absorption and oxidation of chiral molecules





oxidation of Dopa on the surface of PdGa

all the measurement conditions are kept the same except the chirality of the PdGa crystal D-DOPA and L-DOPA show different oxidation behaviors, depending on the chirality of PdGa

electrons – molecules, surfaces and crystals







physics meets chemistry



parity violation



chirality in Charge density wave systems



Switchable chiral transport in charge-ordered CsV_3Sb_5

Chunyu Guo^{*},¹ Carsten Putzke,^{1,2} Sofia Konyzheva,¹ Xiangwei Huang,¹ Martin Gutierrez-Amigo,^{3,4} Ion Errea,^{3,5,6} Dong Chen,⁷ Maia G. Vergniory,^{5,7} Claudia Felser,⁷ Mark H. Fischer^{*},⁸ Titus Neupert[†],⁸ and Philip J. W. Moll^{‡1,2}



chirality in Charge density wave systems



Visualization of Chiral Electronic Structure and Anomalous Optical Response in a Material with Chiral Charge Density Waves

H. F. Yang^{1*}, K. Y. He^{2*}, J. Koo^{3*}, S. W. Shen¹, S. H. Zhang¹, G. Liu², Y. Z. Liu³, C. Chen^{1,4}, A. J. Liang^{1,5}, K. Huang¹, M. X. Wang^{1,5}, J. J. Gao⁶, X. Luo⁶, L. X. Yang⁷, J. P. Liu^{1,5}, Y. P. Sun^{6,8,9}, S. C. Yan^{1,5}, B. H. Yan^{3†}, Y. L. Chen^{1,4,5,7†}, X. Xi^{2,9†}, and Z. K. Liu^{1,5†}

summary

- topologically protected surfaces edge or edge states in crystals
- new quantum effects in crystals
- in semimetals one observes giant effects in response of magnetic, electric field, light etc.
- Fermi arcs
- arcs extended over the recirpoken space in chiral crystals
- high mobilities, free electron path lengths up to mm
- giant Nernst effect and magnetic Seebeck effect
- giant photovoltaic effect quantized
- Weyl semimetals as model systems for high energy and astrophysics
- Parity violation E*B in Weyl semimetals
- chiral anomaly
- axial graviation anomaly
- topological catalysis



Berry Phase



summary

- more than 25% of all inorganic compounds are topological
- quantum simulator for high energy and astro-physics
- paramagnetic Weyl semimetals, which break inversion: chiral anomaly in thermal and electrical transport
- chiral new Fermions: giant Fermi arcs, strong **Berry curvature effects**, new chiral optical effects **outlook**
- chirality and magnetism
- beyond the single particle picture topology in correlated materials
- experiments and understanding of **3D quantum Hall** effects
- connect chiral molecules and catalysis with Berry curvature
 - the interplay between chiral structure/surface state/orbital moment

potential applications

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



arXiv:1511.07672v1

Vision

- Crystal growth of both enantiomers of topological chiral compounds
 - interfaces, grain boundaries, chiral phonons, magnons, ...
 - Investigation of the interplay between structure, chiral surface state, orbital angular 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 over μm
- Chirality plus magnetism, correlations, superconductivity
 - Skyrmions, Antiskyrmions ...













Potentielle Anwendungen



New Konzepte zur Energiekonversion







Neue Elektronik – Spin



Verlustfreier Elektronentransport

Ultraschnelle Quantencomputer

Thank you!



Johannes Gooth



Niels Schröter





Andrei Bernevig



Maia Vergniory




Reaktionskoordinate





•----+



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