Topology – from the materials perspective

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Co-workers in Dresden and elsewhere

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Yulin Chen et al., Oxford; Günter Reiss, Bielfeld
S.C. Zhang et al. and A. Kapitulnik, Stanford
S. S. P. Parkin et al., IBM Almaden, MPI Halle
Topological Insulators
Topology

\[\text{Soccer ball} \cong \text{Bread rolls} \not\cong \text{Donuts} \cong \text{Coffee cup}\]
Molecules with different chiralities can have different physical and chemical properties.

Topologically interesting compounds are 4n aromatics with Möbius geometry, whereas normal 4n compounds are anti-aromatic.
Universe – particles – condensed matter

Theoretician – from model to materials predictions
Family of quantum Hall effects

- **Hall effect**
  - 1879

- **Anomalous Hall effect**
  - 1881

- **Spin Hall effect**
  - 2004

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**1985**
Klaus von Klitzing

**1998**
Horst Ludwig Störmer and Daniel Tsui

**2010**
Andre Geim and Konstantin Novoselov

**2016**
David Thouless, Duncan Haldane and Michael Kosterlitz

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*Science 340 (2013) 153*
Trivial and topological insulators

Trivial semiconductor
CdS

Topological Insulator
Without spin orbit coupling

Topological Insulator
With spin orbit coupling

[Diagram showing the transition from a trivial semiconductor to topological insulators with and without spin orbit coupling]
Topological insulator

**Z₂ 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*

(Received 22 June 2005; published 28 September 2005)

The quantum spin Hall (QSH) phase is a time reversal invariant electronic band gap that supports the transport of charge and spin in gapless edge states. It associated with a novel $Z₂$ topological invariant, which distinguishes it from an $O$ classification, which is defined for time reversal invariant Hamiltonians, is analogous classification of the quantum Hall effect. We establish the $Z₂$ order of the QSH model of graphene and propose a generalization of the formalism applicable to other systems.

Kane and Mele, PRL 95, 146802 (2005)


First success

Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells
B. Andrei Bernevig, et al.
Science 314, 1757 (2006):
DOI: 10.1126/science.1133734

3D: Dirac cone on the surface
2D: Dirac cone in quantum well
3D Topological Insulators

Bi-Sb alloys

$\text{Bi}_2\text{Se}_3$ and relatives

Moore and Balents, PRB 75, 121306(R) (2007)
Fu and Kane, PRB 76, 045302 (2007)
### Table 1. Proposed topological insulator materials grouped into several different material classes.\(^{4,12,13,19,23-29}\)

<table>
<thead>
<tr>
<th>HgTe-type</th>
<th>Bi(_2)Se(_3)-type</th>
<th>Honey Comb Lattice</th>
<th>Bismuth-Alloys</th>
<th>NaCl Structure</th>
<th>Oxides</th>
<th>Correlated Materials</th>
<th>Superconductors</th>
</tr>
</thead>
<tbody>
<tr>
<td>HgTe</td>
<td>Bi(_2)Se(_3), Bi(_2)Te(_3), and Sb(_2)Te(_3)</td>
<td>Graphene</td>
<td>Bi-Sb</td>
<td>SnTe PbTe</td>
<td>Doped BaBiO(_3)</td>
<td>Iridates</td>
<td>Cu(_4)Bi(_5)Se(_3)</td>
</tr>
<tr>
<td>Half-Heuslers such as LaPtBi</td>
<td>Bi(_2)Te(_2)Se</td>
<td>LiAuTe</td>
<td>PuTe AmN</td>
<td>Iridates</td>
<td>SmB(_6)</td>
<td>LaPtBi YPtBi LuPtBi</td>
<td></td>
</tr>
<tr>
<td>α-Sn, HgS, β-HgS</td>
<td>(Bi(_{1-x})Sb(_x))(_2)Te(_3)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chalco-pyrites</td>
<td>TiBiSe(_2) and TiBiTe(_2)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Skutterudites</td>
<td></td>
</tr>
<tr>
<td>AlSb/InAs/GaSb</td>
<td>Bi(_{1-x})Rh(_x)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>PuTe, AmN</td>
<td></td>
</tr>
</tbody>
</table>


\[ \text{Tl}^{+1} \text{ Sn}^{2+} \text{ Bi}^{+3} \]

**Inert pair effect**
Rewriting the text book: Au

On the Surface States Associated with a Periodic Potential

WILLIAM SHOCKLEY
Bell Telephone Laboratories, New York, New York
(Received June 19, 1939)

Binghai Yan at al., Nature Communication 6 (2015) 10167
Rewriting the text book: Au

Cs⁺Au⁻

Binghai Yan at al., Nature Communication 6 (2015) 10167
Heusler compounds

Diamond ZnS Heusler $XYZ \ C_{1b}$ $X_{2}YZ \ L2_{1}$

Graf T, Felser C, Parkin SSP, IEEE TRANSACTIONS ON MAGNETICS 47 (2011) 367
Predicting new compounds

S. Chadow et al., Nat. Mater. 9, 541 (2010).
H. Lin et al., Nat. Mater. 9, 546 (2010).
Predicting new compounds

S. Chadow et al., Nat. Mater. 9, 541 (2010).
H. Lin et al., Nat. Mater. 9, 546 (2010).
Electronic structure

Electronic structure

S. Chadow et al., Nat. Mater. 9, 541 (2010).
H. Lin et al., Nat. Mater. 9, 546 (2010).
ARPES of LnPtBi

The nontrivial Josephson coupling leads to a current-flux relation with a half period in a superconducting quantum interference device geometry.

Topological RPdBi half-Heusler semimetals
A new family of noncentrosymmetric magnetic superconductors

Yasuyuki Nakajima,1 Rongwei Hu,1 Kevin Kirshenbaum,1 Alex Hughes,1 Paul Syers,1
Xiangfeng Wang,1 Kefeng Wang,1 Remxiong Wang,1 Shanta R. Saha,4 Daniel Pratt,3
Jeffrey W. Lynn,2 Johnpierre Paglione1*

Fig. 5. Phase diagram of RPdBi series, indicating evolution of superconducting and antiferromagnetic ground states as a function of de Gennes factor $dG = (g_J - 1)^2(J + 1)$. The superconducting transition $T_c$ increases with $dG$. The inset shows the evolution of the magnetic transition $T_m$.

FIG. 4. Time-reversal symmetry-breaking quintet pairing states: (a) the $E$ pairing state; (b) the $T_2$ pairing state with $I = (1, i, 0)$; (c) the $T_3$ pairing state with $I = (1, -e^{2\pi i/3}, e^{4\pi i/3})$. The color indicates the phase while the saturation gives the gap magnitude. Black points or lines indicate nodes of the gap.
Structure to Property

HgTe

\[ \alpha \text{Ag}_2\text{Te} \]

\[ \text{LaPtBi} \]

\[ \beta \text{Ag}_2\text{Te} \]

\[ \text{Li}_2\text{AgSb} \]

\[ \text{AuTlS}_2 \]

\[ \text{KHgSb} \]
Honeycomb from sp3 to sp2

Band inversion is found in the heavier compounds
No surface state? Why?
Interaction between the two layers in the unit cell and two Dirac Cones

Honeycomb from sp3 to sp2

Honeycomb: Weak T1

Hourglass fermions

Zhijun Wang\textsuperscript{1x}, A. Alexandradinata\textsuperscript{1,2y}, R. J. Cava\textsuperscript{3} & B. Andrei Bernevig\textsuperscript{4}

Weyl Semimetals
Breaking symmetry - TaAs
Dirac and Weyl semimetals

Paul Klee
**Dirac semimetals**

**Normal Insulator**

**Critical**

**Strong TI**

Bohm-Jung Yang and Naoto Nagaosa, arXiv:1404.0754

**Observation of a three-dimensional topological Dirac semimetal phase in high-mobility Cd$_3$As$_2$**

**Observation of Fermi arc surface states in a topological metal**

Su-Yang Xu et al.

*Science 347*, 294 (2015); DOI: 10.1126/science.1256742
Weyl semimetals

Band inversion

SOC

TI

WSM

DSM

Weyl points

Dirac point
**Weyl semimetals in non centro NbP**

**NbP, NbAs, TaP, TaAs**

- NbP is a topological Weyl semimetal
  - with massless relativistic electrons
  - extremely large magnetoresistance of 850,000% at 1.85 K, 9T (250% at room temperature)
  - an ultrahigh carrier mobility of \(5 \times 10^6\) cm\(^2\)/Vs

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NbP, TaP, TaAs

Z. K. Liu et al., Nature Mat. 15 (2016) 27
MoS$_2$ : crystal field

Mo$^{4+}$ (d$^2$)
S$^{2-}$ (s$^2$p$^6$)

2 H  1T  1T', Td

Semiconductor  Metal  Semimetal

d_{xz}, d_{yz}  d_{x^2-y^2}  d_{z^2}, d_{x^2-y^2}

d_{xy}, d_{x^2-y^2}  d_{x^2-y^2}  d_{x^2-y^2}

Semiconductor  Metal  Semimetal
Td-MoTe$_2$

MoTe$_2$: Weyl Semimetal?

MoTe$_2$

![Graph showing the properties of MoTe$_2$ under pressure and temperature, with distinct regions labeled for structure transition and superconductivity.]

Magnetic Weyl Semimetals

Induced

Intrinsic
**Multifunctional properties**

- **RE: Gd Magnetism and TI**
  - Antiferromagnetism with GdPtBi
- **RE: Ce**
  - complex behaviour of the Fermi surface
- **RE: Yb Kondo insulator and TI**
  - YbPtBi is a super heavy fermion with the highest $\gamma$ value

$10 + 3 (f^n) + 5 = 18$

S. Chadov et al., Nat. Mater. 9, 541 (2010).
H. Lin et al., Nat. Mater. 9, 546 (2010).
Weyl semimetals

We need time reversal symmetry breaking (Dirac points are at high symmetry points Weyl points are not at high symmetry points)
- Structural distortion
- Application of magnetic field or magnetism

3D topological Weyl semimetals - breaking Time reversal symmetry – by transport

1. Intrinsic anomalous Hall effect

2. Chiral anomaly

\[ \partial_{\mu} j^{\mu}_{\chi} = \chi \frac{e^3}{4\pi^2 \hbar^2} \mathbf{E} \cdot \mathbf{B} \]

\[ \sigma_a = \frac{e^3 v_f^3}{4\pi^2 \hbar \mu c} B^2 \]

S. L. Adler, Phys. Rev. 177, 2426 (1969)
AA Burkov, L Balents, PRL 107 12720 (2012)
GdPtBi is magnetic

GdPtBi is an Antiferromagnet below 10 K. However, it is very soft and the spins can be tuned in a magnetic field.

Weyl GdPtBi in a magnetic field


In ferromagnets an AHE scales with the magnetic moment.
Antiferromagnet show no AHE.
A Hall angle of 0.2 is exceptional – 1 would be the Quantum AHE.

T. Suzuki, ... & J. G. Checkelsky, Nature Physics (2016) doi:10.1038/nphys3831
Chiral Anomaly – neg. quadratic MR

Magnetic Heusler compounds with and without inversion

[Diagram of magnetic Heusler compounds]

[Diagram of magnetic Heusler compounds with inversion]

[Diagram of magnetic Heusler compounds without inversion]
Magnetic Heusler compounds with and without inversion

26 Valence electrons

Zhijun Wang, et al., arXiv:1603.00479
Guoqing Chang et al., arXiv:1603.01255

Barth et al. PRB 81, 064404 2010
Berry curvature and the anomalous Hall effect in Heusler compounds

Jürgen Kübler\textsuperscript{1,*} and Claudia Felser\textsuperscript{2}

<table>
<thead>
<tr>
<th>Compound\textsuperscript{a}</th>
<th>$N_y$</th>
<th>$a$ (nm)</th>
<th>$M^{\text{exp}}$</th>
<th>$M^{\text{calc}}$</th>
<th>$\sigma_{xy}$</th>
<th>$P$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co$_2$VGa</td>
<td>26</td>
<td>0.5779</td>
<td>1.92</td>
<td>1.953</td>
<td>66</td>
<td>65</td>
</tr>
<tr>
<td>Co$_2$CrAl</td>
<td>27</td>
<td>0.5727</td>
<td>1.7</td>
<td>2.998</td>
<td>438</td>
<td>100</td>
</tr>
<tr>
<td>Co$_2$VSn</td>
<td>27</td>
<td>0.5960</td>
<td>1.21</td>
<td>1.778</td>
<td>$-1489$</td>
<td>35</td>
</tr>
<tr>
<td>Co$_2$MnSn</td>
<td>78</td>
<td>0.5749</td>
<td>4.04</td>
<td>4.045</td>
<td>1800</td>
<td>75</td>
</tr>
<tr>
<td>Rh$_2$MnAl</td>
<td>28</td>
<td>0.6022</td>
<td>4.066</td>
<td>1500</td>
<td>94</td>
<td></td>
</tr>
<tr>
<td>Mn$_2$PtSn\textsuperscript{b}</td>
<td>28</td>
<td>0.4509 (1.3477)</td>
<td>6.66</td>
<td>1108</td>
<td>91</td>
<td></td>
</tr>
<tr>
<td>Co$_2$MnSi</td>
<td>29</td>
<td>0.5984</td>
<td>5.08</td>
<td>5.00</td>
<td>118</td>
<td>82</td>
</tr>
<tr>
<td>Co$_2$MnSi</td>
<td>29</td>
<td>0.5645</td>
<td>4.90</td>
<td>4.98</td>
<td>228</td>
<td>100</td>
</tr>
</tbody>
</table>

\textsuperscript{a} \text{See Ref. 2.}  \textsuperscript{b} \text{See Ref. 3.}

FIG. 4. (Color online) Band structure near the Fermi edge of Co$_2$VSn. Majority-spin electron states appear in red, minority-spin states in black. Note the Dirac cone at the $\Gamma$ point at about $-0.22$ eV.

Kübler, Felser, PRB 85 (2012) 012405
Kübler, Felser, Europhys. Lett. 114 (2016) 47005
AHE in half metallic ferromagnets

Giant AHE in Co$_2$MnAl

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

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

Weyl points are the origin for a large Berry phase and a Giant AHE.

Kübler, Felser, PRB 85 (2012) 012405
**ITRI’s MRAM Roadmap**

**2007-2014**
- STT MRAM

**2015 -**
- SHE MRAM

**Embedded-Memory for IoT**
- ultra-low voltage (<0.3V)
- high endurance (>1E16)
Structural distortion of Heusler

\[ l4/mmm \ (D_{0_{22}}) \quad Fm\bar{3}m \ (L_2_1) \quad P6_3/mmc \ (D_{0_{19}}) \]

tetragonal \quad \text{cubic} \quad \text{hexagonal}
Non-collinear antiferromagnets and the anomalous Hall effect

J. Kübler and C. Felser

Anomalous Hall Effect Arising from Noncollinear Antiferromagnetism

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

Kübler and Felser EPL 108 (2014) 67001
Non-collinear AFM in metallic Mn$_3$Ge

The anomalous Hall conductivities are normally assumed to be proportional to magnetization.
Large anomalous Hall effect in a non-collinear antiferromagnet at room temperature

Kiyohara, Nakatsuji, preprint: arXiv:1511.04619,
Nakatsuji, Kiyohara, & Higo, Nature, doi:10.1038/nature15723
Fermiarcs in the Weyl AFM

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”
New Fermions

Fermions in condensed-matter systems are not constrained by Poincare symmetry. Instead, they must only respect the crystal symmetry of one of the 230 space groups. Hence, there is the potential to find and classify free fermionic excitations in solid-state systems that have no high-energy counterparts.

What comes next? Magnetic Space groups
Can we do something useful - Catalysis

- Dirac and Weyl semimetals
  - Linear bands – electron and holes with high mobilities
  - High mobility of electrons and holes – reduces the probability of recombination of electron hole pairs in redox reaction
- Topological connection between the two surfaces via Fermi arcs
Hydrogen evolution reaction
Weyl and catalysis

Graphs showing the evolution of H₂ with time for different catalysts and materials, including NbP, TaP, NbAs, and TaAs, with data points indicating the added time periods.
## Comparison with other catalysts

<table>
<thead>
<tr>
<th>Materials</th>
<th>Gibbs free energy ((\Delta G^*_\text{H} (\text{eV})))</th>
</tr>
</thead>
<tbody>
<tr>
<td>NbP</td>
<td>-0.31</td>
</tr>
<tr>
<td>TaP</td>
<td>-0.38</td>
</tr>
<tr>
<td>TaAs</td>
<td>-0.74</td>
</tr>
<tr>
<td>NbAs</td>
<td>-0.96</td>
</tr>
<tr>
<td>Pt</td>
<td>-0.1</td>
</tr>
<tr>
<td>Ni (111)</td>
<td>-0.27</td>
</tr>
<tr>
<td>2H-TaS(_2)</td>
<td>0.24</td>
</tr>
<tr>
<td>1T-TaS(_2)</td>
<td>0.82</td>
</tr>
<tr>
<td>Td-MoTe(_2)</td>
<td>0.84</td>
</tr>
<tr>
<td>2H-MoS(_2)</td>
<td>2.19</td>
</tr>
</tbody>
</table>

### Reactivity

- \(\Delta G^*_\text{H}\) vs. Reactivity
- Pt, NbP, TaP, TaAs, NbAs, TaS\(_2\) (2H), TaS\(_2\) (1T)

### Activity

<table>
<thead>
<tr>
<th>Catalysts</th>
<th>Activity ((\text{µmol g}^{-1}))</th>
<th>TOF (h(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>NbP powder</td>
<td>88.7</td>
<td>0.06</td>
</tr>
<tr>
<td>NbP crystal</td>
<td>8.4</td>
<td>0.02</td>
</tr>
<tr>
<td>Ni</td>
<td>0.9</td>
<td>0.02</td>
</tr>
</tbody>
</table>

### Activity (\(\text{µmol m}^{-2}\))

<table>
<thead>
<tr>
<th>Catalysts</th>
<th>Activity ((\text{µmol m}^{-2}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>NbP</td>
<td>88.7</td>
</tr>
<tr>
<td>Ni</td>
<td>8.4</td>
</tr>
<tr>
<td>Sr0.9NbO(_3)</td>
<td>0.9</td>
</tr>
</tbody>
</table>
Solid State Chemistry can have an impact on topological effects

- Topological insulators (Oxides, correlated systems)
- Weyl and Dirac semimetals
- ..

Applications in

- Electronics AHE SHE QAHE
- chemistry (catalysis)