Nodal-line semimetals in high magnetic field

a study of ZrSiS

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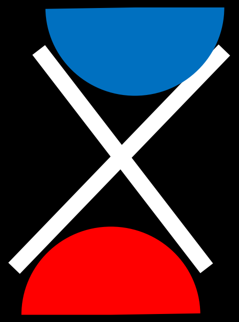
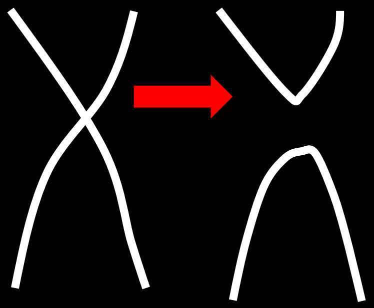
Topological insulators



Time inversion symmetry protected surface states

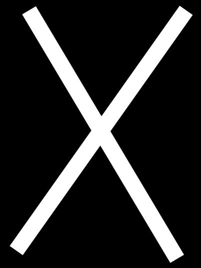
„Ordinary metals”



Band repulsion

Symmetry protection

Dirac semimetals

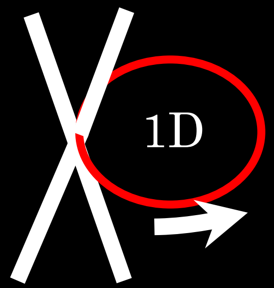


Spin degenerated

Weyl semimetals

Spin non-degenerated

Nodal-line semimetals



Spin degenerated

…

How to study topological materials?

What does theory say?

ARTICLE

https://doi.org/10.1038/s41586-019-0954-4

A complete catalogue of high-quality topological materials

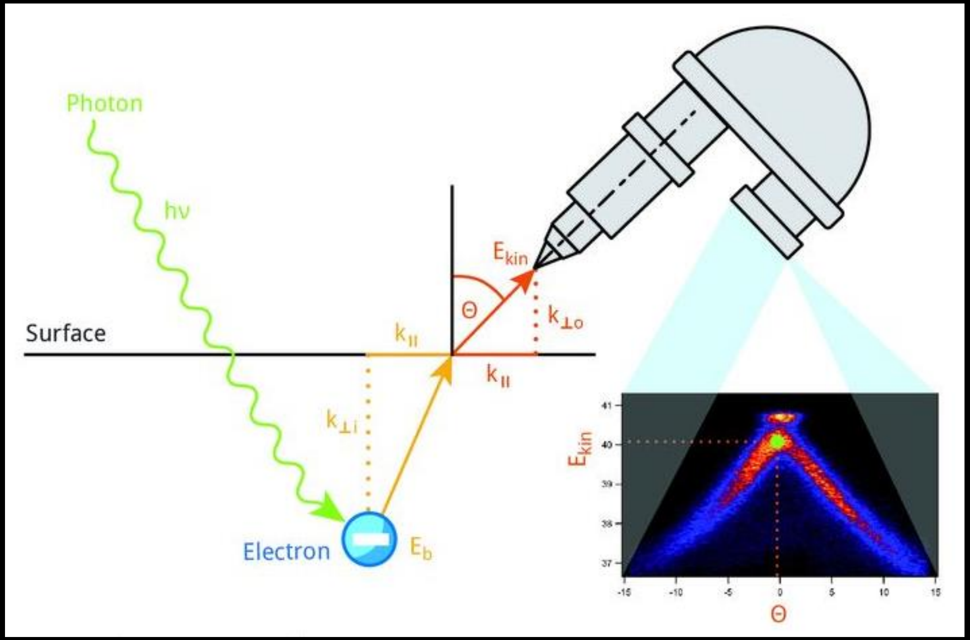
M. G. Vergniory[1,2,3,11], L. Elcoro[4,11], Claudia Felser[5], Nicolas Regnault[6], B. Andrei Bernevig[7,8,9]* & Zhijun Wang[7,10]*

Using a recently developed formalism called topological quantum chemistry, we perform a high-throughput search of 'high-quality' materials (for which the atomic positions and structure have been measured very accurately) in the Inorganic Crystal Structure Database in order to identify new topological phases. We develop codes to compute all characters of all symmetries of 26,938 stoichiometric materials, and find 3,307 topological insulators, 4,078 topological semimetals and no fragile phases. For these 7,385 materials we provide the electronic band structure, including some electronic properties (bandgap and number of electrons), symmetry indicators, and other topological information. Our results show that more than 27 per cent of all materials in nature are topological. We provide an open-source code that checks the topology of any material and allows other researchers to reproduce our results.

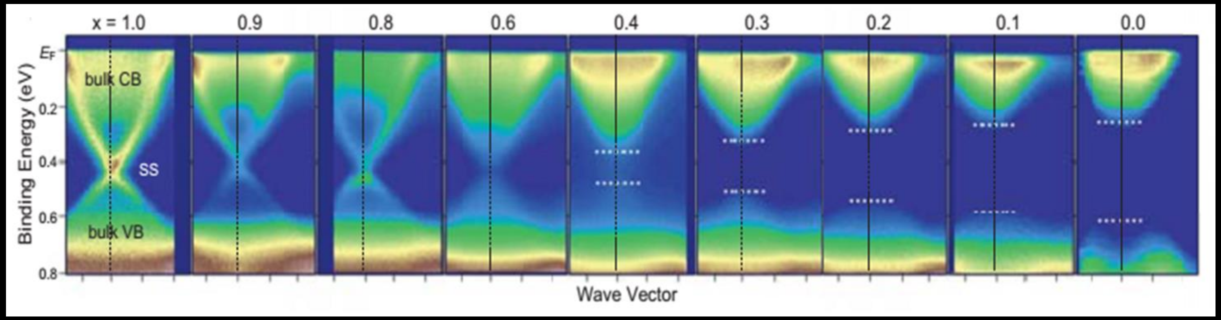
How to study topological materials?

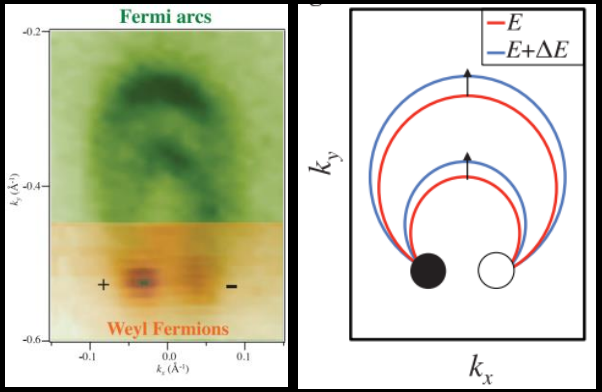
Angle resolved photoemission spectroscopy ARPES

- We can identify SS and spin polarization

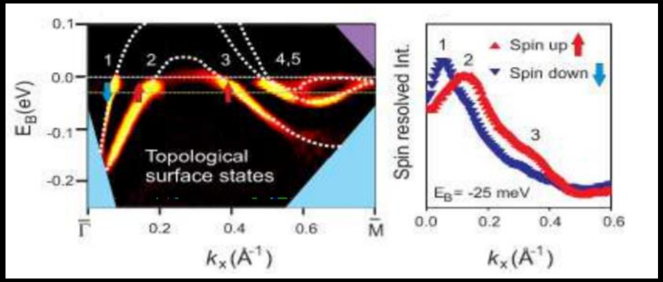


TlBiSSe - Nature Physics 7 840 (2011)





TaAs – Science 349 613 (2015)

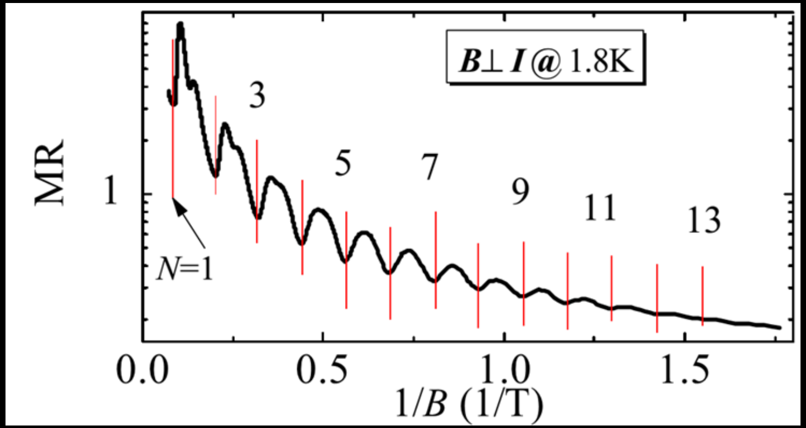


Bi_{1-x} Sb – Science 323 919 (2009)

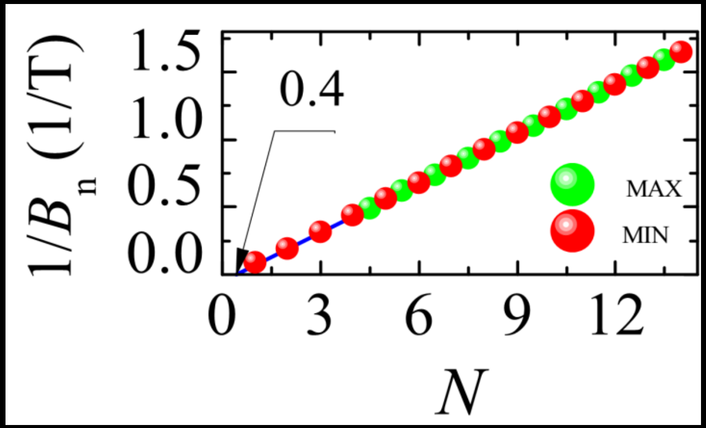
How to study topological materials?

Transport properties
Magnetic properties under high magnetic field
Optical properties

Quantum oscillations



Landau level diagram



$\frac{1}{2} - \frac{1}{8}$ =0.375

Osanger's relation

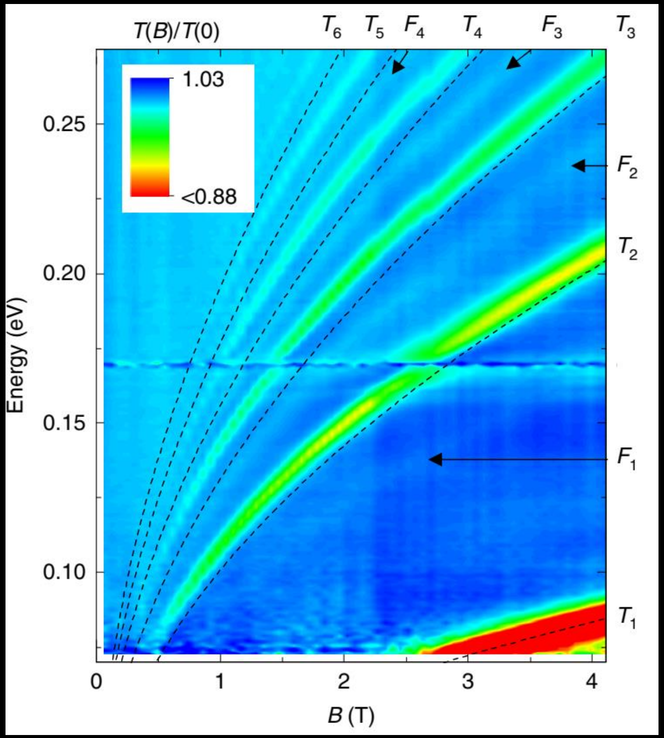
$$A_{\boldsymbol{k}}(\epsilon_{\boldsymbol{k}}) = (n+\gamma)2\pi eB/\hbar$$

Berry phase

$$\phi_B = 2\pi\left(\frac{1}{2} - \gamma\right)$$

How to study topological materials?

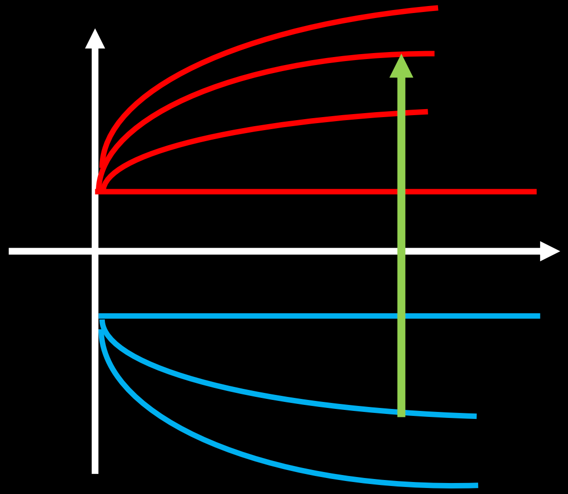
Transport properties
Magnetic properties under high magnetic field
Optical properties



Kuzmenko et al. Nature nano.

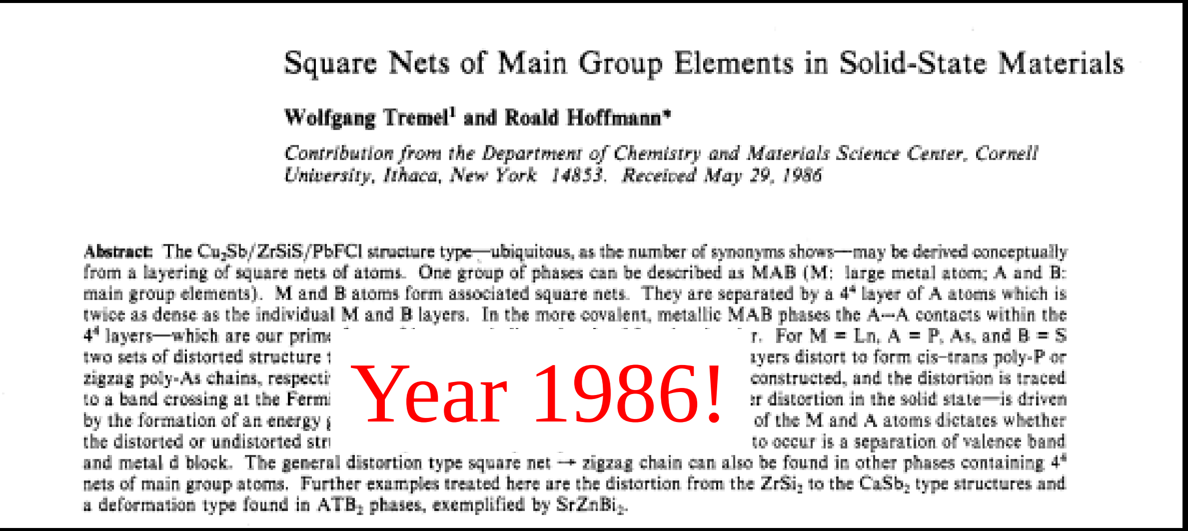
Landau levels in (masive) Dirac system

$$E_N = \sqrt{\Delta^2 + 2v_F^2 BN}$$



Nodal-line Dirac system under study:

ZrSiS



Square Nets of Main Group Elements in Solid-State Materials

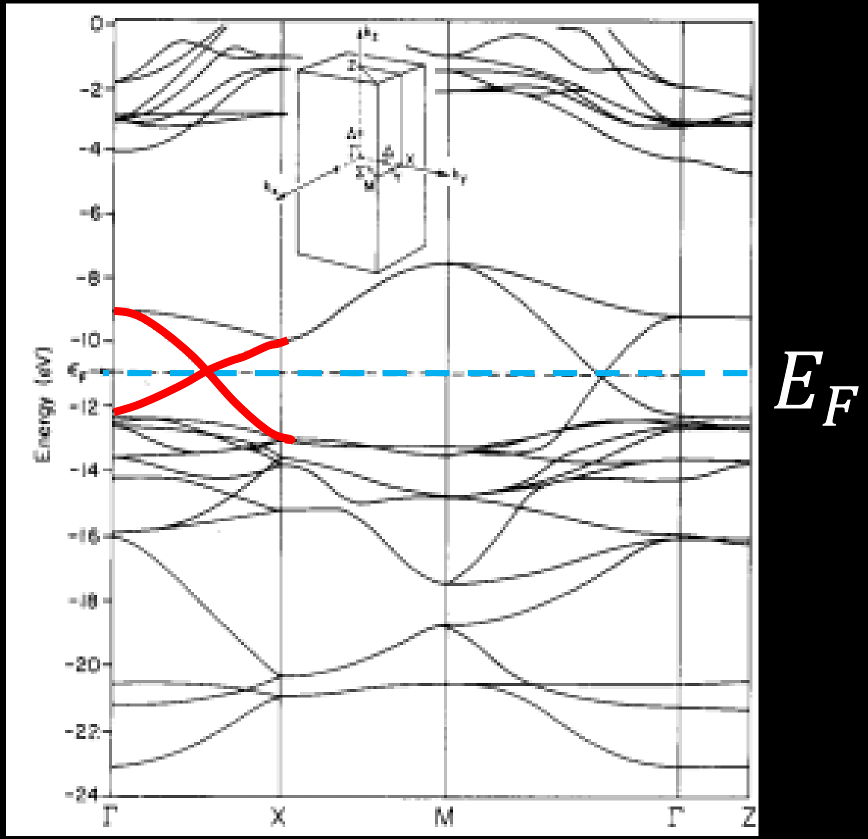
Wolfgang Tremel[1] and Roald Hoffmann*

Contribution from the Department of Chemistry and Materials Science Center, Cornell University, Ithaca, New York 14853. *Received May 29, 1986*

Abstract: The Cu_2Sb/ZrSiS/PbFCl structure type—ubiquitous, as the number of synonyms shows—may be derived conceptually from a layering of square nets of atoms. One group of phases can be described as MAB (M: large metal atom; A and B: main group elements). M and B atoms form associated square nets. They are separated by a 4^4 layer of A atoms which is twice as dense as the individual M and B layers. In the more covalent, metallic MAB phases the A–A contacts within the 4^4 layers—which are our prim r. For M = Ln, A = P, As, and B = S two sets of distorted structure t ayers distort to form cis–trans poly-P or zigzag poly-As chains, respecti constructed, and the distortion is traced to a band crossing at the Fermi er distortion in the solid state—is driven by the formation of an energy g of the M and A atoms dictates whether the distorted or undistorted str to occur is a separation of valence band and metal d block. The general distortion type square net → zigzag chain can also be found in other phases containing 4^4 nets of main group atoms. Further examples treated here are the distortion from the $ZrSi_2$ to the $CaSb_2$ type structures and a deformation type found in ATB_2 phases, exemplified by $SrZnBi_2$.

Year 1986!

- Prototypical nodal-line Dirac semimetal

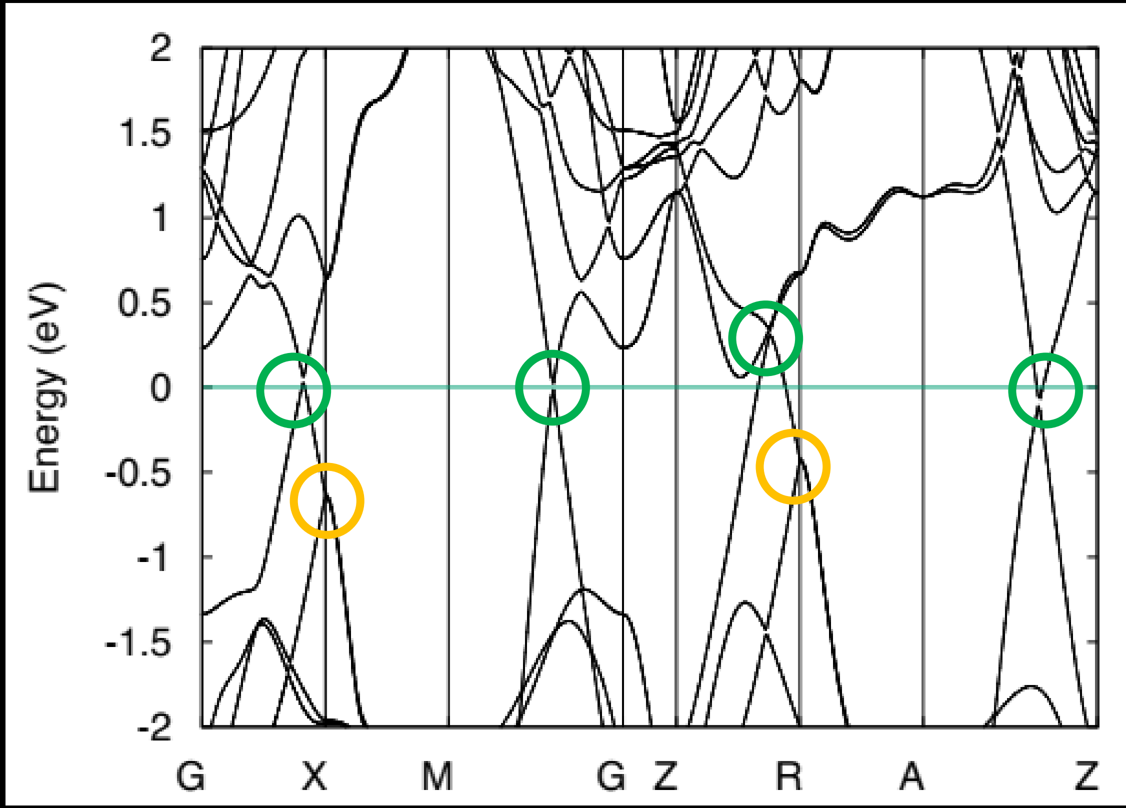


- Early band structure

Nodal-line Dirac system under study:

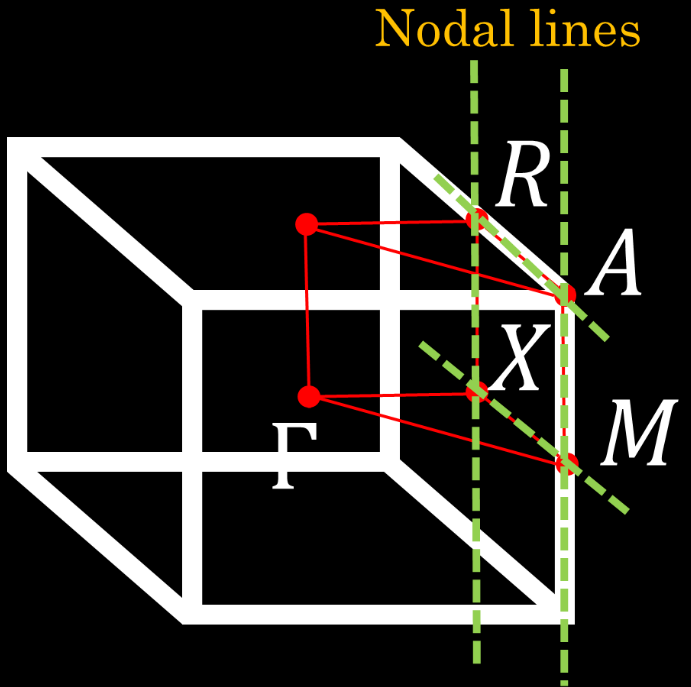
ZrSiS

- Modern DFT calculations



Nonsymmorphic symmetry protected nodal lines

C2 protected nodal lines
SOC opens a gap



Nodal-line Dirac system under study:

ZrSiS

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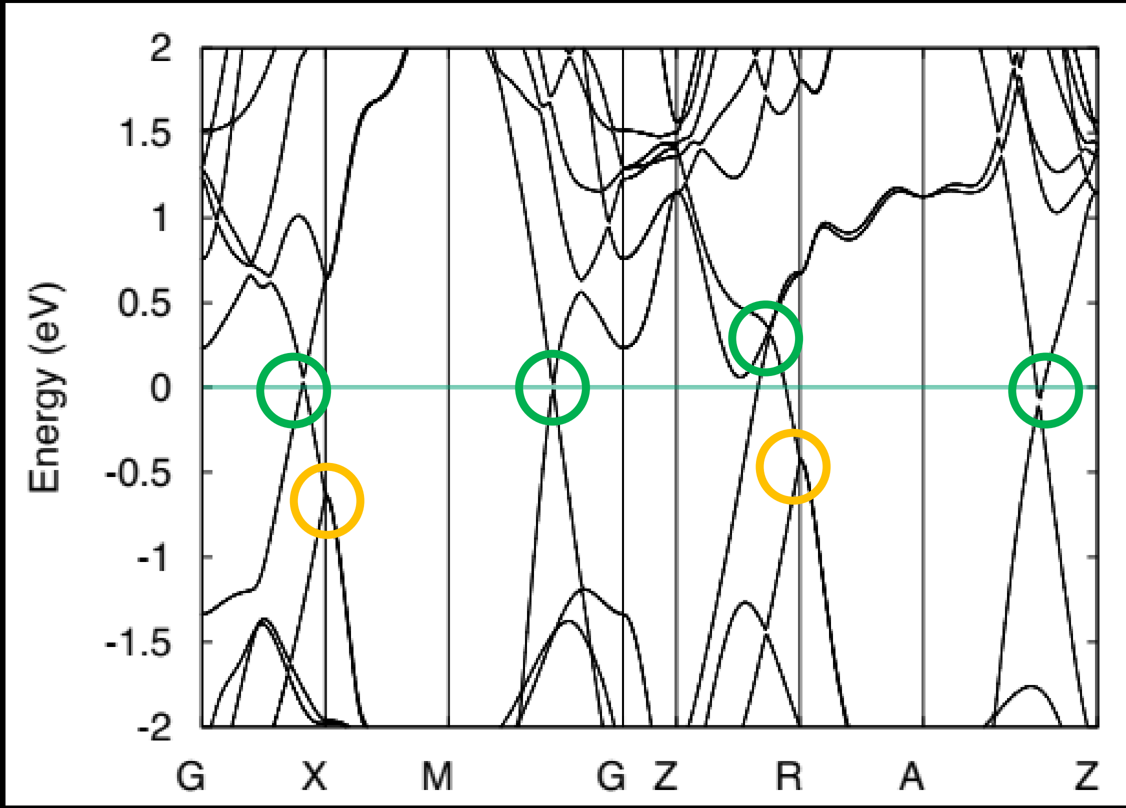

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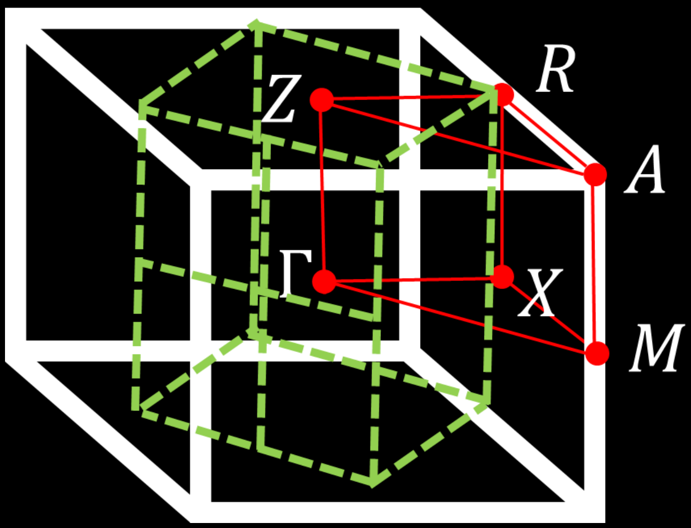
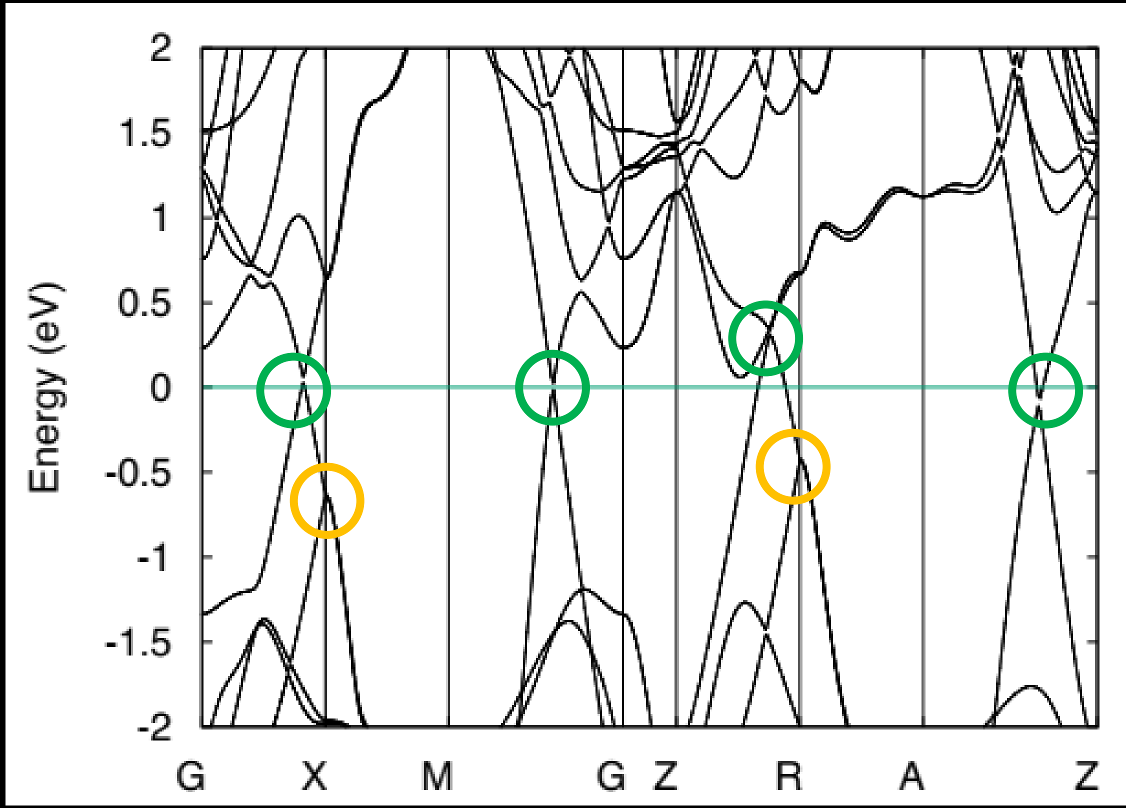


Nodal-line Dirac system under study:

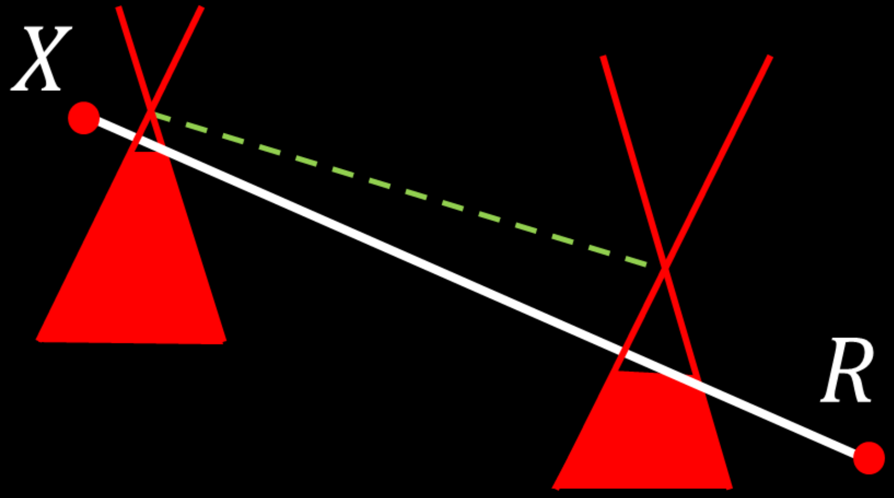
ZrSiS

- Modern DFT calculations



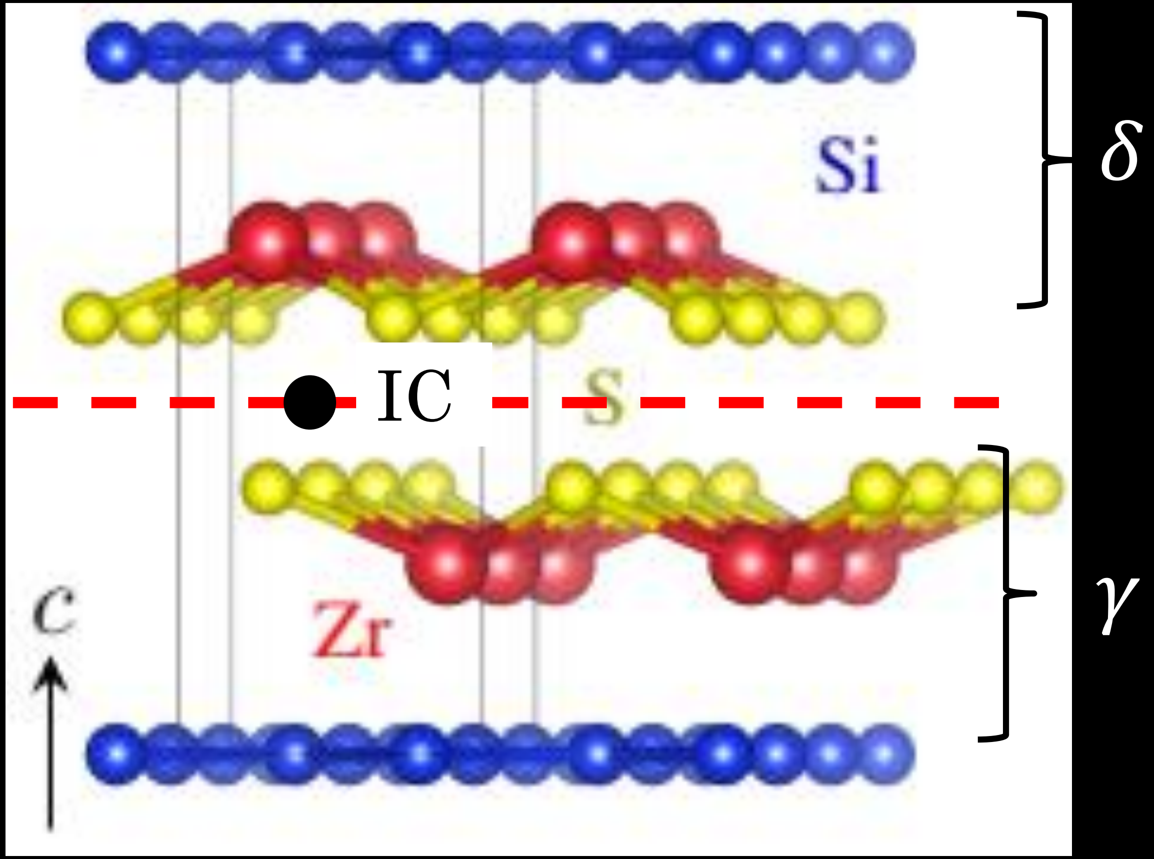
Nonsymmorphic symmetry protected nodal lines

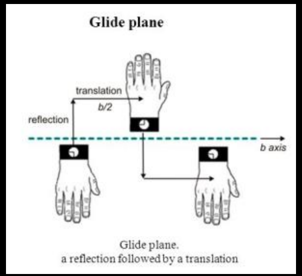
C4 protected nodal lines
SOC opens a gap



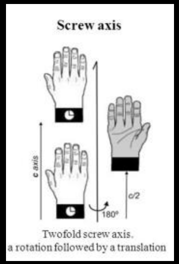
Why is ZrSiS interesting?

- Tetragonal crystal structure
- Nonsymmorphic symmetry
- Van der Waals gap





Glide plane



Screw axis

- P4/nmm SG

nature physics | ARTICLES

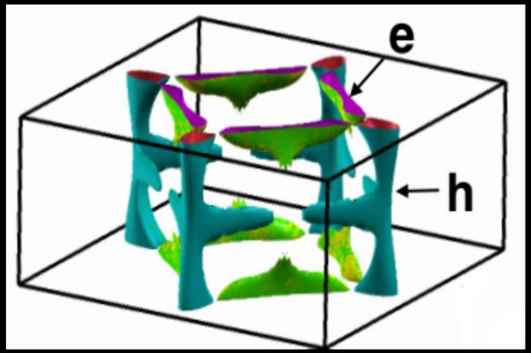
PUBLISHED ONLINE: 13 APRIL 2014 | DOI: 10.1038/NPHYS2933

Hidden spin polarization in inversion-symmetric bulk crystals

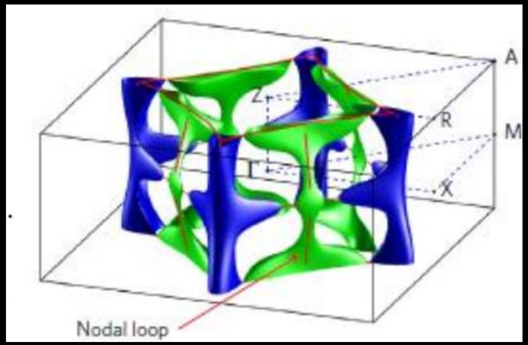
Xiuwen Zhang[1,2,3†], Qihang Liu[1,4†], Jun-Wei Luo[3*], Arthur J. Freeman[4] and Alex Zunger[1*]

How does Fermi surface look like?

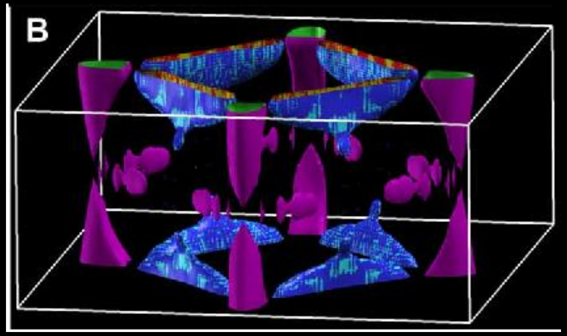
- Exact Fermi surface very sensitive to position of the parameters of DFT modeling

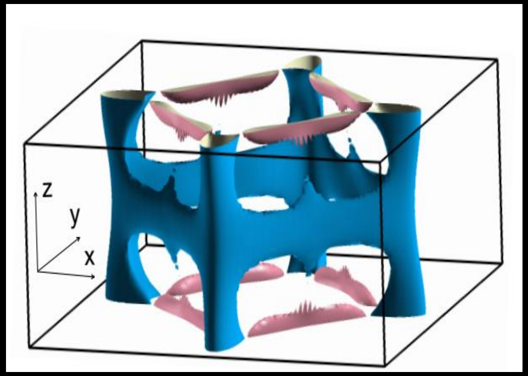


Our calculations



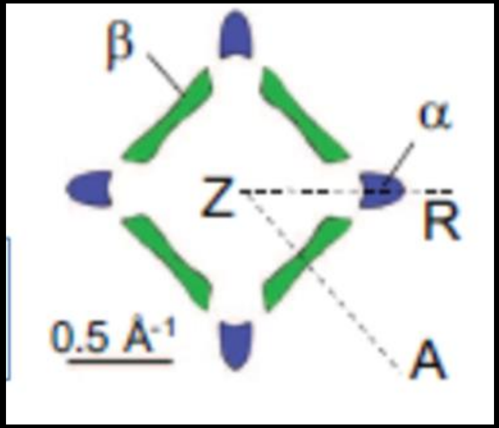
Nature Physics 14, 178 (2018)





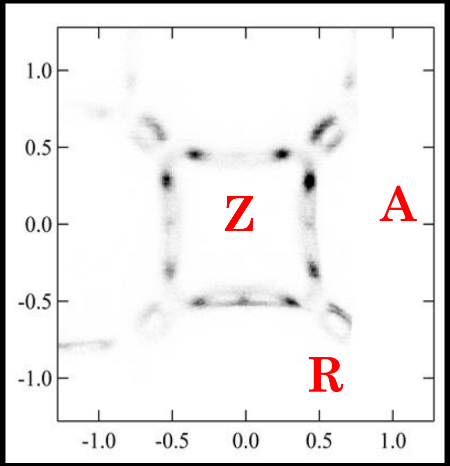
- Magnetoresitance is very sensitive to FS shape and topology

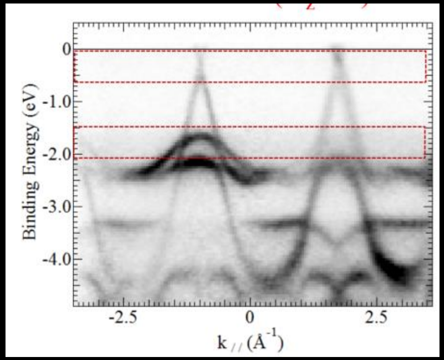
Top view of the FS



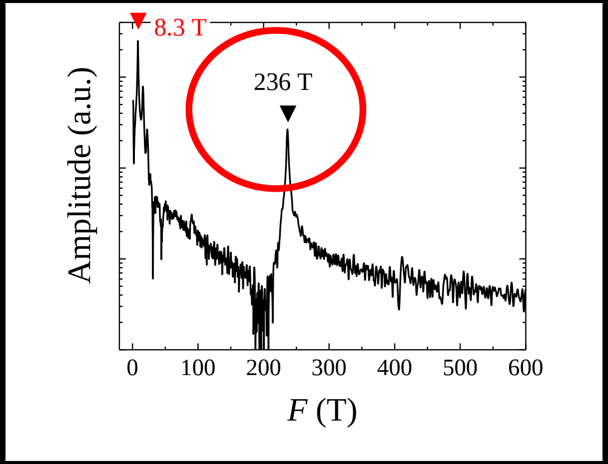
Quantum oscillations and AREPS

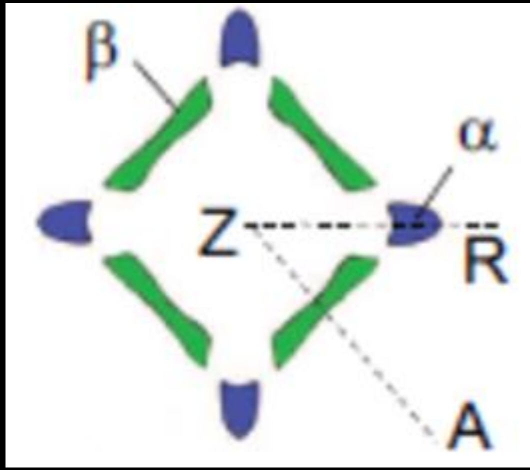
- ARPES measurements
- $k_z = \frac{\pi}{c}$





- Quantum oscillations (SdH, dHvA)
  -at moderate magnetic fields-





- 8.3 T pocket has also linear dispersion
- Early work indicated 236 T is q-2D pocket

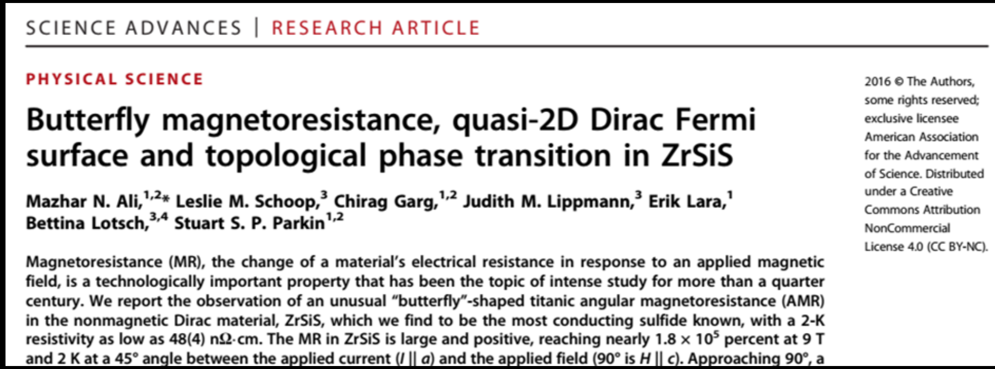
- All pocket at the FS have linear dispersion

Angular magnetoresistance measurements

- Magnetoresistance measurement are very sensitive to Fermi surface shape

$$v_k = \nabla_k E_k$$

- It has been known that in plane magnetoresistance exabits unusual behavior


SCIENCE ADVANCES | RESEARCH ARTICLE

PHYSICAL SCIENCE

Butterfly magnetoresistance, quasi-2D Dirac Fermi surface and topological phase transition in ZrSiS

Mazhar N. Ali,[1,2]* Leslie M. Schoop,[3] Chirag Garg,[1,2] Judith M. Lippmann,[3] Erik Lara,[1] Bettina Lotsch,[3,4] Stuart S. P. Parkin[1,2]

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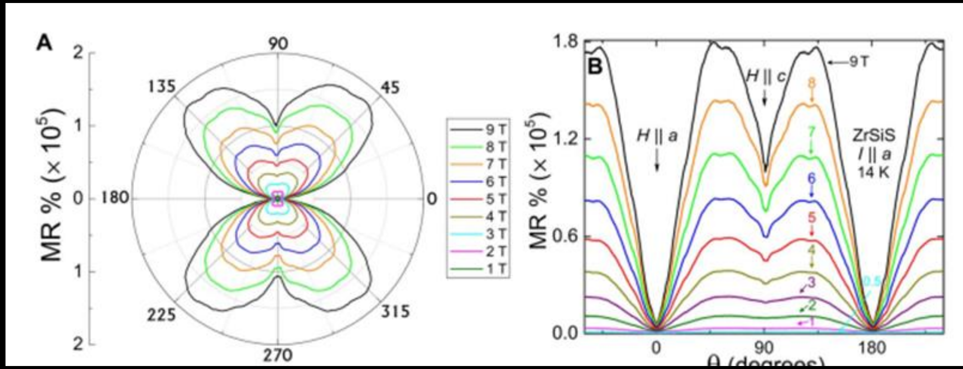
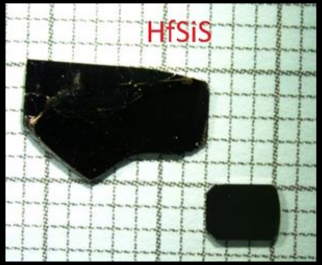
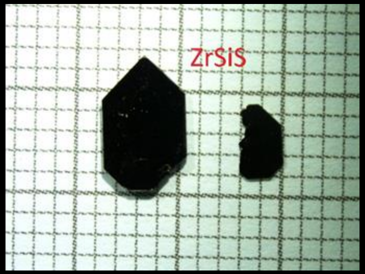
Magnetoresistance (MR), the change of a material's electrical resistance in response to an applied magnetic field, is a technologically important property that has been the topic of intense study for more than a quarter century. We report the observation of an unusual "butterfly"-shaped titanic angular magnetoresistance (AMR) in the nonmagnetic Dirac material, ZrSiS, which we find to be the most conducting sulfide known, with a 2-K resistivity as low as 48(4) nΩ·cm. The MR in ZrSiS is large and positive, reaching nearly 1.8 × 10[5] percent at 9 T and 2 K at a 45° angle between the applied current (I || a) and the applied field (90° is H || c). Approaching 90°, a



- We manage to synthesized crystals of bigger lateral size and thickness

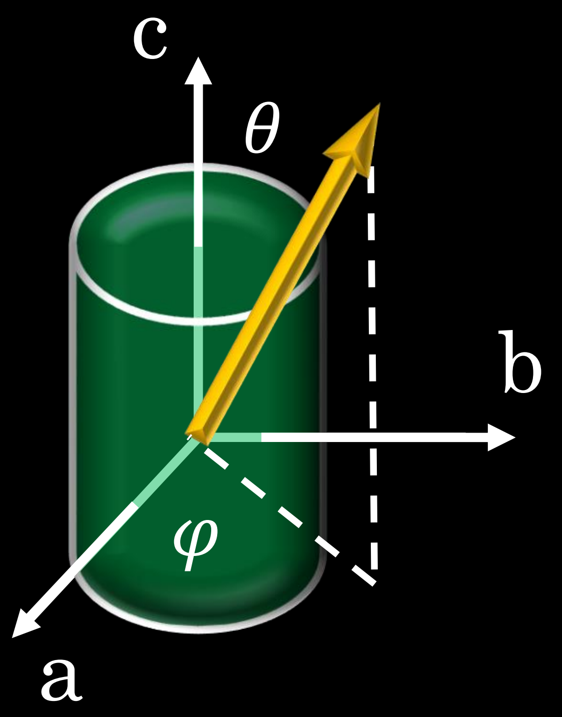


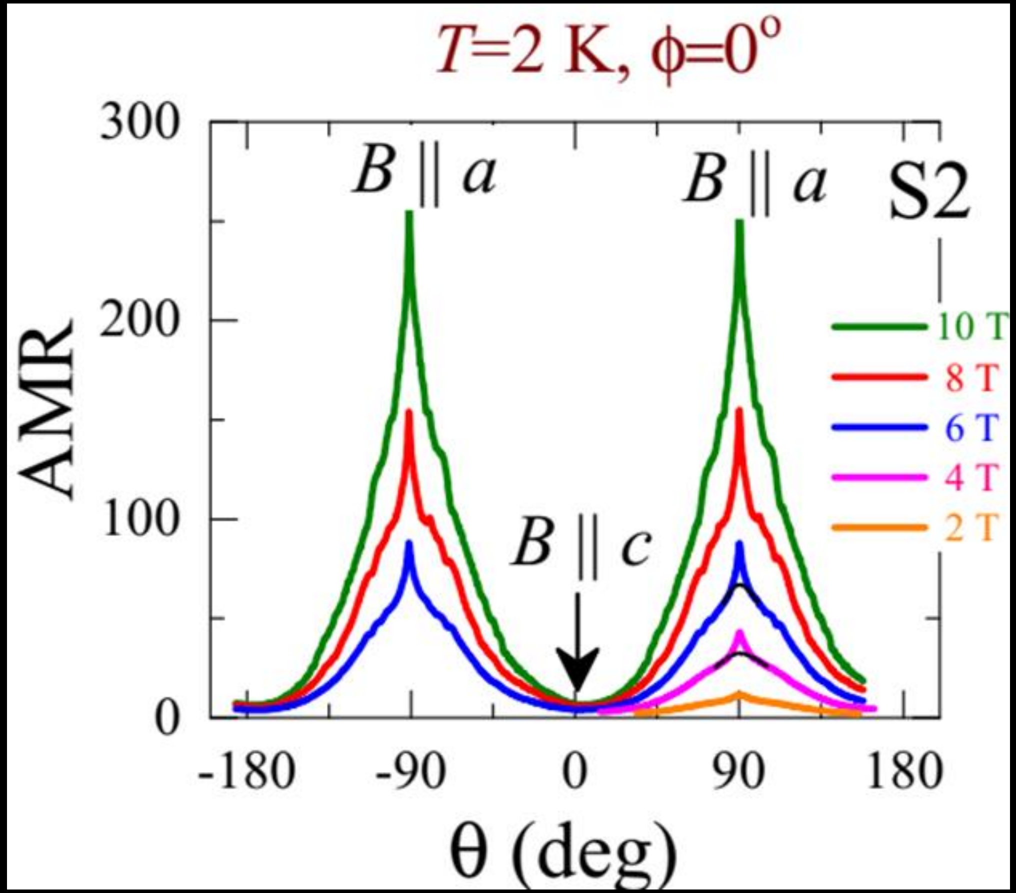


- Good for c-axis transport measurements
- Good for optical measurements

Angular magnetoresistance measurements

- Angular magnetoresistance in out-of-plane direction (detail mapping)





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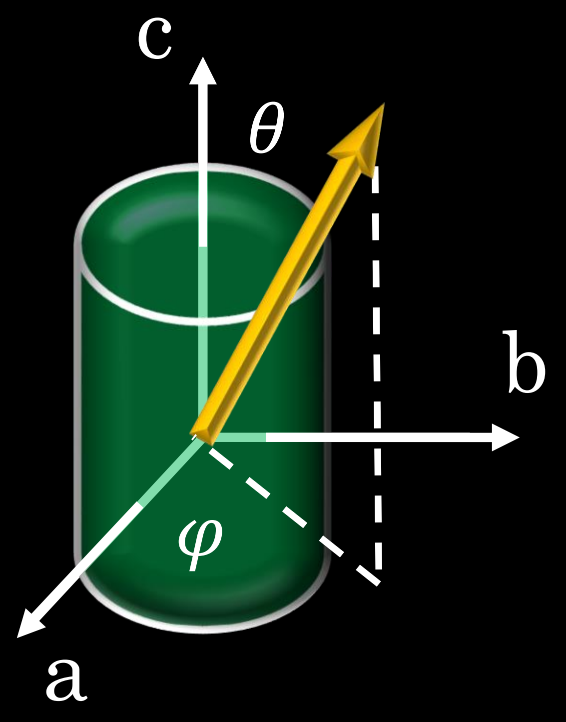

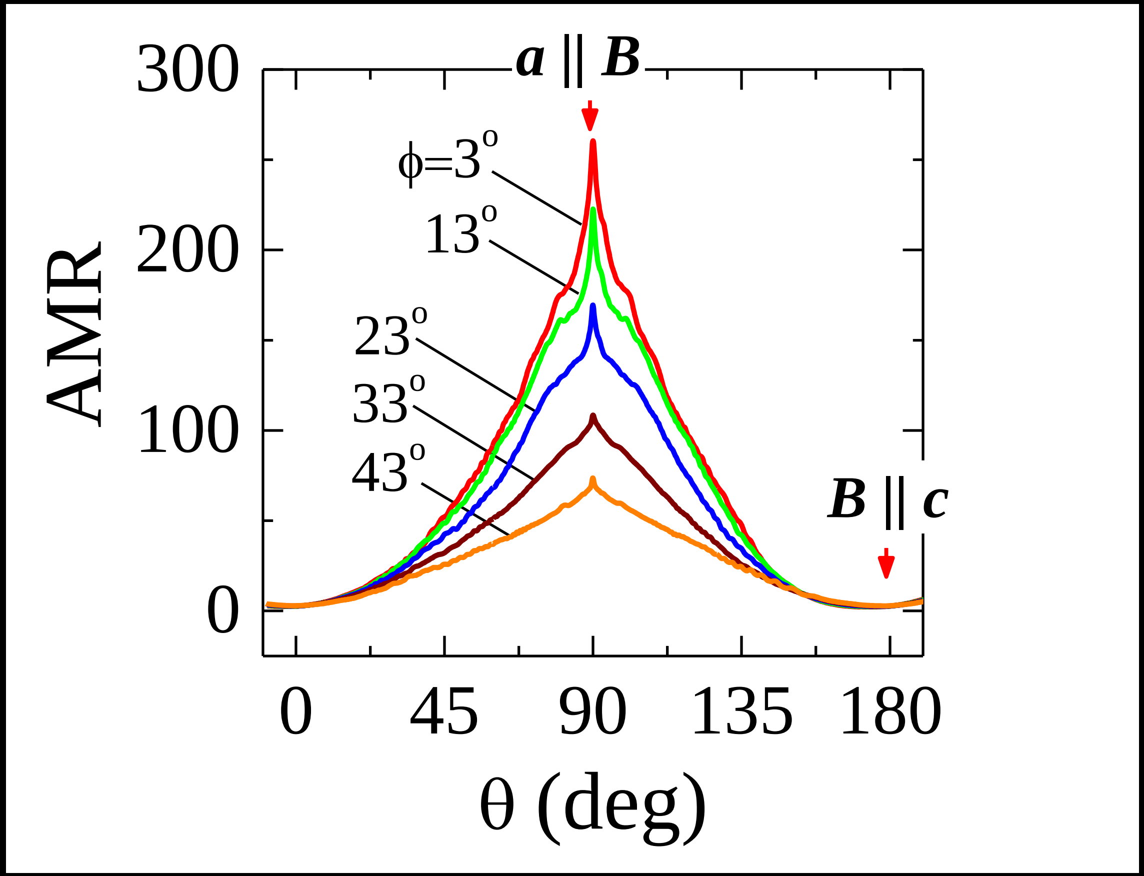

Angular magnetoresistance measurements

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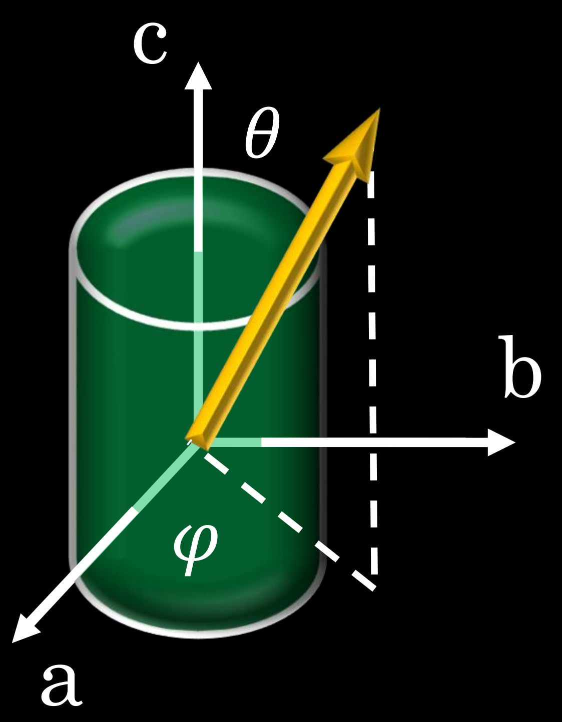
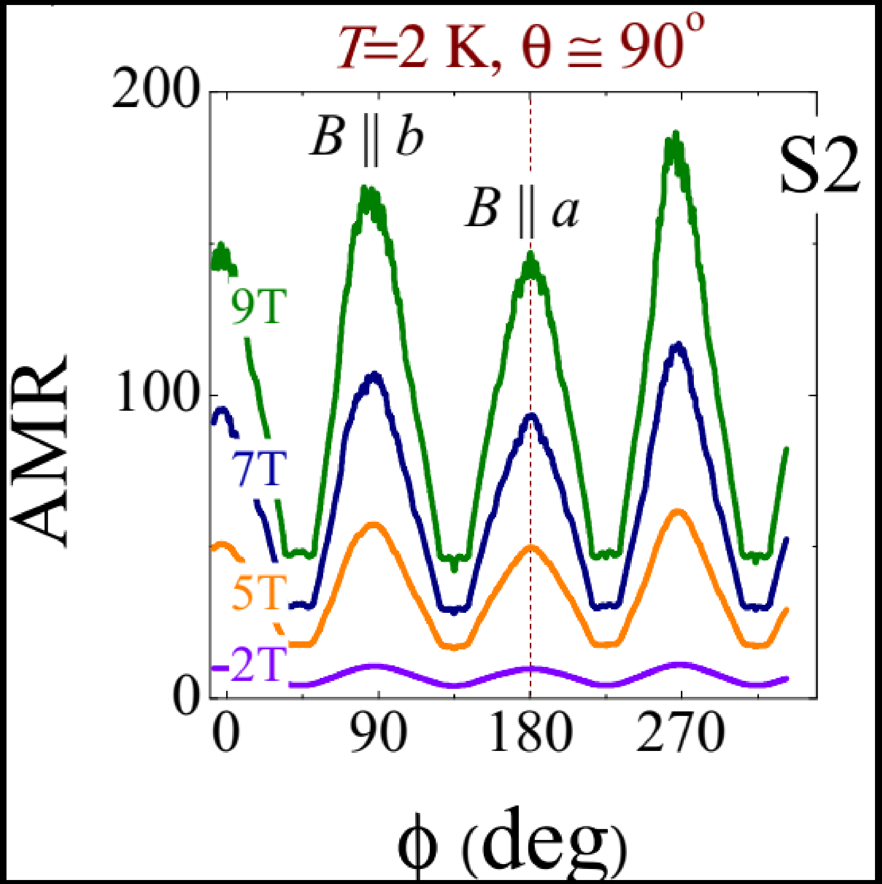




Angular magnetoresistance measurements

- Structurally similar compounds

nature COMMUNICATIONS

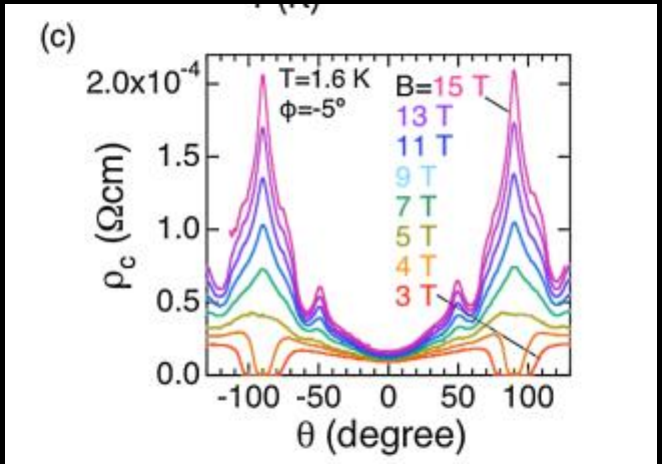
ARTICLE

DOI: 10.1038/s41467-017-00673-7 OPEN

Unusual interlayer quantum transport behavior caused by the zeroth Landau level in $YbMnBi_2$

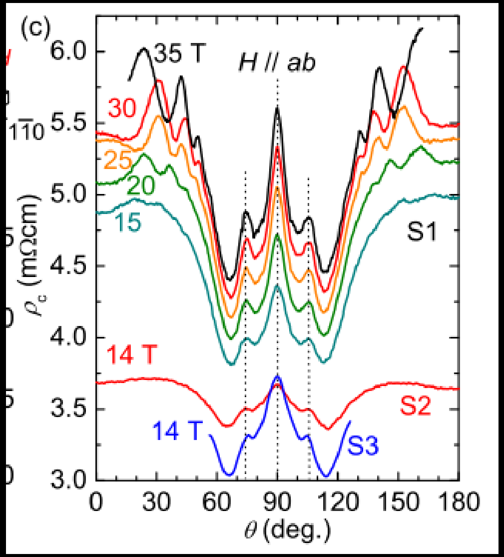
J.Y. Liu[1], J. Hu[1], D. Graf[2], T. Zou[3], M. Zhu[3], Y. Shi[4], S. Che[5], S.M.A. Radmanesh[6], C.N. Lau[5], L. Spinu[6], H.B. Cao[7], X. Ke[3] & Z.Q. Mao[1]

KFe2As2

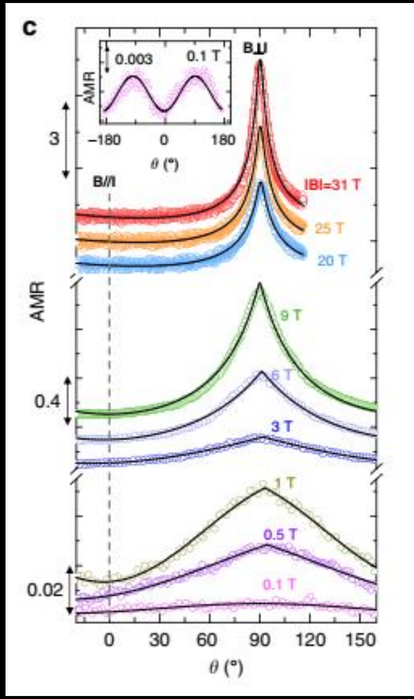


PRL **105**, 246403 (2010)

SrMnBi2



PRL **113**, 156602 (2014)



YbMnBi2

Isostructural to ZrSiS

How can we understand present AMR?

Calculations done by Shengnan Zhang at EPFL

- Approach:

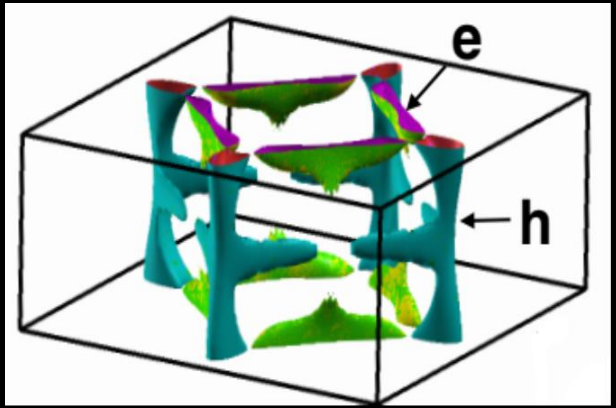
DFT (ab initio) Quantum model → Fermi surface shape → Boltzmann transport equation Semiclassical model

$$\rightarrow \sigma_{ij}^{(n)} = e^2 \int \frac{d\boldsymbol{k}}{4\pi} \tau^{(n)} v_i^{(n)}(\boldsymbol{k}) \overline{v_j^{(n)}}(\boldsymbol{k}) \left(-\frac{\partial f}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon(\boldsymbol{k})}$$

$$\downarrow$$

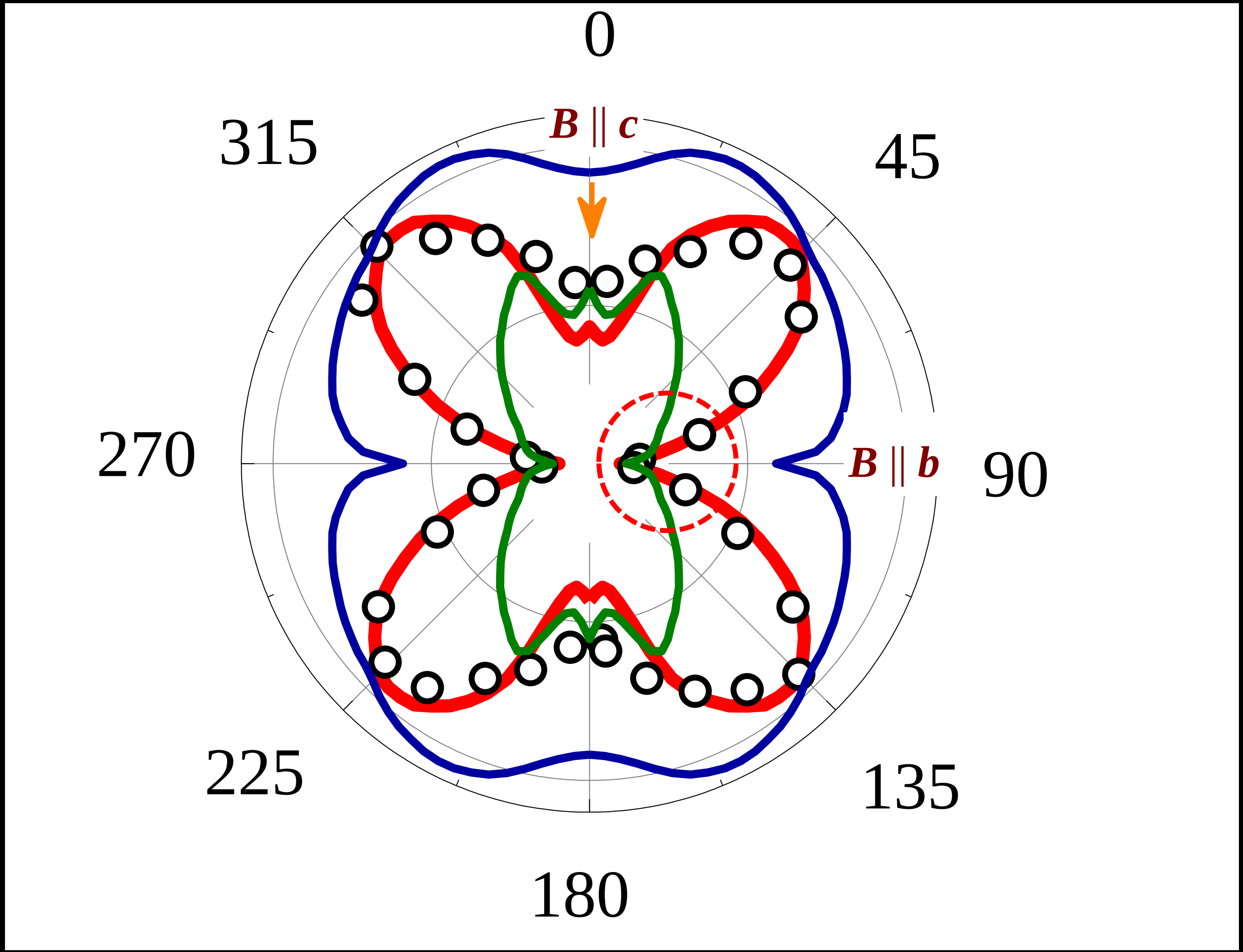
$$\sum [\sigma_{ij}] \Rightarrow [\rho_{ij}]$$

4+4 independent elements



- Model which worked excellently for the Q-2D organics

Origin of the butterfly AMR



ρ_{xx}

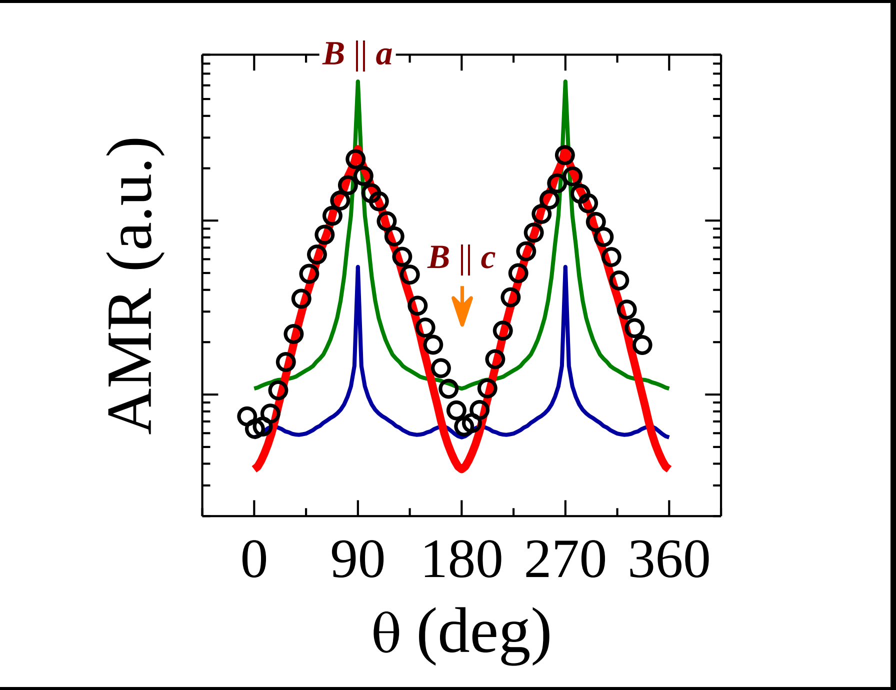
Electrons
Holes
Total

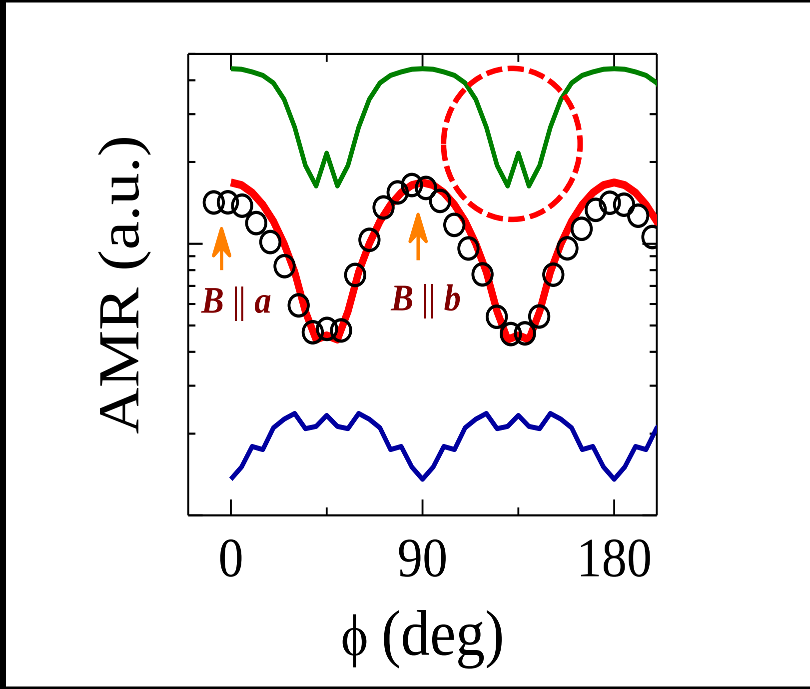
- Off-diagonal matrix elements are not small

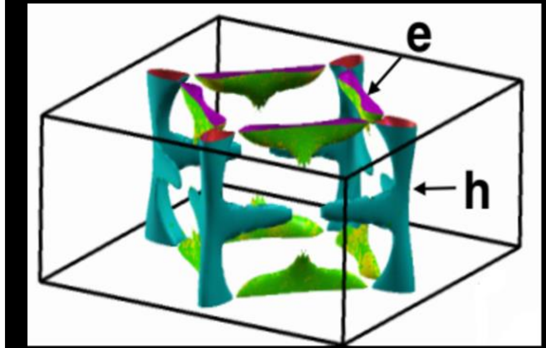
$$\frac{1}{\rho_{tot}} \neq \frac{1}{\rho_{ele}} + \frac{1}{\rho_{hole}}$$

Origin of the polar and azimuthal anisotropy of AMR

- Hole pocket dominates AMR
- Open and closed orbits







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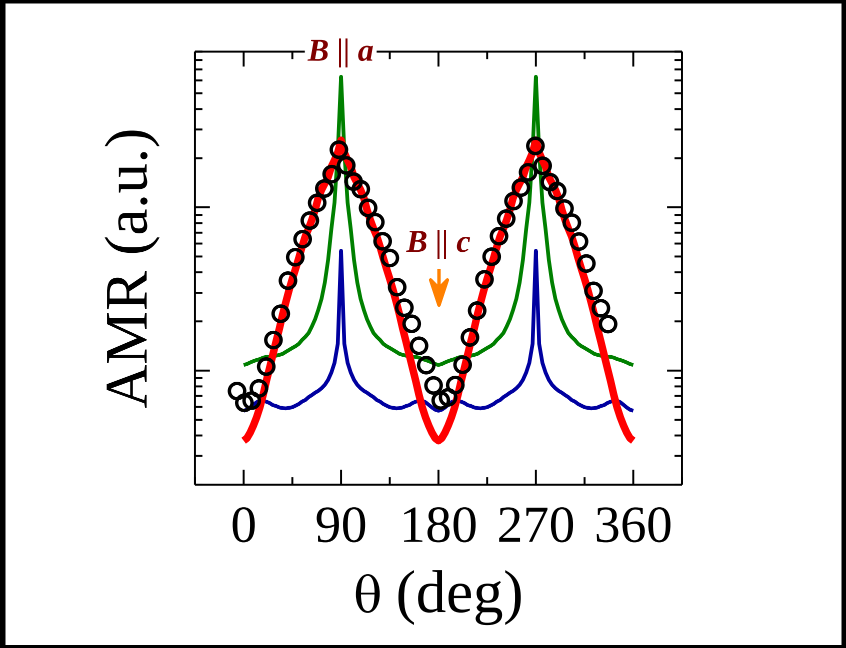
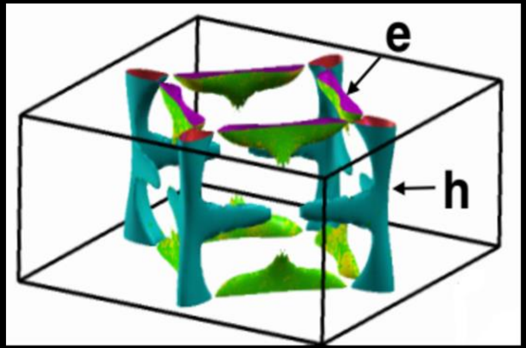
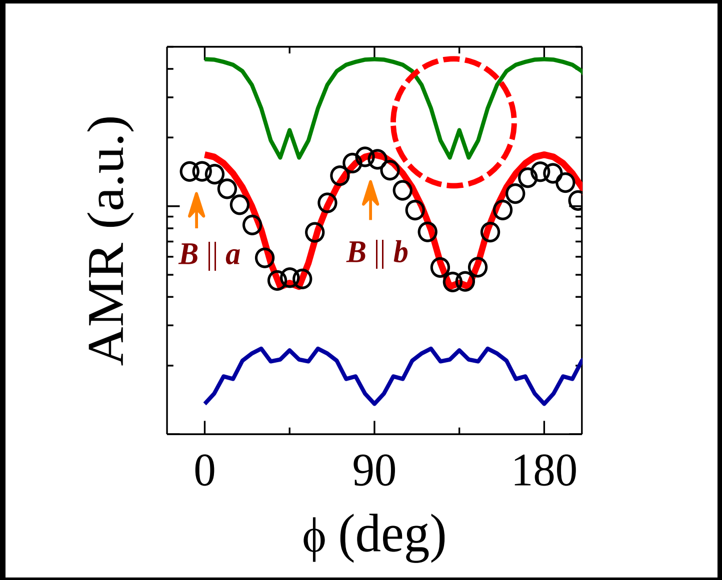
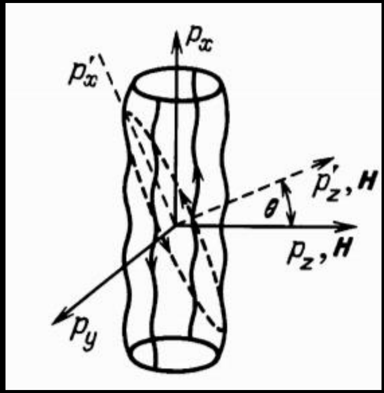




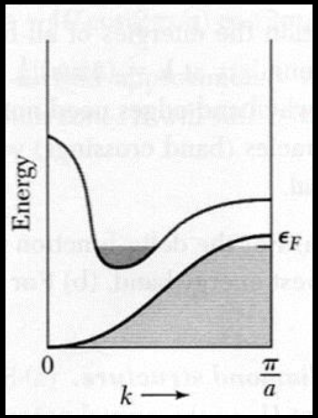


- Origin of unusual AMR

Open orbits

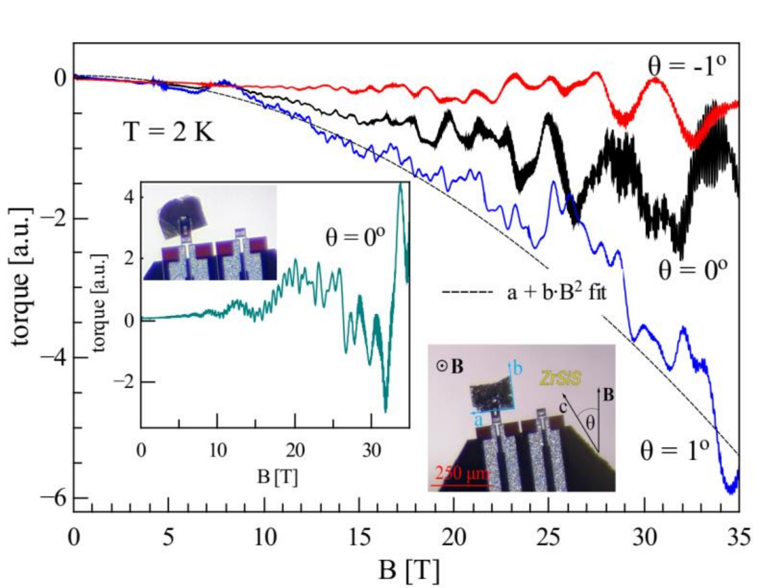


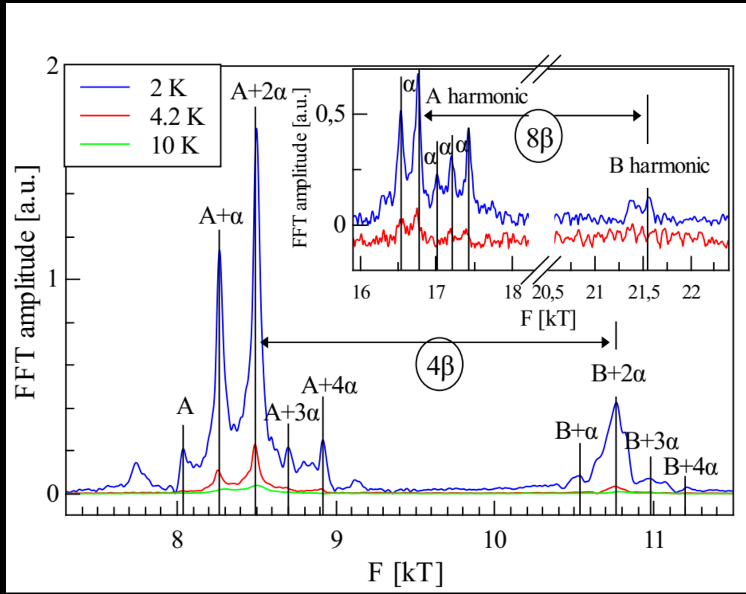
Effect of compensation

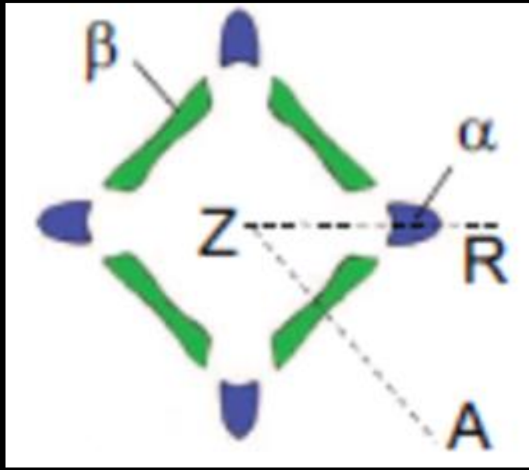


High magnetic field measurements

- Magnetic field up to 35T
- Magnetic torque measurements







- Magnetic breakdown usually occurs between SO-split bands

- S. Pezzini et al., Nat. Phys. **14**, 178 (2018).
(Nijmegen group)

Unconventional mass enhancement around the Dirac nodal loop in ZrSiS

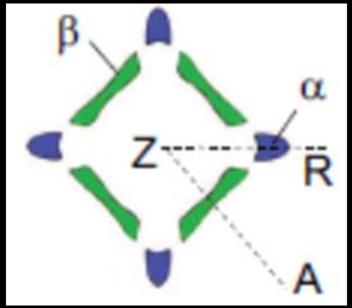
S. Pezzini, M. R. van Delft, L. M. Schoop, B. V. Lotsch, A. Carrington, M. I. Katsnelson, N. E. Hussey & S. Wiedmann

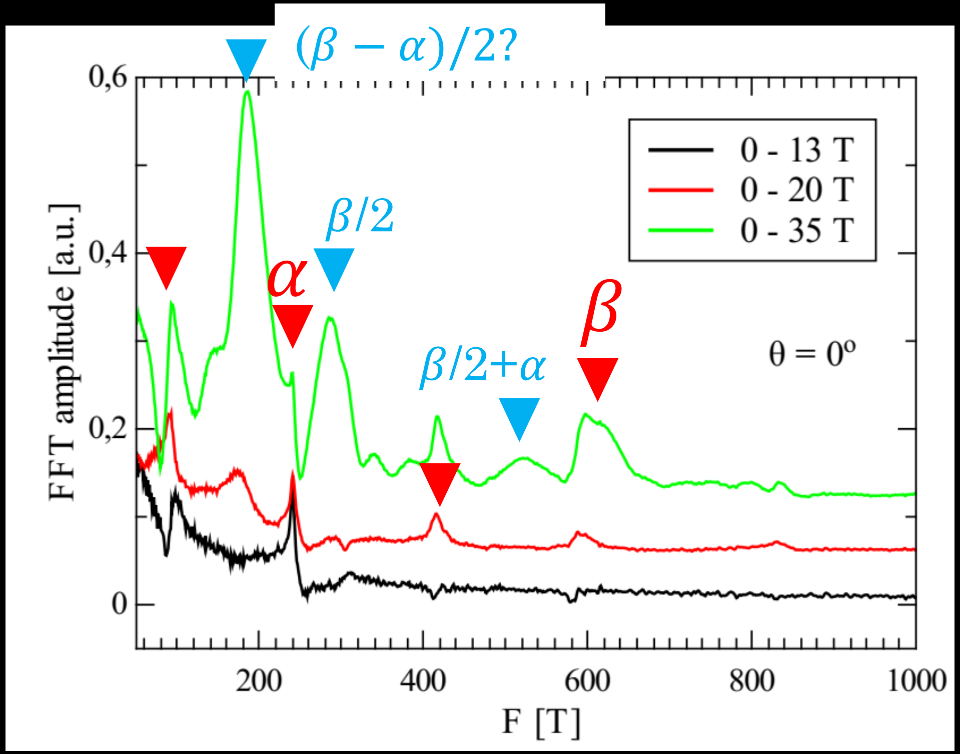
Nature Physics **14**, 178–183 (2018) | Download Citation

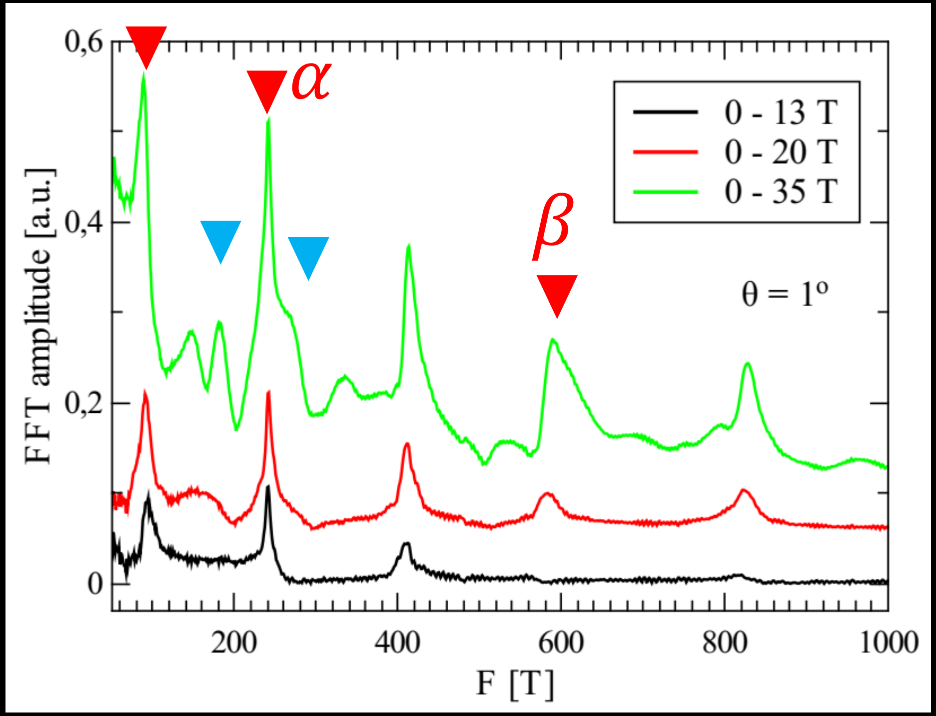
High magnetic field measurements

- Magnetic field up to 35T
- Magnetic torque measurements

- Low-*F* oscillation spectrum







Summary:

- Magnetotransport properties as moderate $\boldsymbol{B}$ can be described by the semiclassical theory
- Fermi surface shape is pinpointed

- Deviation for the semiclassical theory in high magnetic fields?

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Thank you for your attention!