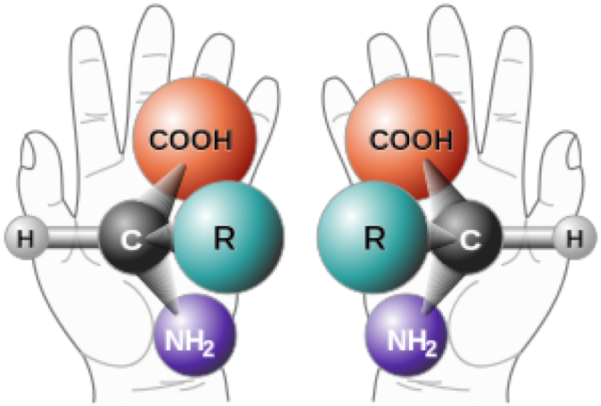
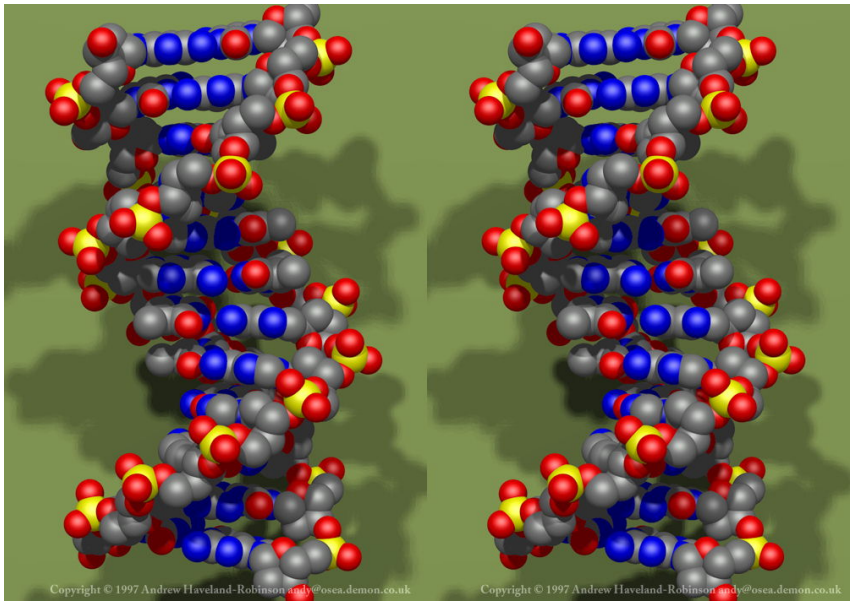
Topology: Introduction

Claudia Felser

Topology in Chemistry

Molecules with different chiralities can have different physical and chemical properties

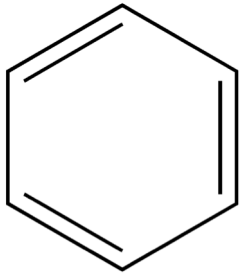


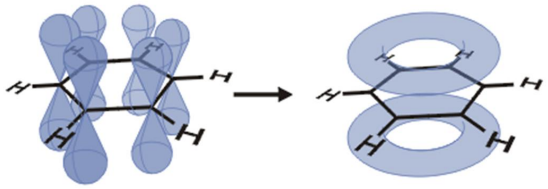


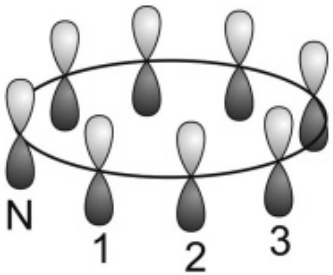
Topology in Chemistry

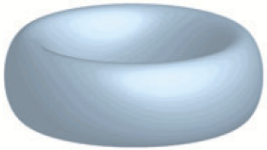
Aromatic compounds

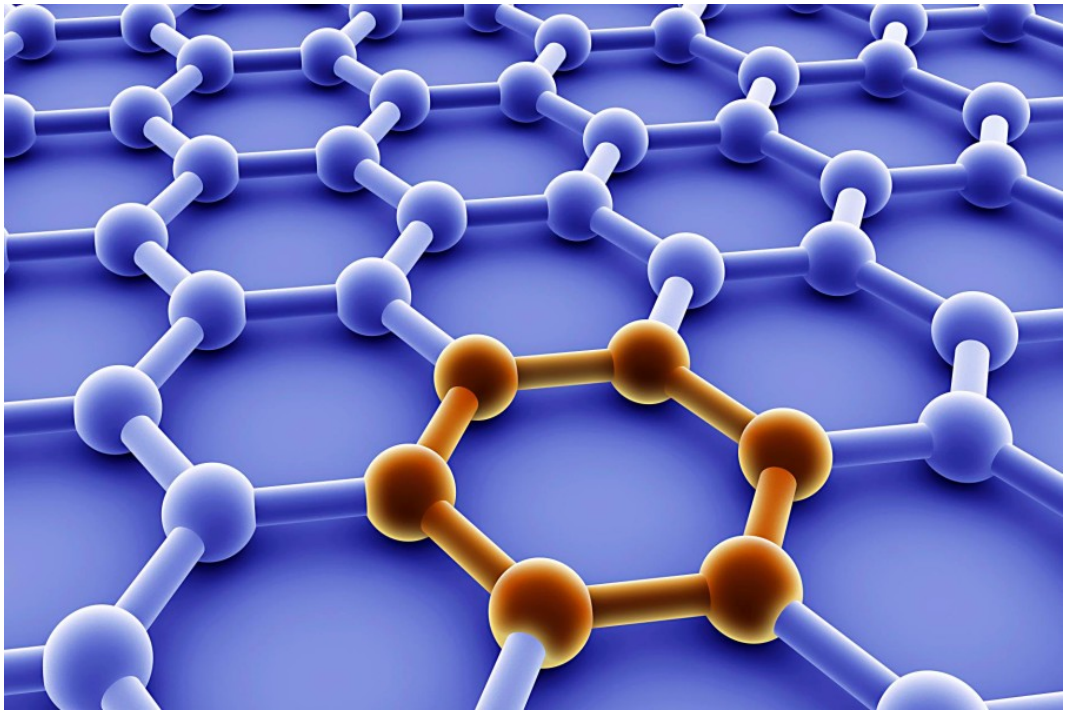
- Aromatic with (**4 n + 2) π-electrons**
- The symmetry counts



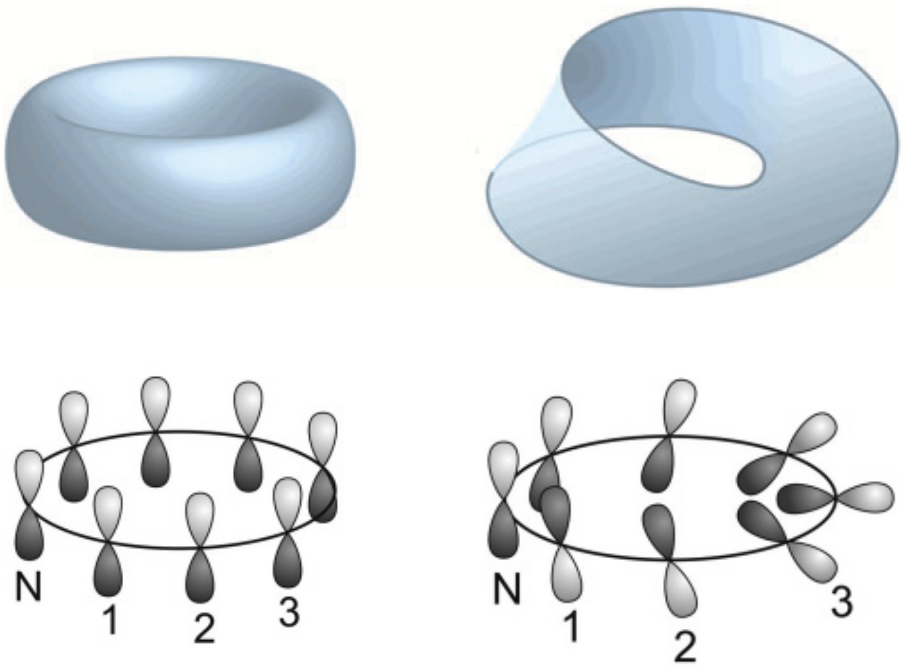








Topology in Chemistry

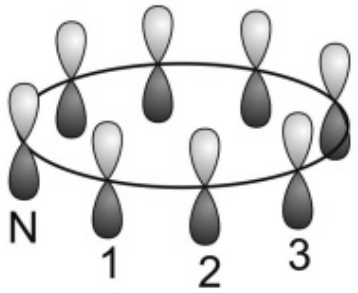


Magic electron numbers

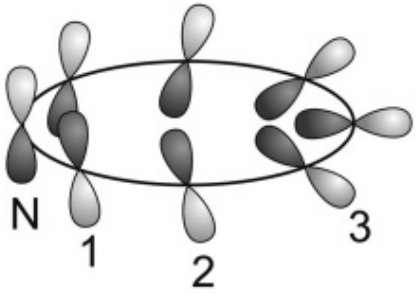
Hückel:
4n+2 aromatic
4n antiaromatisc

Möbius
4n aromatic
4n+2 antiaromatic

Hückel and Möbius Aromaticity



Möbius Annulenes



ORGANIC CHEMISTRY

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.

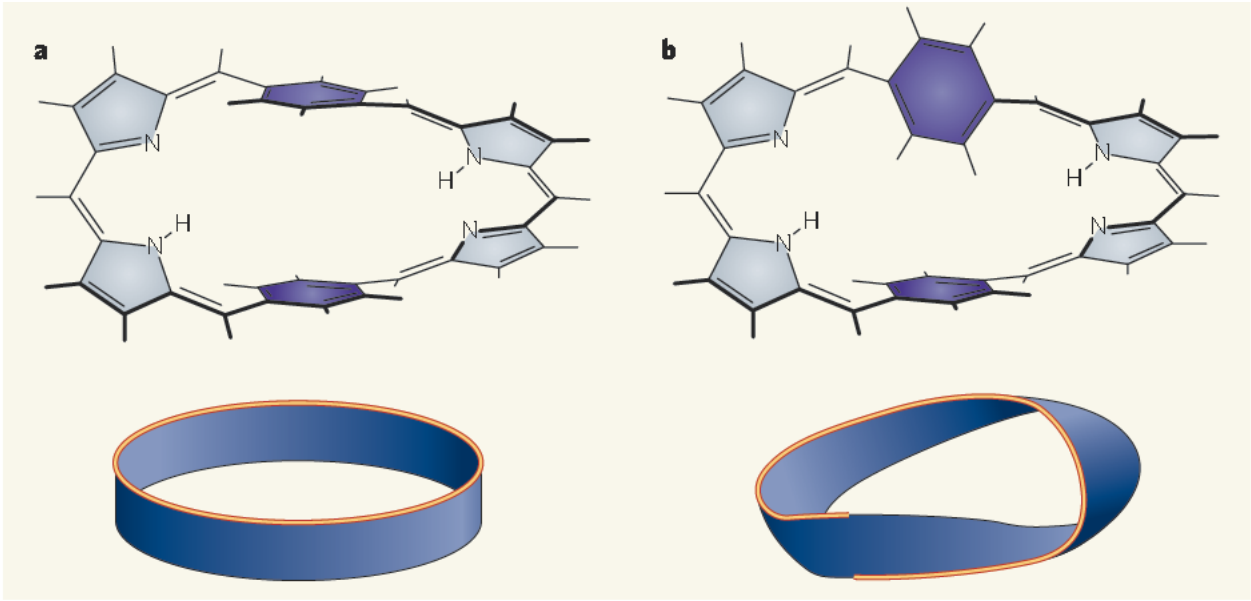


Figure 2 | A molecular topological switch. Latos-Grażyński and colleagues[1] have made a compound that is antiaromatic in nonpolar solvents, but not in polar solvents. **a**, In nonpolar solvents, the two benzene rings (purple) in the molecule are parallel, and the molecule is a two-sided, non-twisted 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.

The result

Catalogue of Topological Electronic Materials

Tiantian Zhang,[1,2,*] Yi Jiang,[2,1,*] Zhida Song,[1,2,*] He Huang,[3]
Yuqing He,[3,2] Zhong Fang,[1] Hongming Weng,[1,†] and Chen Fang[1,4,‡]

[1] *Beijing National Labratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*
[2] *University of Chinese Academy of Sciences, Beijing 100049, China*
[3] *Computer Network Information Center, Chinese Academy of Sciences, China*
[4] *CAS Centre for Excellence in Topological Quantum Computation, Beijing, China*

Preprints 1807.08756, 1807.10271

The ("High-Quality") Topological Materials In The World

M. G. Vergniory[1,2,3*]
[1] *Donostia International Physics Center, P. Manuel de Lardizabal 4, 20018 Donostia-San Sebastián, Spain*
[2] *IKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, 48013 Bilbao, Spain and*
[3] *Applied Physics Department II, University of the Basque Country UPV/EHU, Apartado 644, 48080 Bilbao, Spain*

L. Elcoro[1*]
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Claudia Felser
[1] *Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany*

B. Andrei Bernevig[†]
[1] *Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*
[2] *Physics Department, Freie Universitat Berlin, Arnimallee 14, 14195 Berlin, Germany and*
[3] *Max Planck Institute of Microstructure Physics, 06120 Halle, Germany*

Zhijun Wang[1‡]
[1] *Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*
(Dated: July 26, 2018)

Bilbao crystallographics server

FCT/ZTF

bilbao crystallographic server

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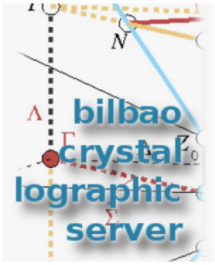


ECM31-Oviedo Satellite

Crystallography online: workshop on the use and applications of the structural tools of the Bilbao Crystallographic Server

20-21 August 2018

News:

- **New program: mCIF2PCR**
  01/2018: Transformation from mCIF to PCR format. The

Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

Solid State Theory Applications

Structure Utilities

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Quick access to some tables

Space Groups

Plane Groups

Layer Groups

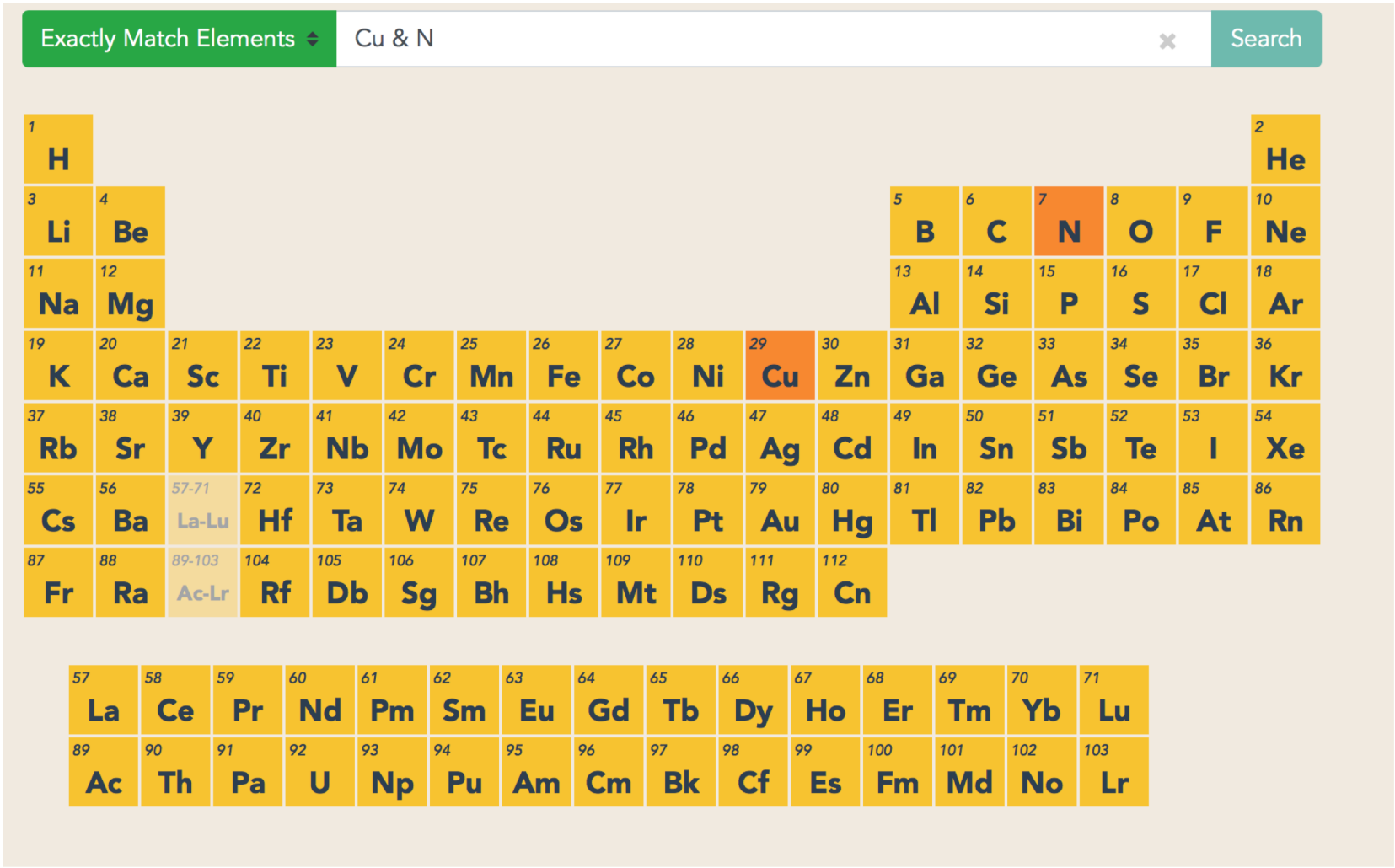
Rod Groups

Frieze Groups

2D Point Groups

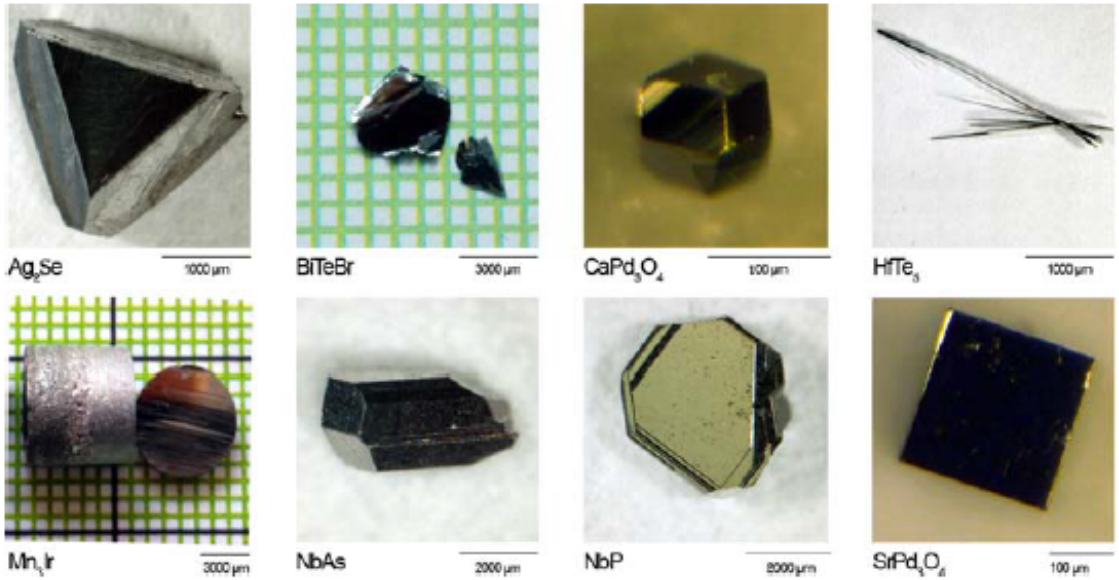
3D Point Groups

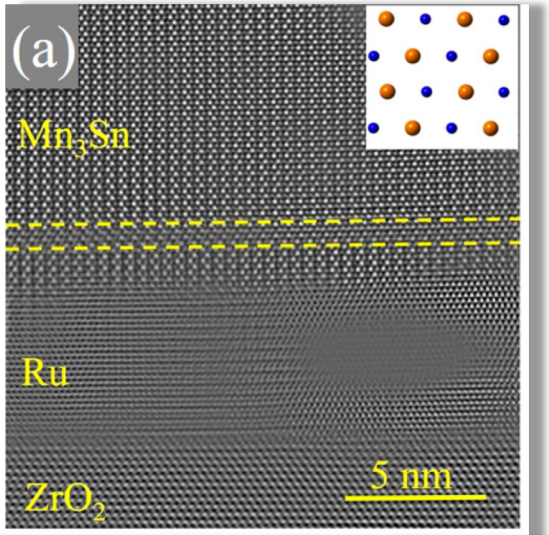
http://materiae.iphy.ac.cn

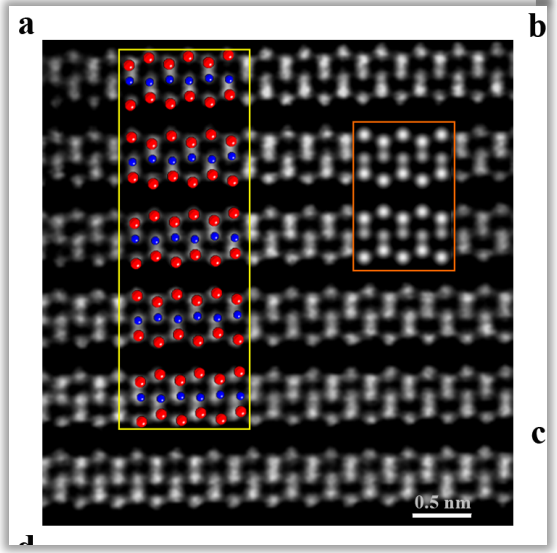


Novel topological materials

- **Explorative search for new materials** & **predictive design** (Yan Sun)
- **200** high quality **single crystal growth** (Shekhar Chandra)
- **Epitaxial growth** of thin films (Anastasious Markou)
- **2D materials – Nanowires** (Johannes Gooth)





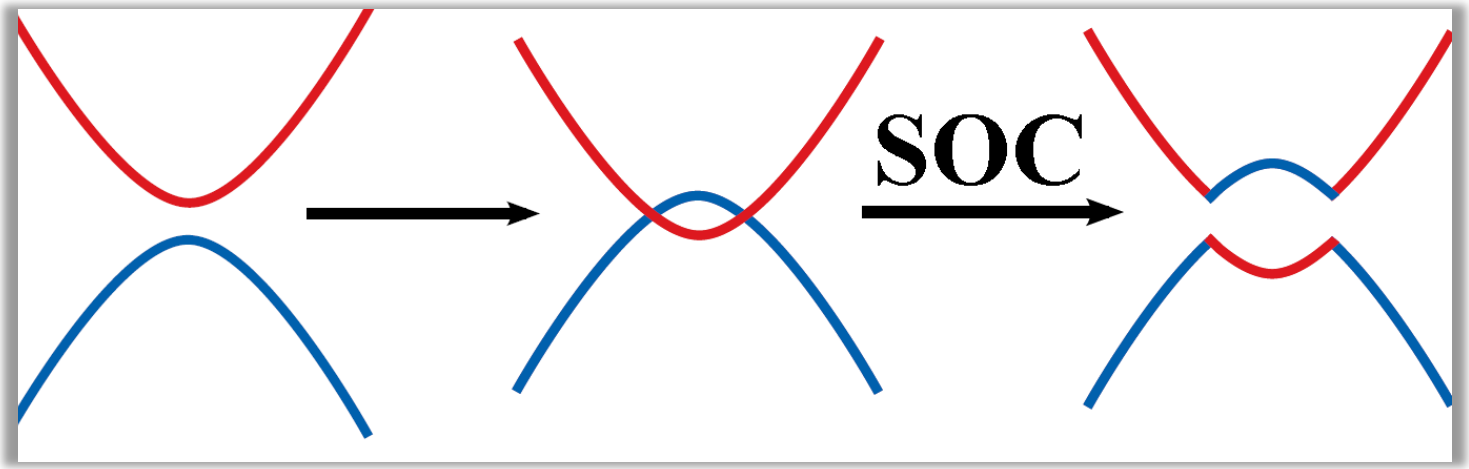


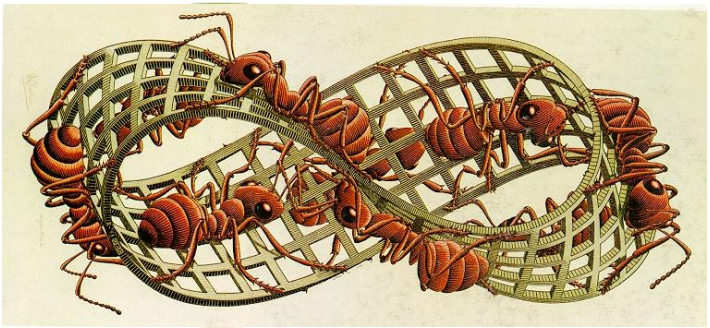
Trivial and Topological Insulators

Trivial semiconductor
CdS

Topological Insulator
Without spin orbit coupling

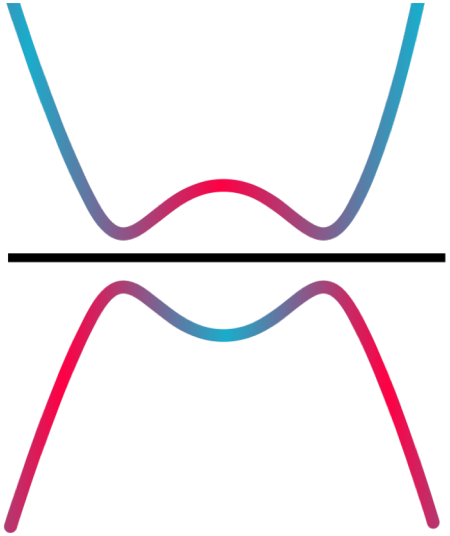
Topological Insulator
Withspin orbit coupling





M. C. Escher

Topological Insulators



Topological Insulators

Z_2 Topological Order and the Quantum Spin Hall Effect

C. L. Kane and E. J. Mele

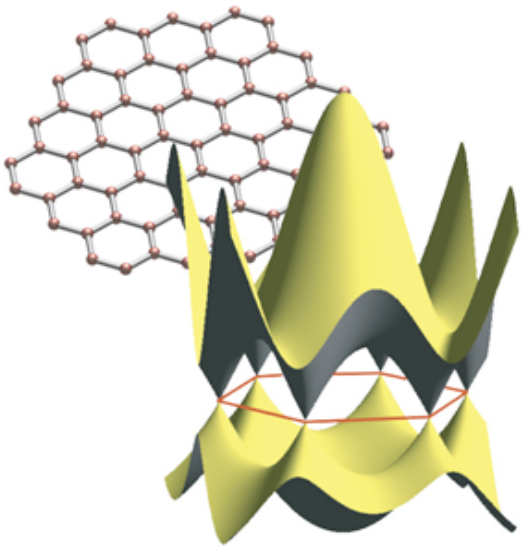
Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA

(Received 22 June 2005; published 28 September 2005)

The quantum spin Hall (QSH) phase is a time reversal invariant electronic state with a bulk electronic band gap that supports the transport of charge and spin in gapless edge states. We show that this phase is associated with a novel Z_2 topological invariant, which distinguishes it from an ordinary insulator. The Z_2 classification, which is defined for time reversal invariant Hamiltonians, is analogous to the Chern number classification of the quantum Hall effect. We establish the Z_2 order of the QSH phase in the two band model of graphene and propose a generalization of the formalism applicable to multiband and interacting systems.

Heavy insulating elements?

Strained α-Sn and Bi-bilayer



First prediction in graphene by Kane

H 2.20																	He
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00
Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.60	Mo 2.16	Tc 1.90	Ru 2.20	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.10	I 2.66	Xe 2.60
Cs 0.79	Ba 0.89		Hf 1.30	Ta 1.50	W 1.70	Re 1.90	Os 2.20	Ir 2.20	Pt 2.20	Au 2.40	Hg 1.90	Tl 1.80	Pb 1.80	Bi 1.90	Po 2.00	At 2.20	Rn
Fr 0.70	Ra 0.90																
		La 1.10	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.20	Gd 1.20	Tb 1.10	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.10	Lu 1.27	
		Ac 1.10	Th 1.30	Pa 1.50	U 1.70	Np 1.30	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.30	Cf 1.30	Es 1.30	Fm 1.30	Md 1.30	No 1.30	Lr 1.30	

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

Kane and Mele, PRL 95, 146802 (2005)

Topological Insulators

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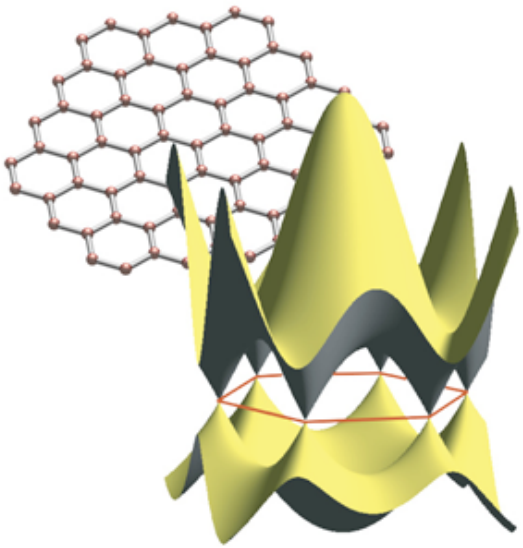
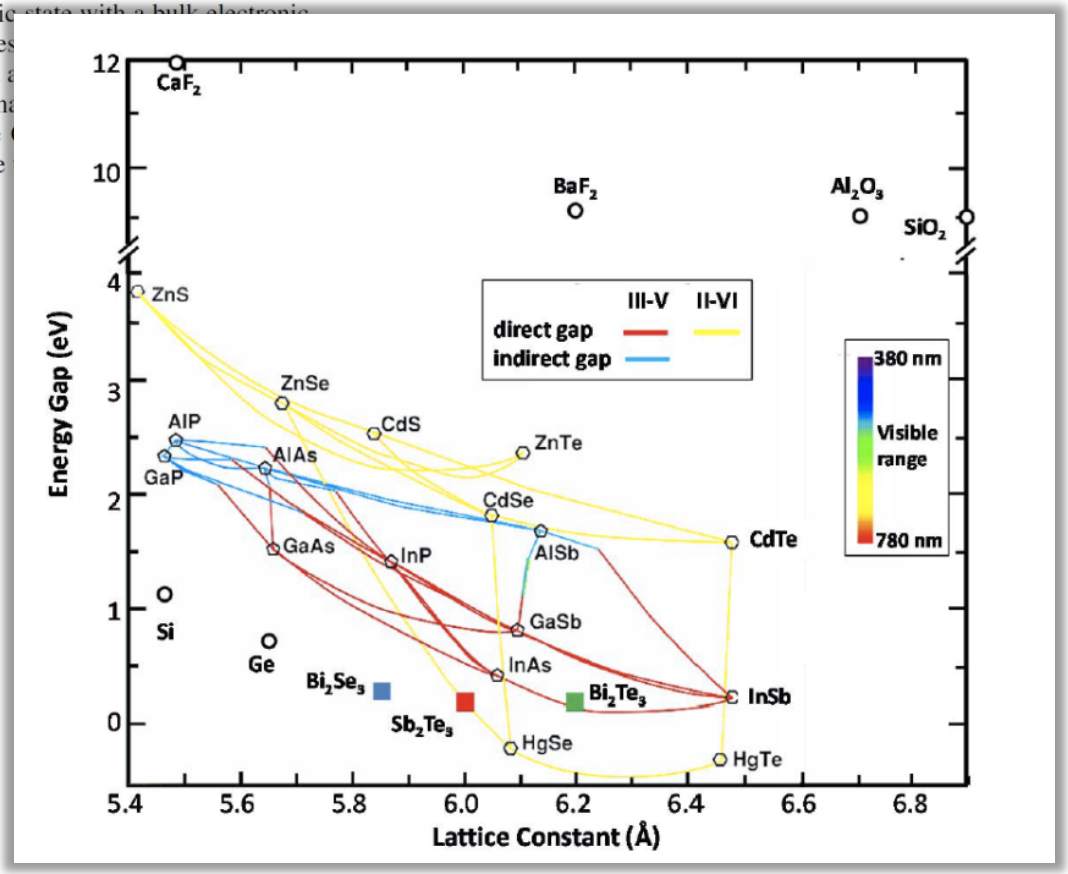


First prediction in graphene by Kane

Heavy insulating binaries

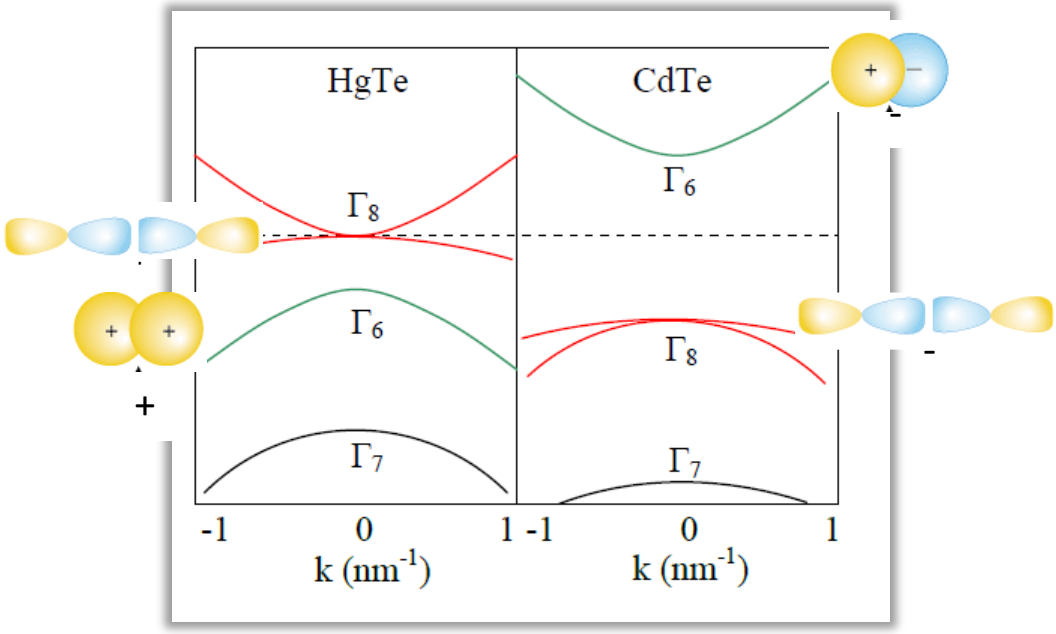


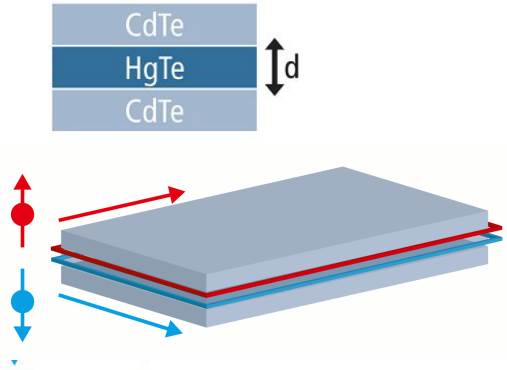
Kane and Mele, PRL 95, 146802 (2005)
Bernevig, et al., Science 314, 1757 (2006)
Bernevig, S.C. Zhang, PRL 96, 106802 (2006)
König, et al. Science 318, 766 (2007)

Quantum Spin Hall

Science
AAAS

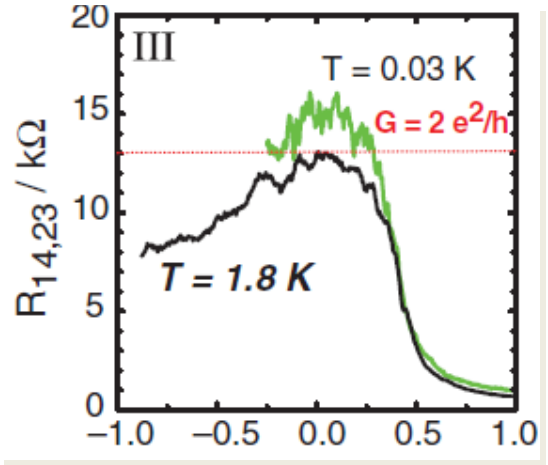
Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells
B. Andrei Bernevig, *et al.*
Science **314**, 1757 (2006);
DOI: 10.1126/science.1133734





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

Inert pair effect



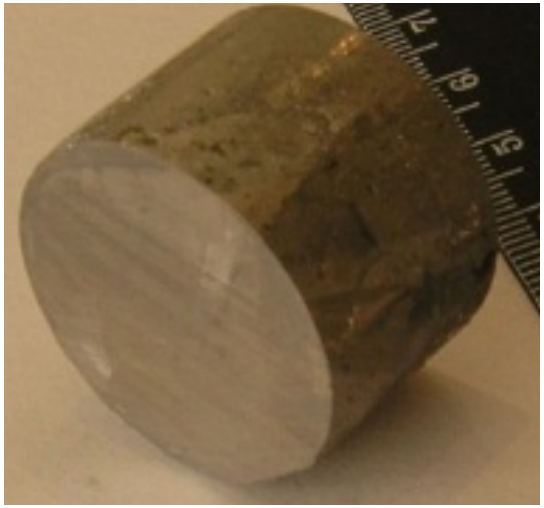
Bernevig,et al., Science 314, 1757 (2006)
Bernevig, S.C. Zhang, PRL 96, 106802 (2006)
König, et al. Science 318, 766 (2007)

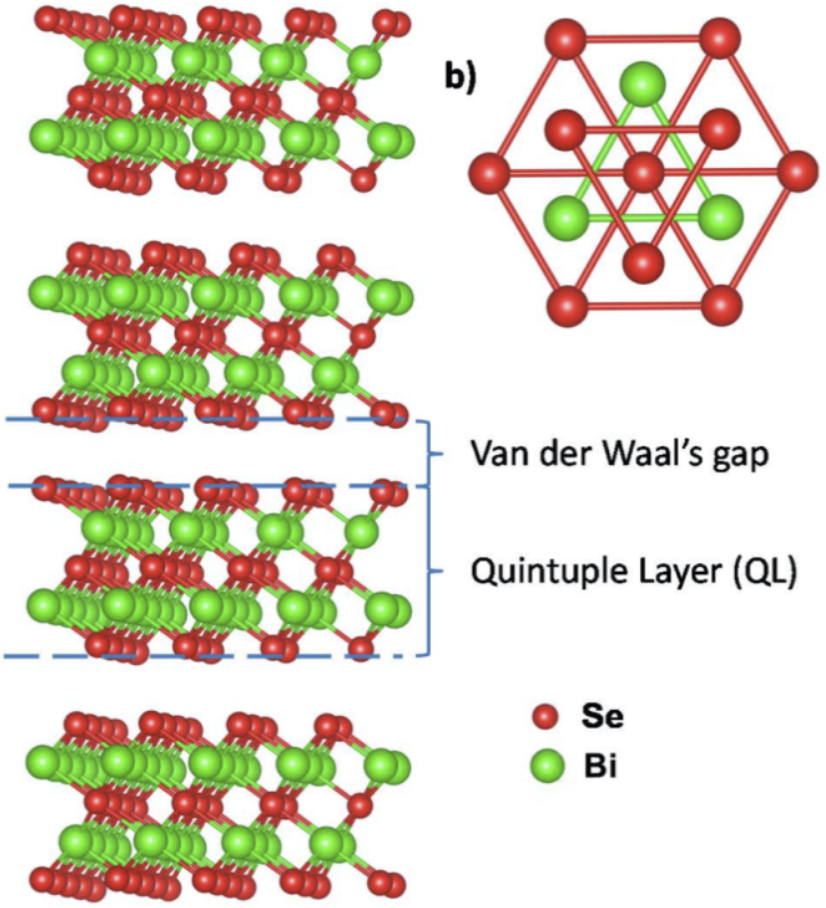
Topologische Isolatoren

Starting with Bismuth

Bi-Sb Legierungen

Bi_2Se_3 und verwandte Strukturen





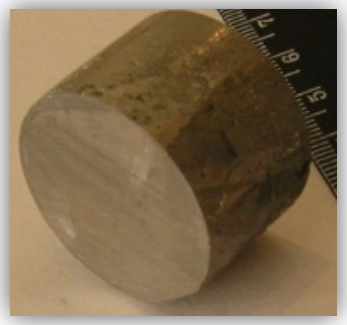
Moore and Balents, PRB 75, 121306(R) (2007)
Fu and Kane, PRB 76, 045302 (2007)
Murakami, New J. Phys. 9, 356 (2007)
Hsieh, et al., Science 323, 919 (2009)
Xia, et al., Nature Phys. 5, 398 (2009); Zhang, et al., Nature Phys. 5, 438 (2009)

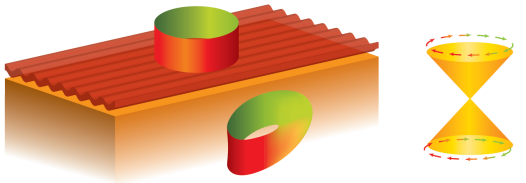
Theory and experiment

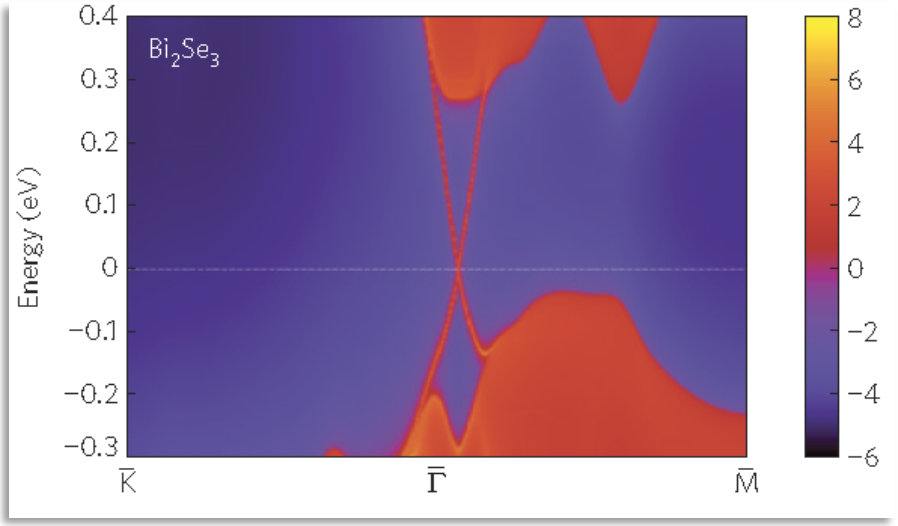
3D topological insulators

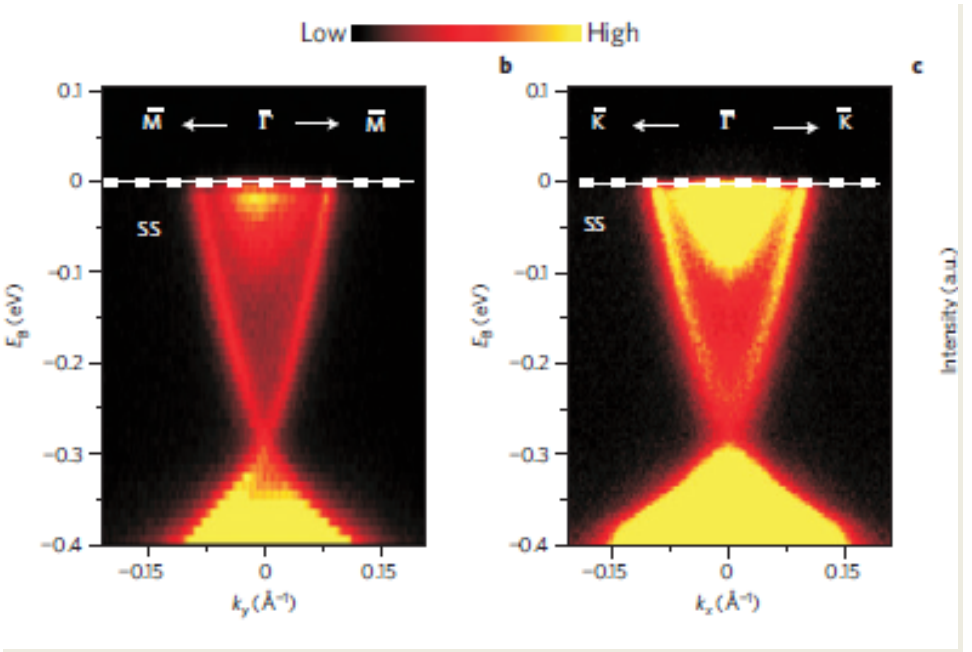
Bi-Sb alloy

Bi_2Se_3 and relatives









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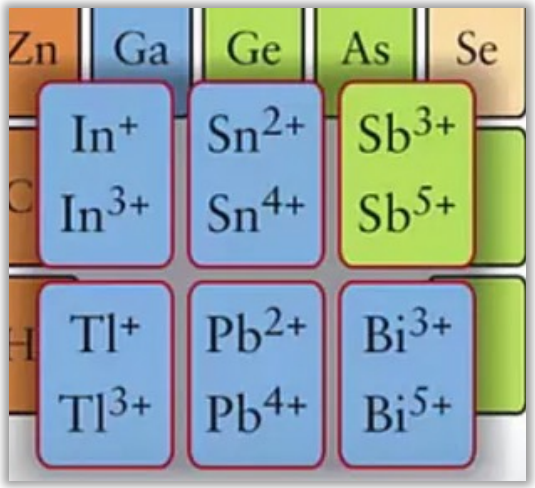
Murakami, New J. Phys. 9, 356 (2007)
Hsieh, et al., Science 323, 919 (2009)
Xia, et al., Nature Phys. 5, 398 (2009); Zhang, et al., Nature Phys. 5, 438 (2009)

Materials

Table I. Proposed topological insulator materials grouped into several different material classes.[4,12,13,19,23–29]

HgTe-type	Bi_2Se_3-type	Honey Comb Lattice	Bismuth-Alloys	NaCl Structure	Oxides	Correlated Materials	Super-conductors
HgTe	Bi_2Se_3, Bi_2Te_3, and Sb_2Te3	Graphene	Bi-Sb	SnTe PbTe	Doped $BaBiO_3$	Iridates	$Cu_xBi_2Se_3$
Half-Heuslers such as LaPtBi	Bi_2Te_2Se	LiAuTe		PuTe AmN	Iridates	SmB_6	LaPtBi YPtBi LuPtBi
α-Sn, HgSe β-HgS	$(Bi_xSb_{1-x})_2Te_3$					YbPtBi	$TlBiSe_2$ $TlBiTe_2$
Chalco-pyrites	$TlBiSe_2$ and $TlBiTe_2$					Skutterudites	
AlSb/InAs/GaSb	$Bi_{14}Rh_3I_9$					PuTe, AmN	



Claudia Felser and Xiao-Liang Qi , Guest Editors, MRS Bull. 39 (2014) 843.

$Tl^{+1}\ Sn^{2+}\ Bi^{+3}$

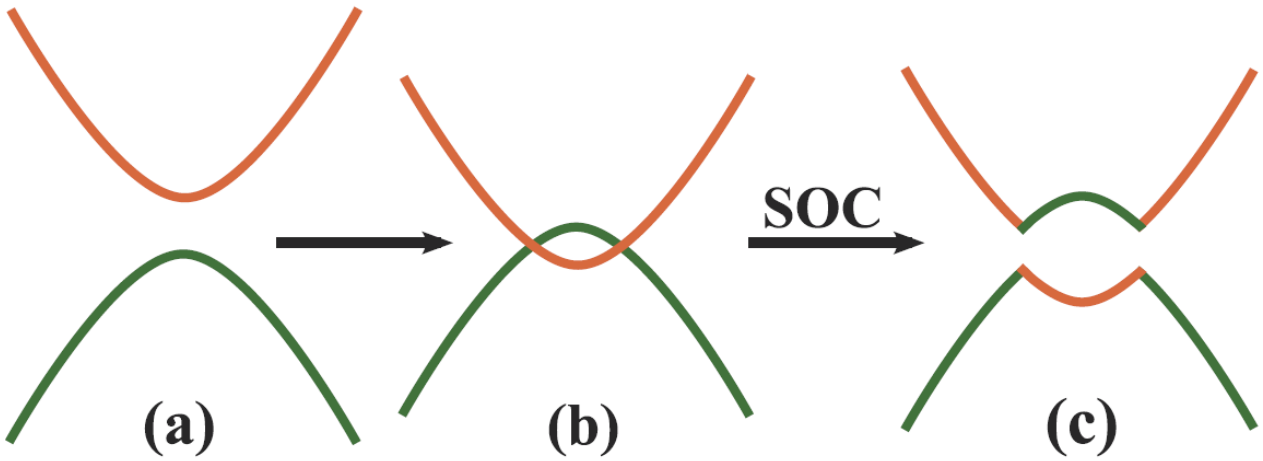
Inert pair effect

Trivial and topological insulators

Trivial semiconductor
CdS

Topological Insulator
Without spin orbit coupling

Topological Insulator
Withspin orbit coupling



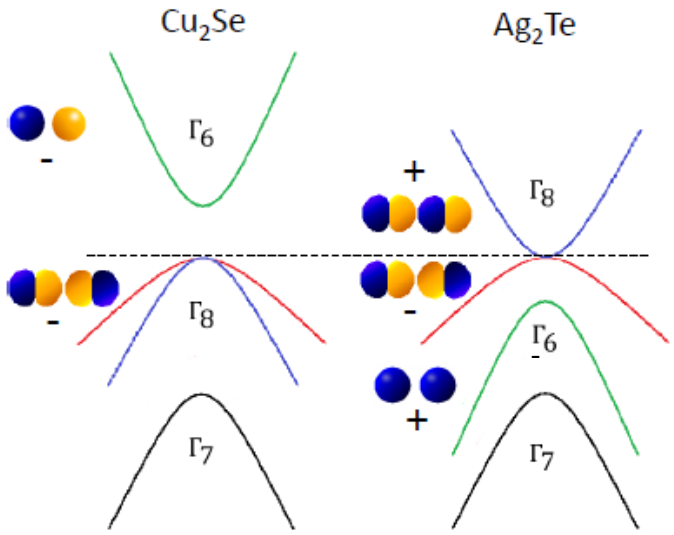
Sufficient condition:

Parity change

Centro symmetric ➡ **Eigenvalues**

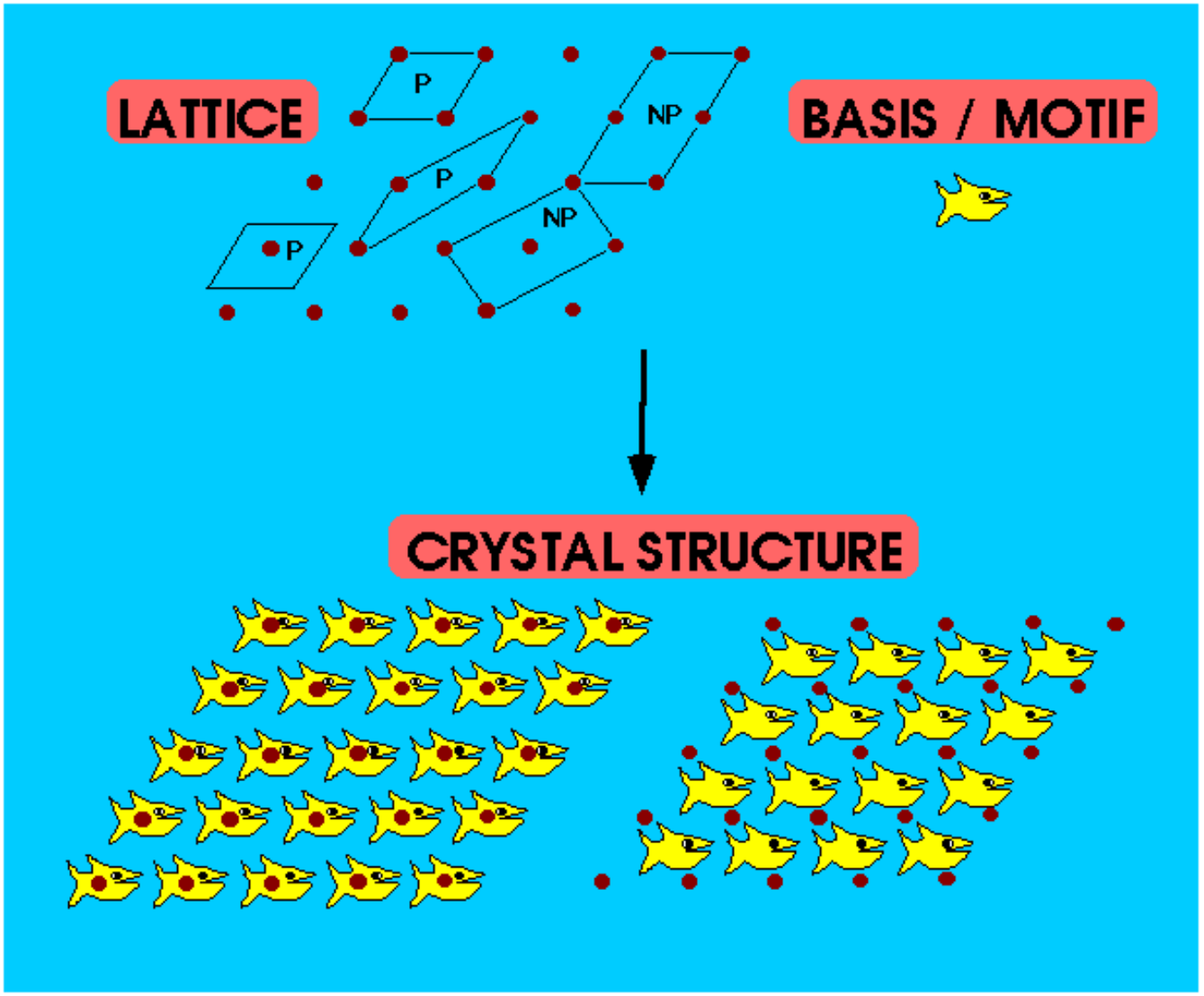
Noncentro sym. ➡ Z2 classification

Inert pair effect



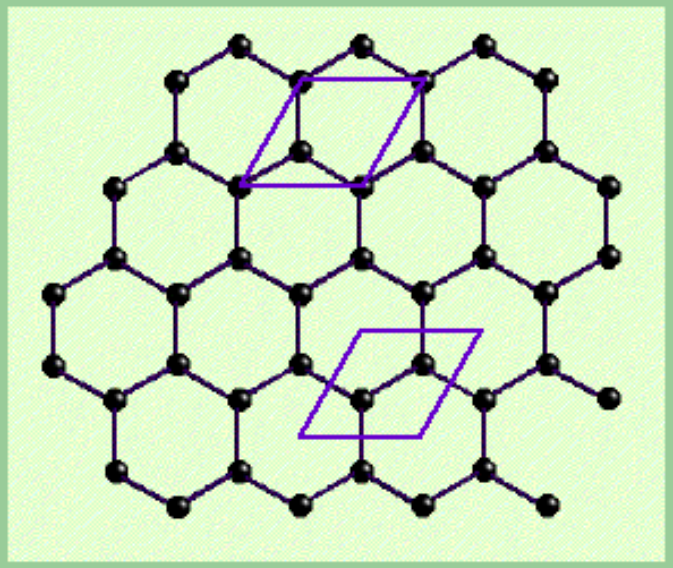
Crystal structure

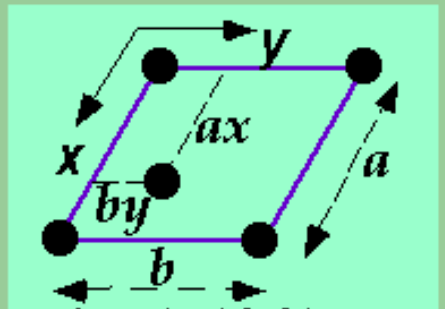
Definitions



Graphene

2D LATTICE

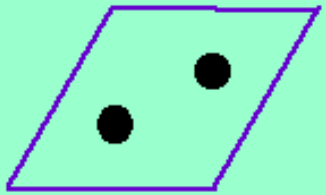




Atom 1: (0, 0)

Atom 2: ($^{2}/_{3}$, $^{1}/_{3}$)

Unit Cells

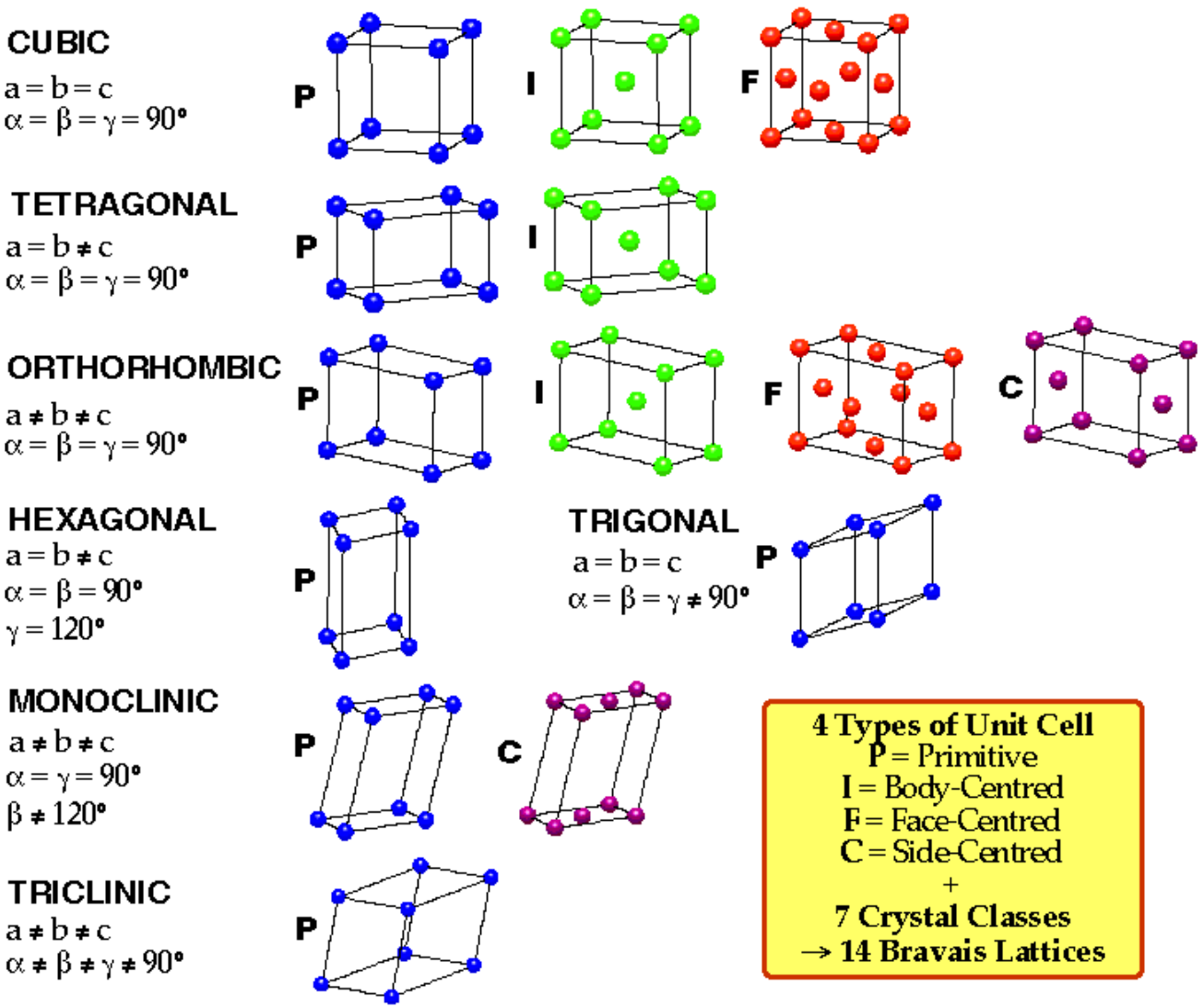


Atom 1: ($^{2}/_{3}$, $^{1}/_{3}$)

Atom 2: ($^{1}/_{3}$, $^{2}/_{3}$)

FRACTIONAL Atomic (x,y) coordinates
(As a fraction of unit cell dimension)
i.e. true dimensions are *ax* and *by*

Space groups



230 space groups

ICSD data base

FIZ Karlsruhe ICSD

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ICSD - Inorganic Crystal Structure Database

FIZ Karlsruhe provides the scientific and the industrial community with the world's largest database for completely identified inorganic crystal structures, ICSD. The ICSD data are of excellent quality and its first records date back to 1913. Only data which have passed thorough quality checks are included.

Quality Management

As the world's leading provider of scientific information on inorganic crystal structures, we take full responsibility for database production, maintenance and quality control, and we ensure that the ICSD database and our software solutions meet the highest possible quality standards.

Around 6,000 new structures are added every year. Through our continuous quality assurance, existing content is modified, supplemented or duplicates removed. As a result, and by filling gaps from previous years, even the older content is not static.

Highlights:

- All important crystal structure data are available, including unit cell, space group, complete atomic parameters, site occupation factors, Wyckoff sequence, molecular formula and weight, ANX formula, mineral group, etc.
- 80 % of the structures are allocated to about 9,000 structure types. This allows for searches for substance classes.
- Continuous selection and evaluation of theoretical structures. They can serve as a basis for developing new materials through data mining processes.
- Keywords to describe to physical and chemical properties are provided.
- Abstracts for a quick grasp of the article content are available.
- Simulation of Powder Diffraction Data

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ICSD enables scientists to search for text in titles in combination with chemical compound information, e.g., compound classes which cannot be described through specific compound information such as the molecular formula. An interesting example for such a compound class is provided by the spinel compounds.

Read more

- Closed packed structures
  - Cubic
  - Hexagonal

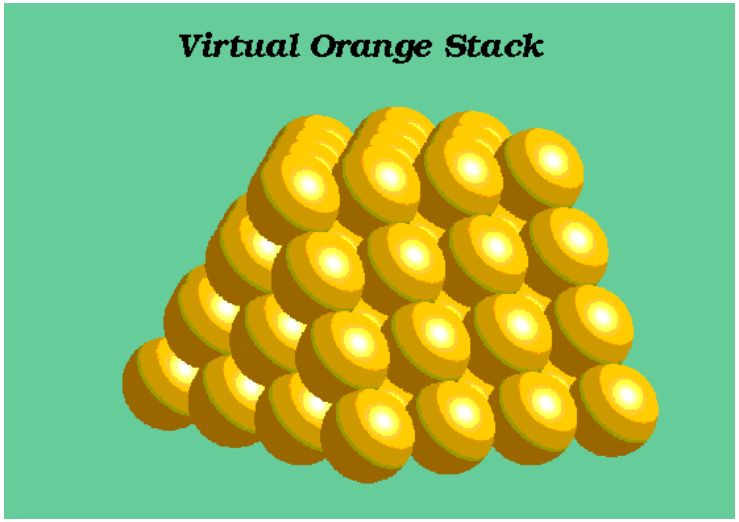
The anion (neg. charged atom and therefore big) builds the closed packed structure

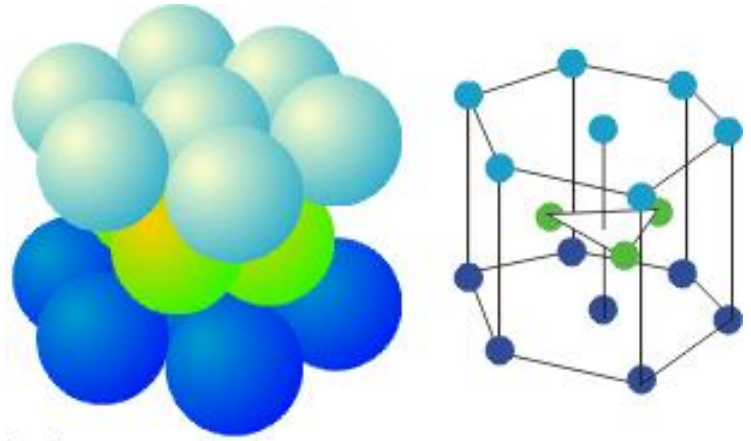
The cation is found in the voids

How structures are made

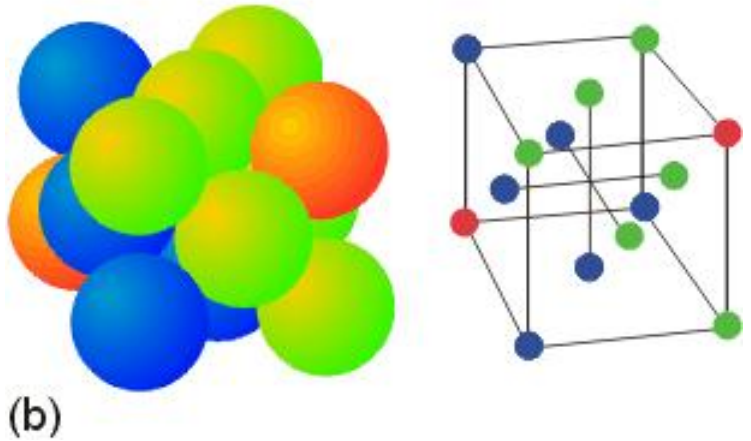
Anions always are the largest spheres, they build a closed packed lattice

In oxides: O^{2-}





(a) **hexagonal close packing**

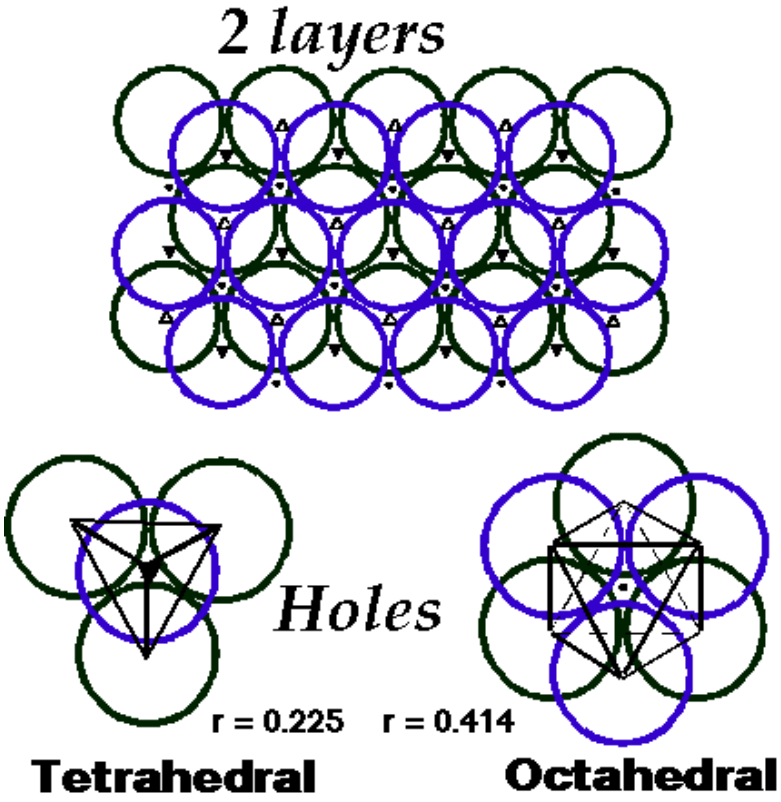


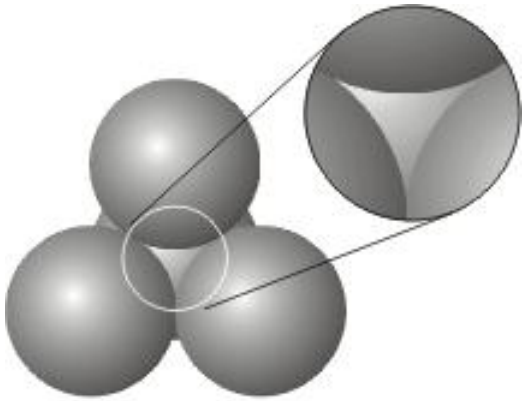
(b) **cubic close packing**

How structures are made: holes

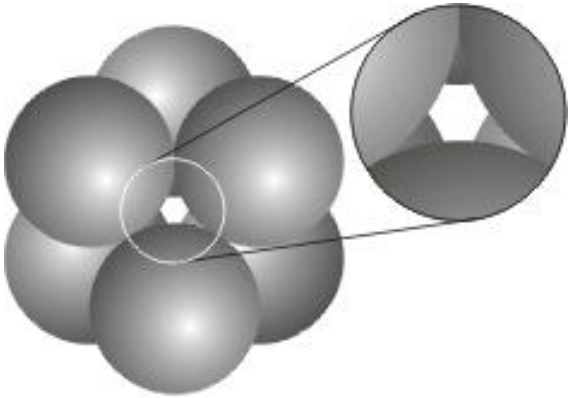
Anions always are the largest spheres, they build a closed packed lattice

Cations are stuffed in the holes



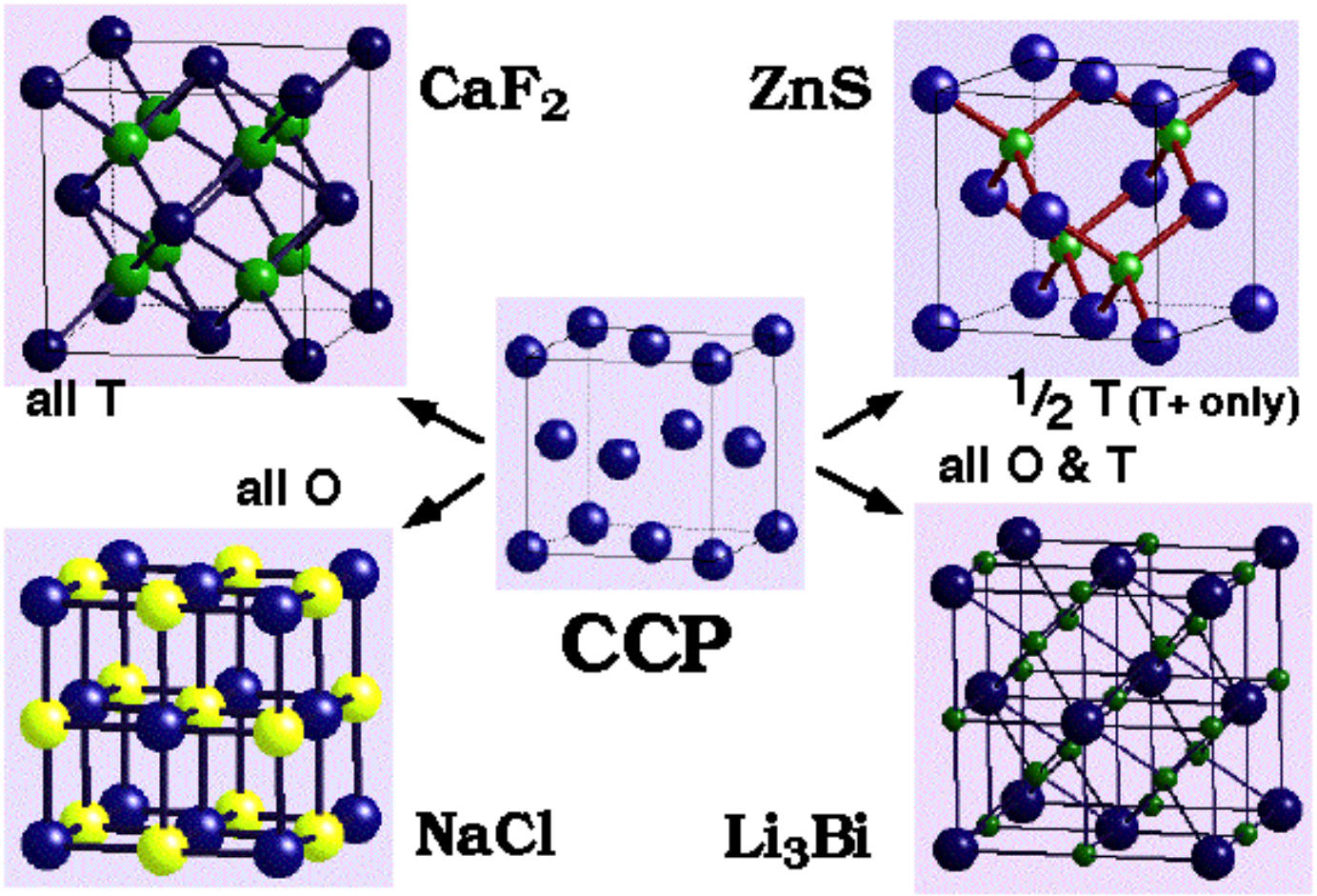


5 Tetrahedral hole

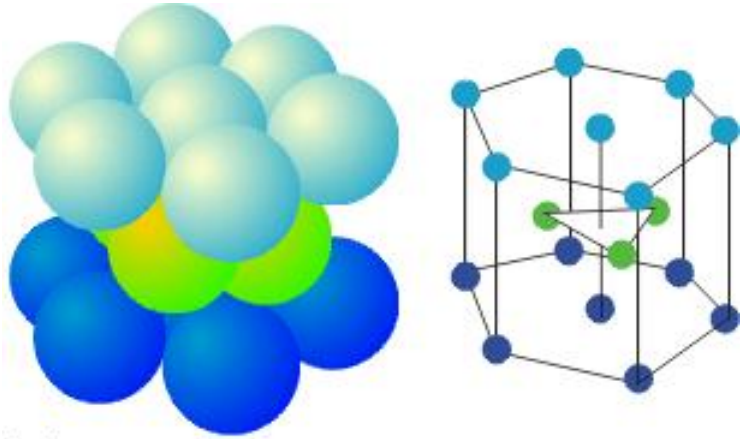


2 Octahedral hole

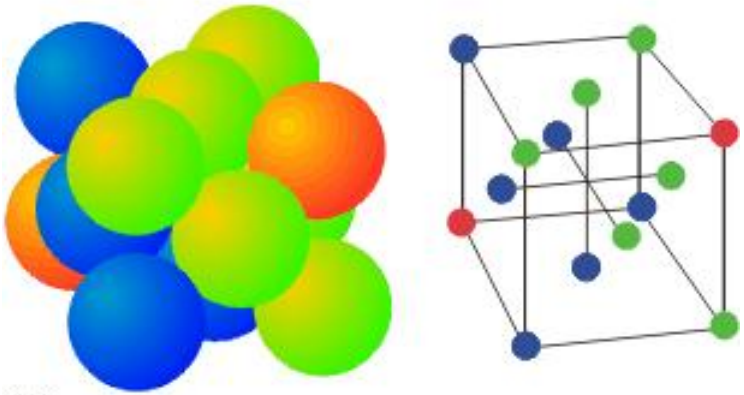
Simple ionic structures



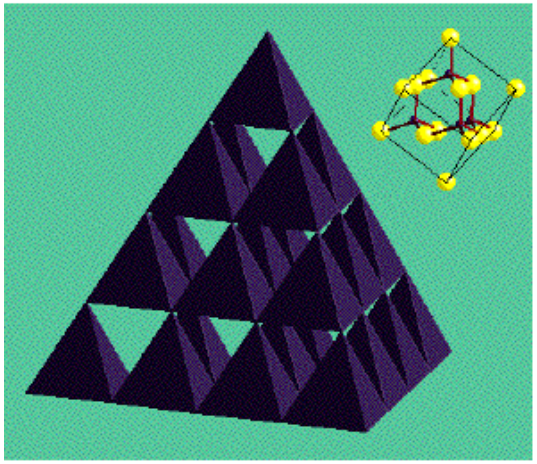
Filled voids in the hexagonal lattice



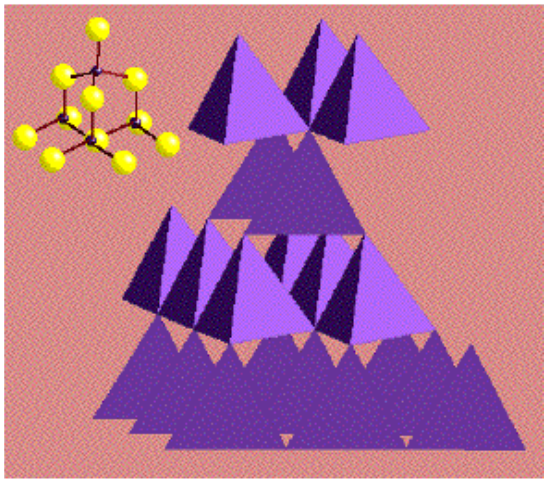
(a)



(b)

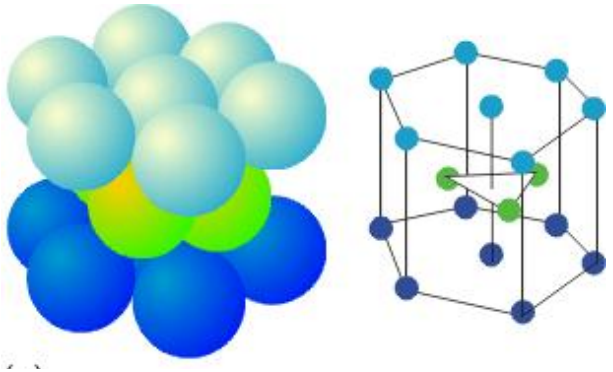


Zinc Blende

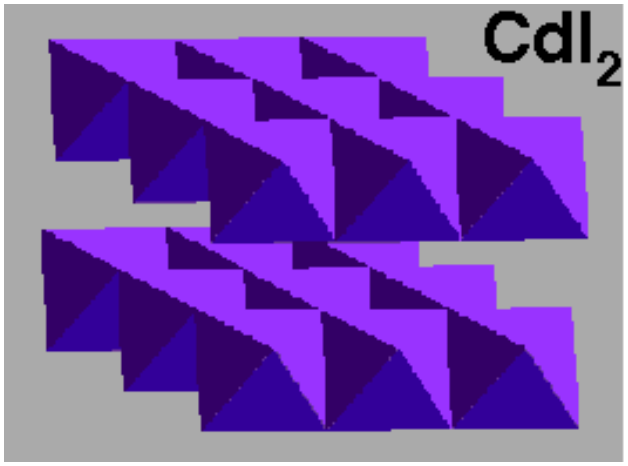


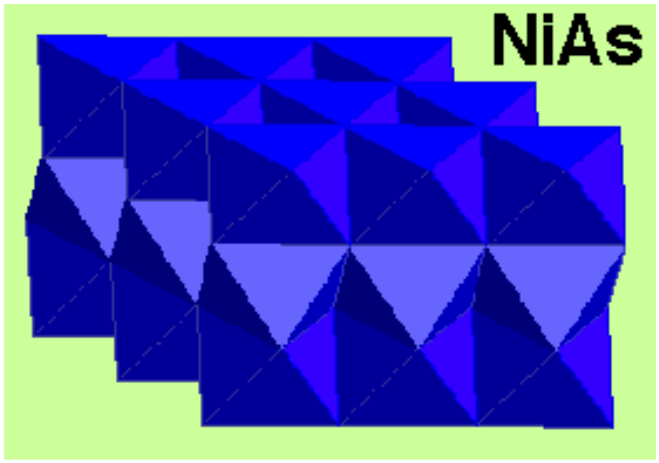
Wurtzite

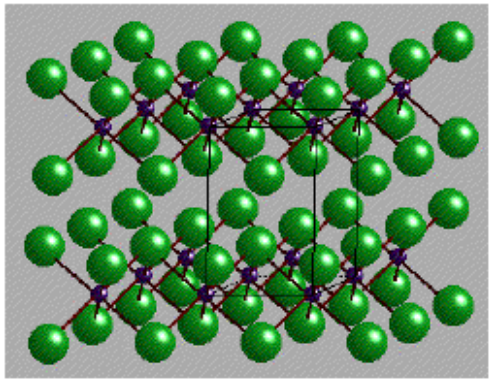
Formula	Type/fraction of sites occ.	HCP	CCP
AB	All octahedral	NiAs Nickel Arsenide	NaCl Rock Salt
	Half tetrahedral	ZnS Wurtzite	ZnS Zinc Blende
A_2B	All tetrahedral	Not known	CaF_2/Mg_2Si (Fluorite/Anti-Fluorite)
A_3B	All octahedral & tetrahedral	Not known	Li_3Bi

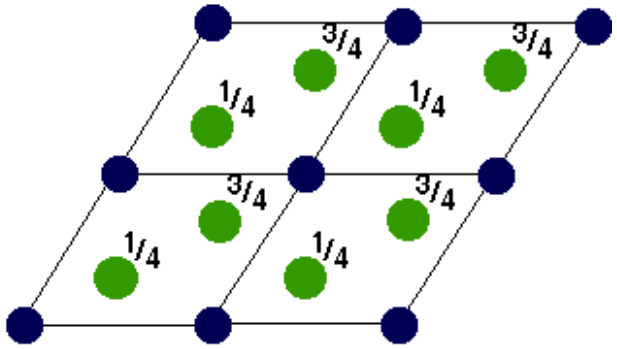


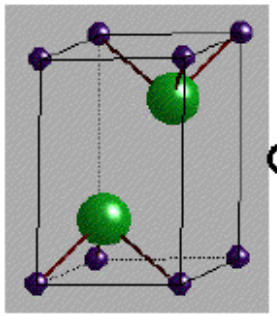
Layered structure





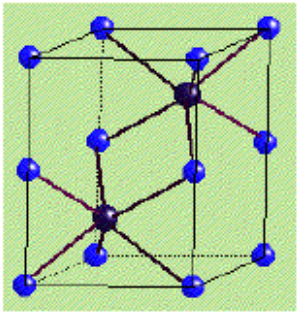






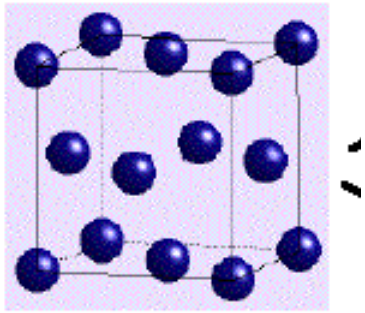
Comparison

CdI_2 *vs* NiAs

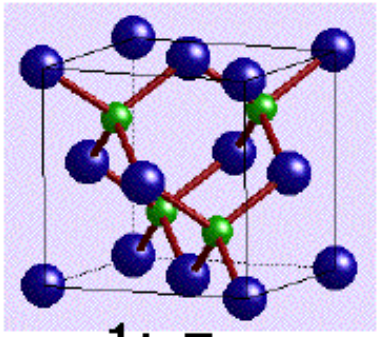


Formula	Type/fraction of sites occ.	HCP	CCP
AB	All octahedral	NiAs Nickel Arsenide	NaCl Rock Salt
	Half tetrahedral	ZnS Wurtzite	ZnS Zinc Blende
A_2B	All tetrahedral	Not known	CaF_2/Mg_2Si (Fluorite/Anti-Fluorite)
A_3B	All octahedral & tetrahedral	Not known	Li_3Bi
AB_2	Half octahedral (Alternate layers full/empty)	CdI_2 Cadmium Chloride	$CdCl_2$ Cadmium Chloride
	Half octahedral (ordered framework arrangement)	$CaCl_2$ TiO_2 (Rutile)	TiO_2 (Anatase)
AB_3	1/3 octahedral Alternate layers 2/3 empty	BiI_3	$AlCl_3$
A_2B_3	2/3 octahedral (Ordered framework)	$Al_2O_3/FeTiO_3$ Corundum/Ilmenite	

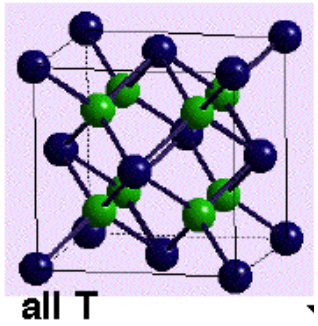
Filled fcc



CCP

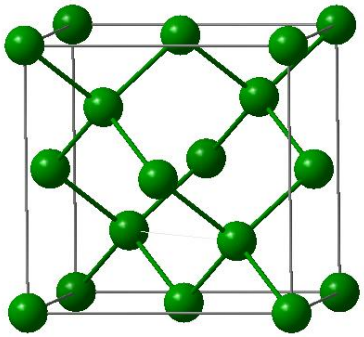


1/2 T (T+ only)

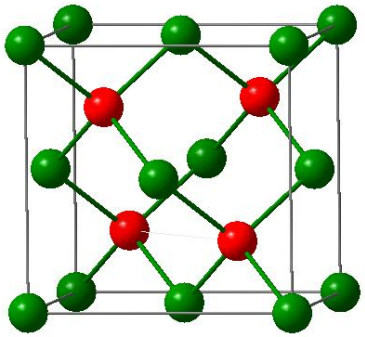


all T

Diamond

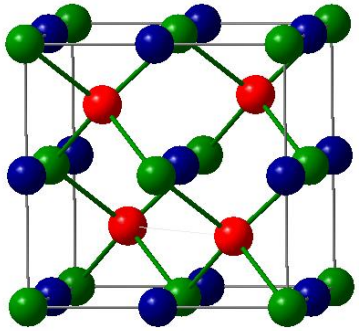


ZnS



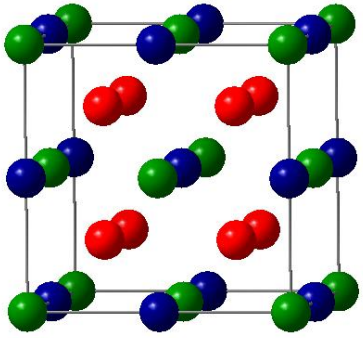
2 interpenetrating fcc
with half of the tetrahedral sites filled

Heusler XYZ $C1_b$



3 interpenetrating fcc
half of the tetrahedral sites
and the octahedral sites

X_2YZ $L2_1$

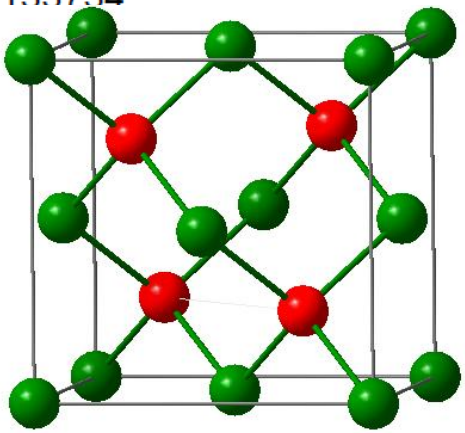


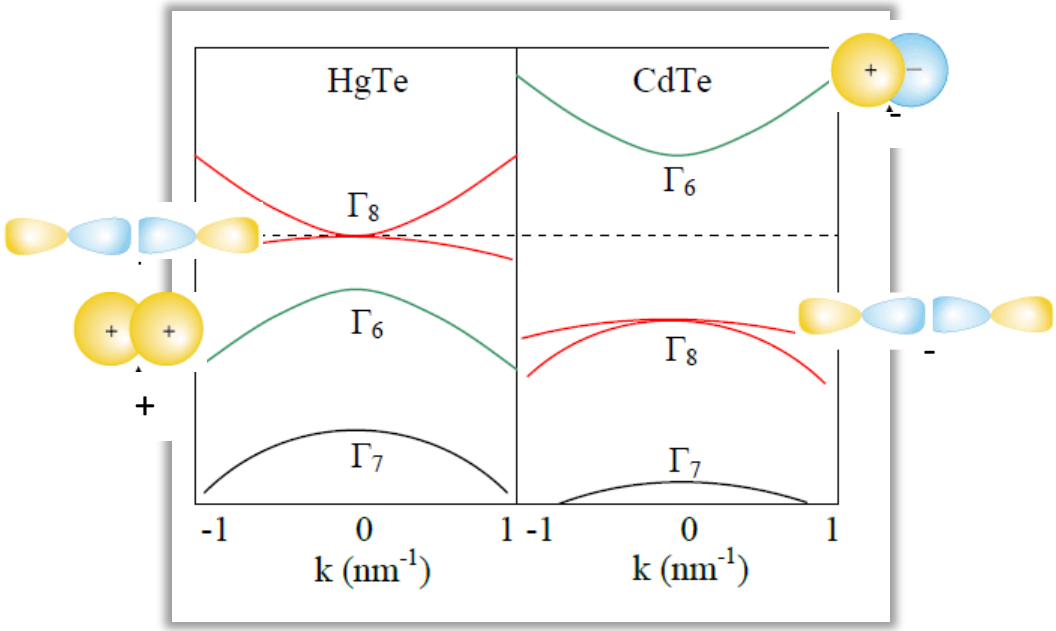
4 interpenetrating fcc
all tetrahedral sites filled
and the octahedral sites

Quantum Spin Hall

Science
AAAS

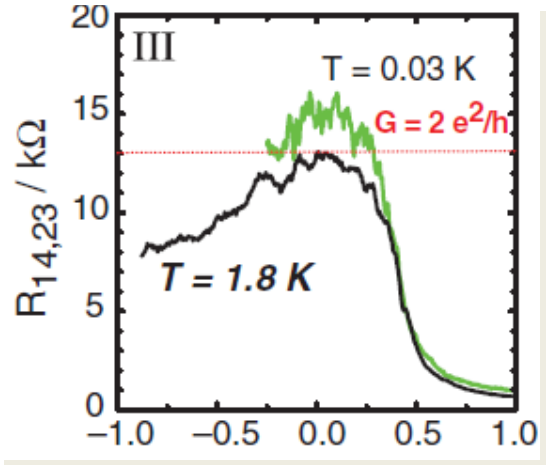
Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells
B. Andrei Bernevig, *et al.*
Science **314**, 1757 (2006);
DOI: 10.1126/science.1133734





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

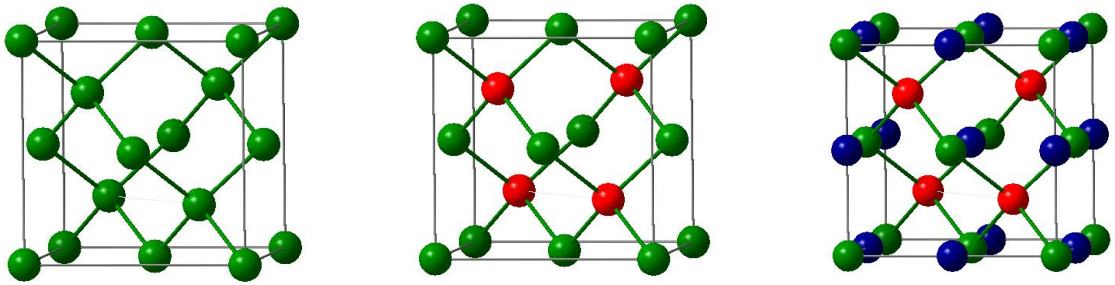
Inert pair effect

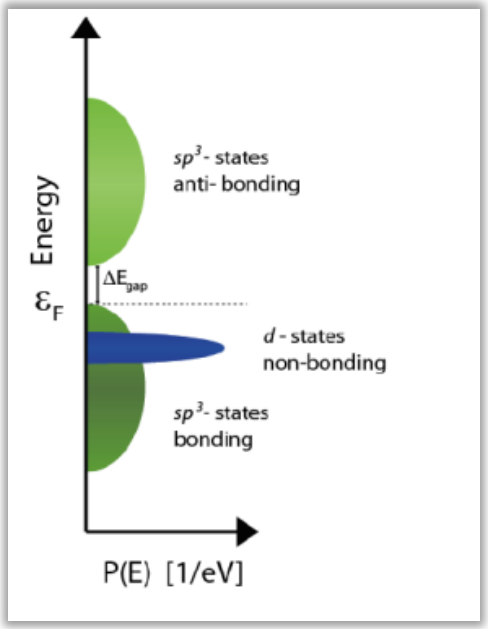


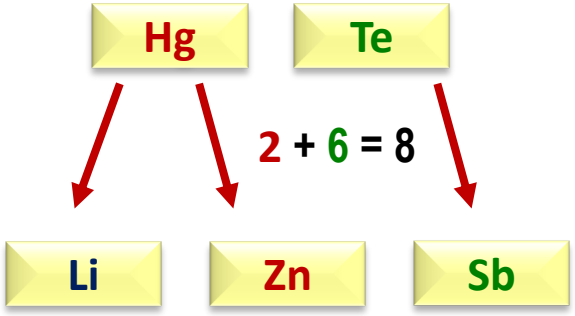
Bernevig,et al., Science 314, 1757 (2006)
Bernevig, S.C. Zhang, PRL 96, 106802 (2006)
König, et al. Science 318, 766 (2007)

Heusler compounds

Diamond **ZnS** **Heusler XYZ $C1_b$**

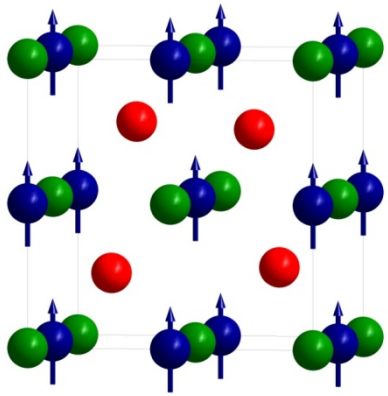






Counting electrons

From wide to low band gap semiconductor



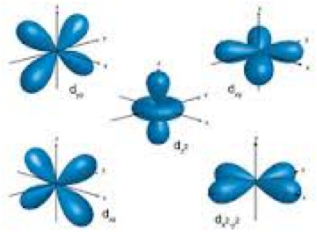
Hg Te

2 + 6 = 8

2 s
6 p

Li Mg As

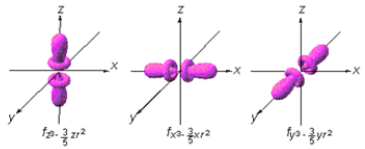
1 + 2 + 5 = 8



Zr Ni Sn

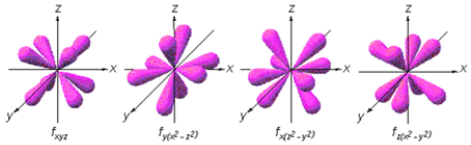
10 d

4 + 10 + 4 = 18



RE Pt Bi

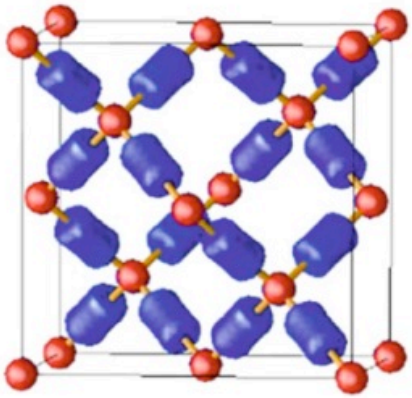
14 f



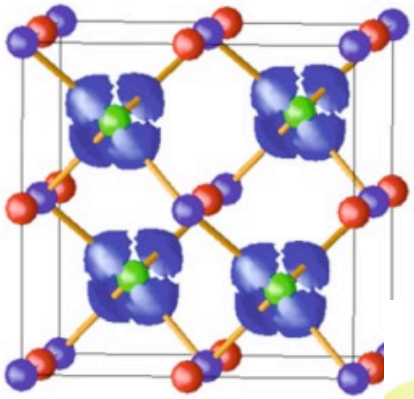
3 (+f^n) + 10 + 5 = 18 + n

Graf, Felser, Parkin, Progress in Solid State Chemistry **39** 1 (2011)
Kandpal et al., J. Phys. D **39** 776 (2006)

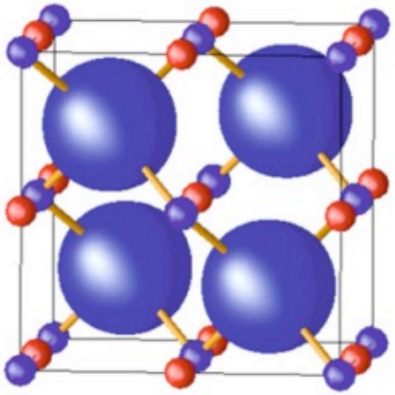
Ionic and covalent structure



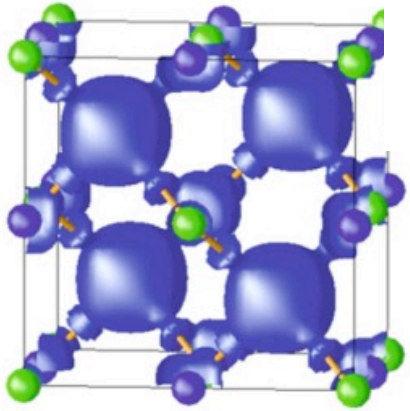
Si



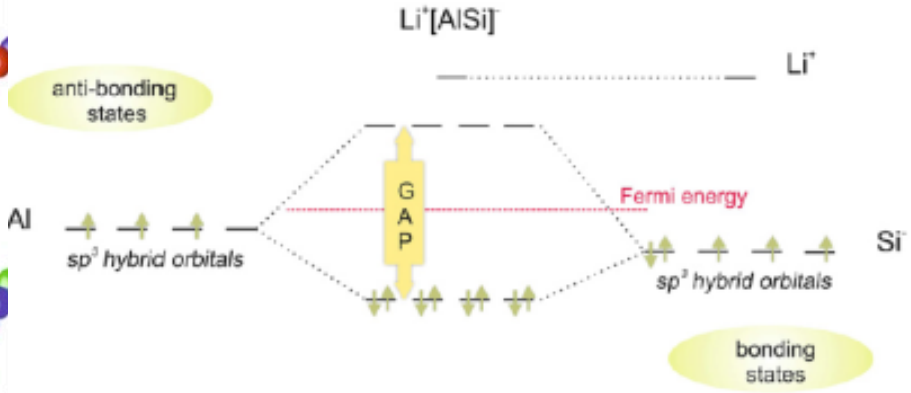
LiAlSi



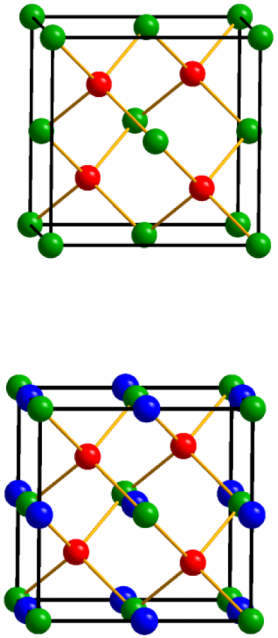
LiMgN

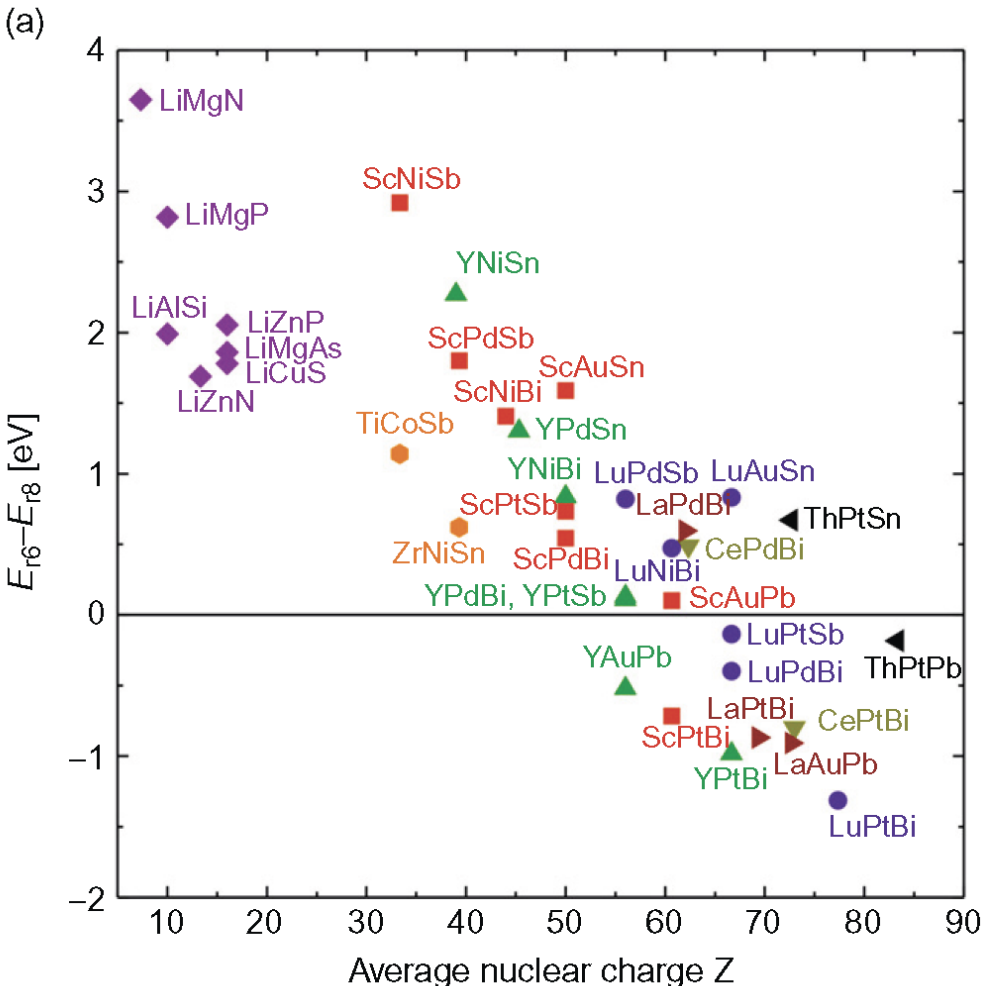


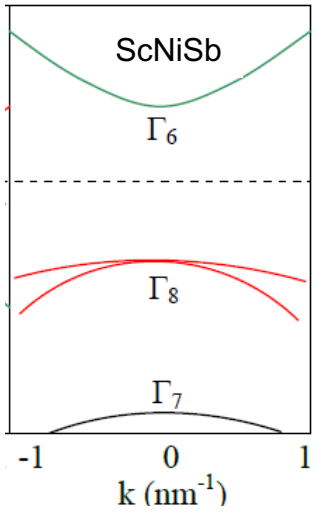
TiCoSb

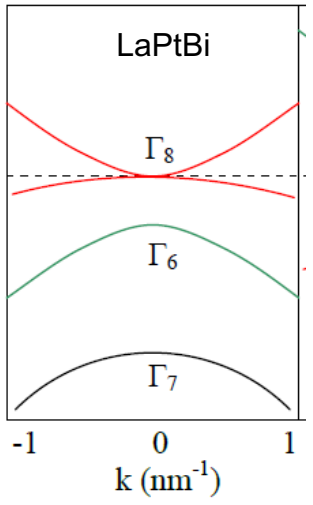


Predicting topological insulators



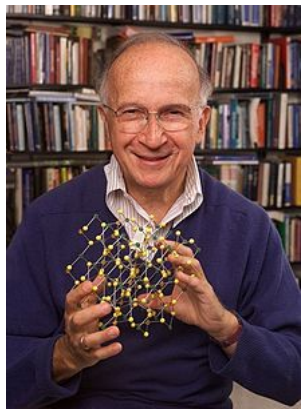






S. Chadov et al., Nat. Mater. **9** 541 (2010).
H. Lin et al., Nat. Mater. **9** 546 (2010).

From Orbitals to Bands

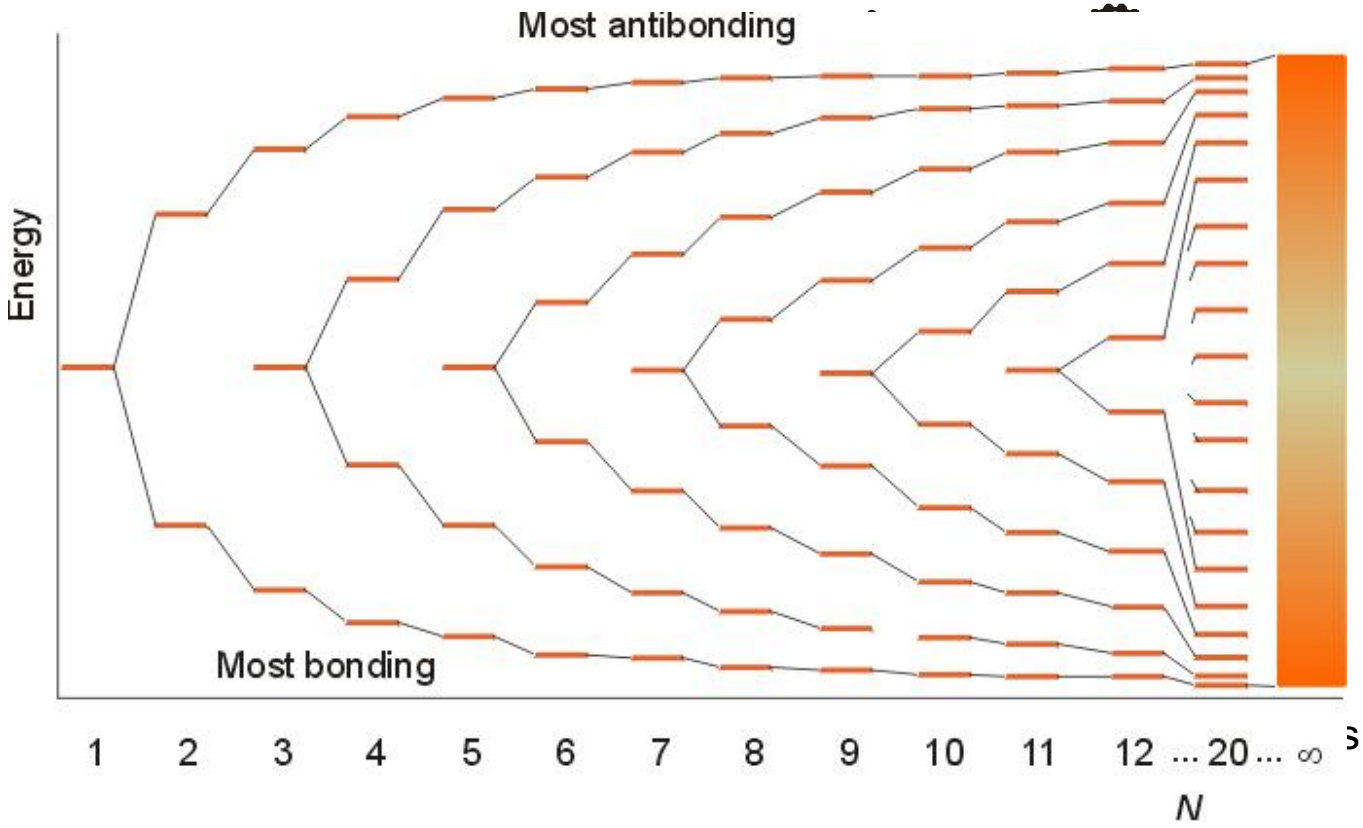


How Chemistry and Physics Meet in the Solid State

By Roald Hoffmann*

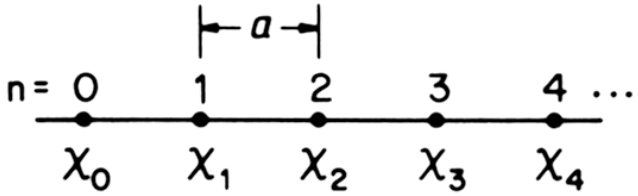
Hoffmann Angewandte. Chem. 26 (1987) 846

Energy bands in solids arise from overlapping atomic orbitals
$\Rightarrow$ crystal orbitals (which make up the bands)
Recipe: use LCAO (tight binding) approach
Crystal = regular periodic array $\Rightarrow$ translational symmetry



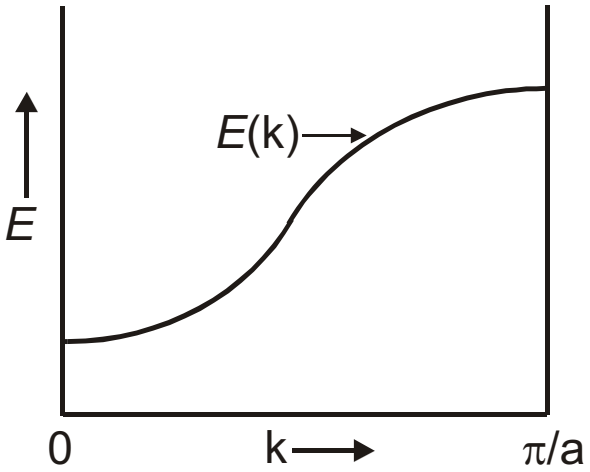
How to find a band structure

We start from atomic orbitals – localized picture: linear chain of hydrogen atoms
Using the translational symmetry of the solid we can set up the n terms of symmetry with a 1s basis function for two special values of k



$$\psi_k = \sum_n e^{ikna} \chi_n$$

Test with a 1s basis function for two special values of k



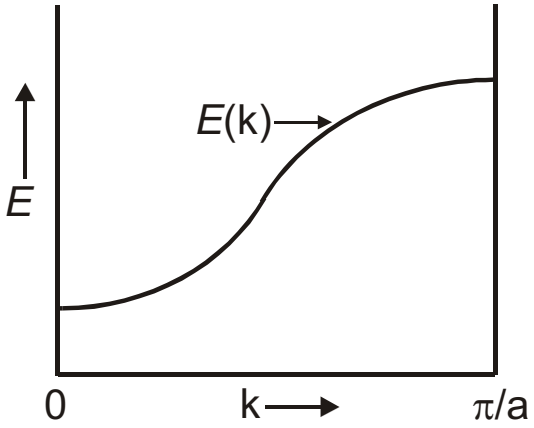
$k = 0 \qquad \Psi_0 = \sum_n e^0 \chi_n = \sum_n \chi_n = \chi_0 + \chi_1 + \chi_2 + \chi_3 \ldots$

$k = \frac{\pi}{a} \qquad \Psi_{\frac{\pi}{a}} = \sum_n e^{\pi i n} \chi_n = \sum_n (-1)^n \chi_n = \chi_0 - \chi_1 + \chi_2 - \chi_3 \ldots$

Hoffmann Angewandte. Chem. 26 (1987) 846

How to find a band structure

The topology of the orbital interaction determines how a band runs



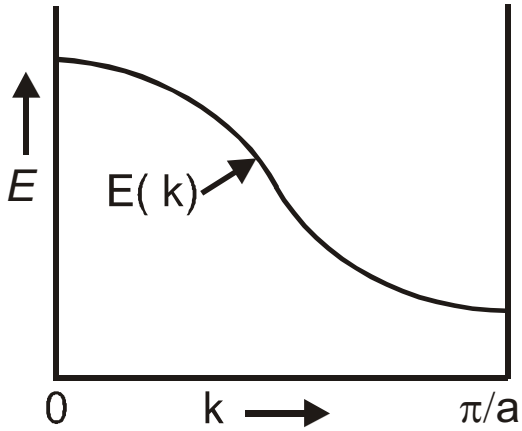
$k = 0 \quad \Psi_0 = \sum_n e^0 \chi_n = \sum_n \chi_n = \chi_0 + \chi_1 + \chi_2 + \chi_3 \ldots\ldots$

$k = \frac{\pi}{a} \quad \Psi_{\frac{\pi}{a}} = \sum_n e^{\pi i n} \chi_n = \sum_n (-1)^n \chi_n = \chi_0 - \chi_1 + \chi_2 - \chi_3 \ldots\ldots$

k = 0 bonding interaction ⇒ band runs „uphill“

$\Psi_0 = \chi_0 + \chi_1 + \chi_2 + \chi_3 + \ldots\ldots$

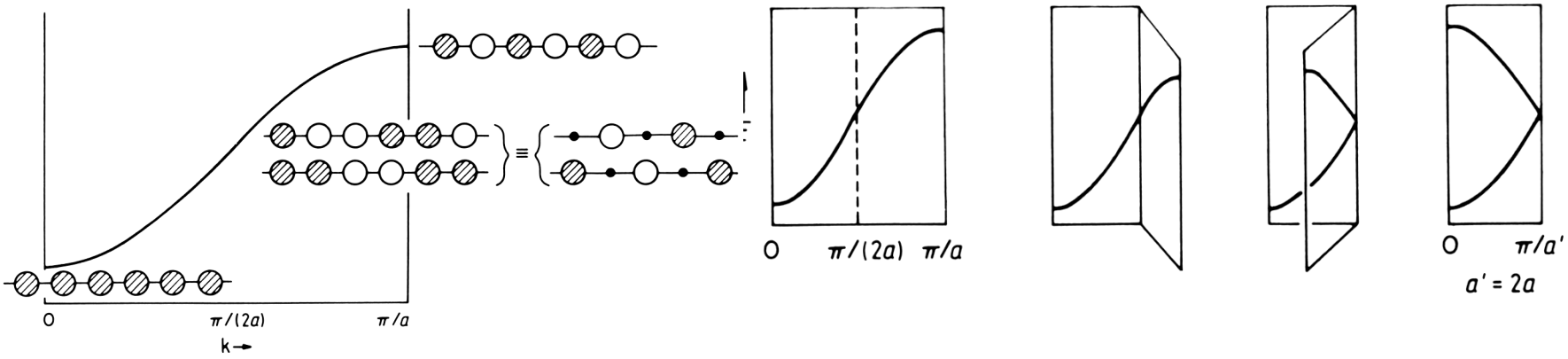
$\Psi_{\frac{\pi}{a}} = \chi_0 - \chi_1 + \chi_2 - \chi_3 + \ldots$

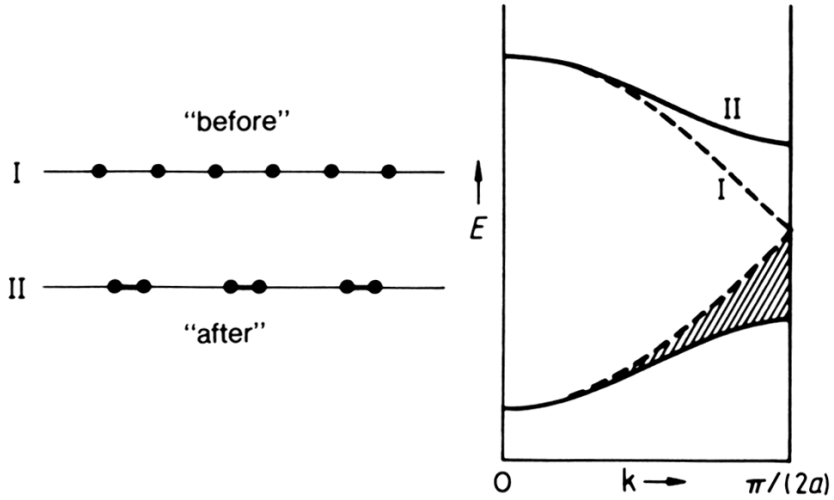


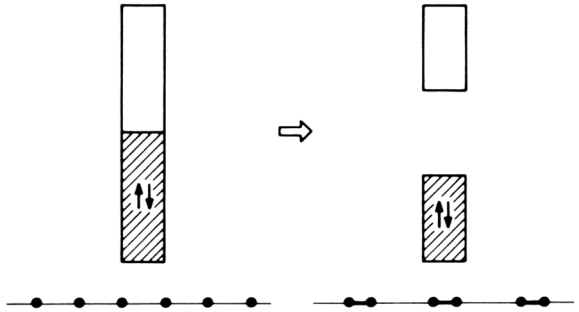
k = 0 antibonding interaction ⇒ band runs „downhill“

Hoffmann Angewandte. Chem. 26 (1987) 846

Why is Hydrogen a molecule



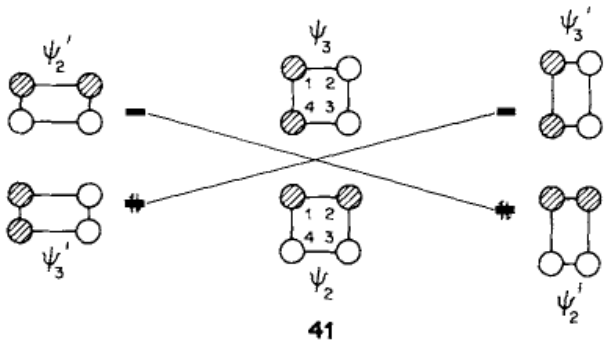


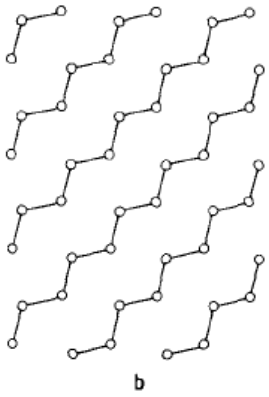


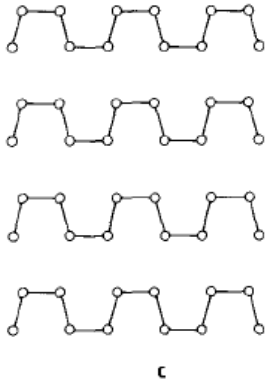
Peierls Distortion

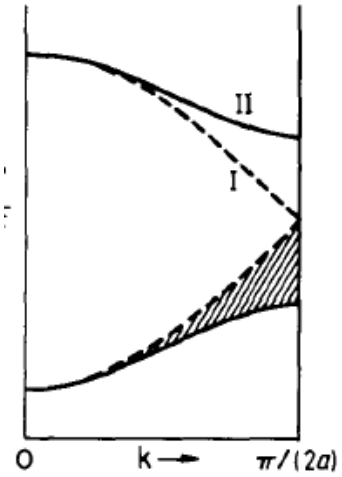
Hoffmann Angewandte. Chem. 26 (1987) 846

Square nets







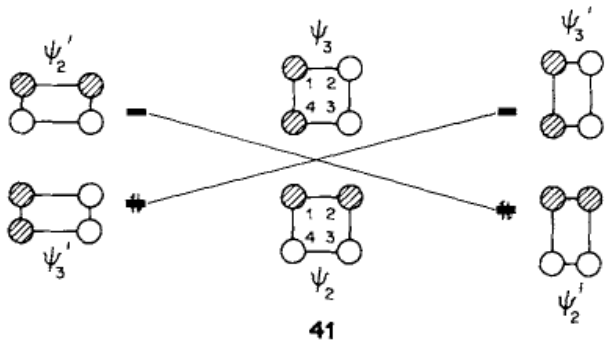


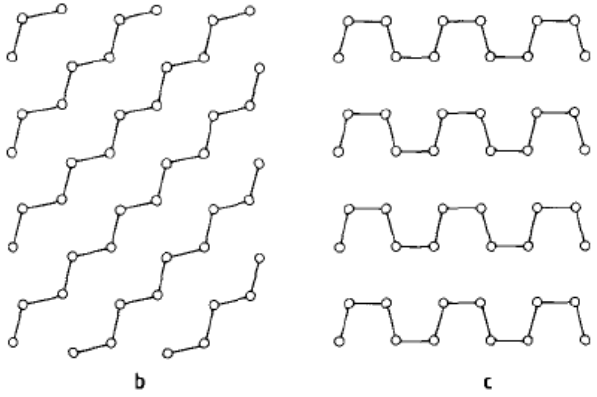
Square Nets of Main Group Elements in Solid-State Materials

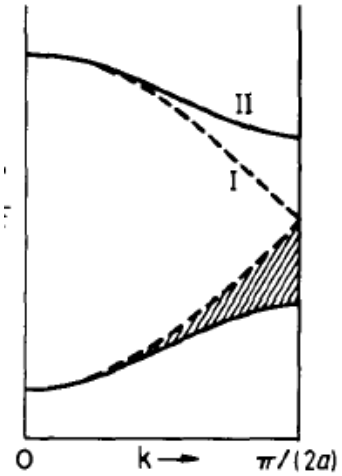
Wolfgang Tremel[1] and Roald Hoffmann*

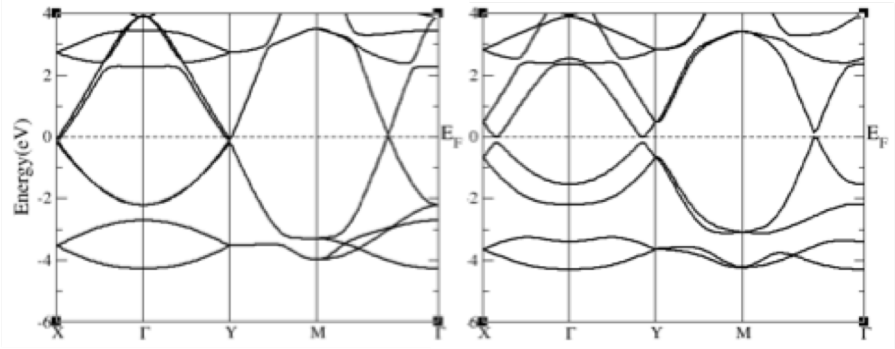
Contribution from the Department of Chemistry and Materials Science Center, Cornell University, Ithaca, New York 14853. *Received May 29, 1986*

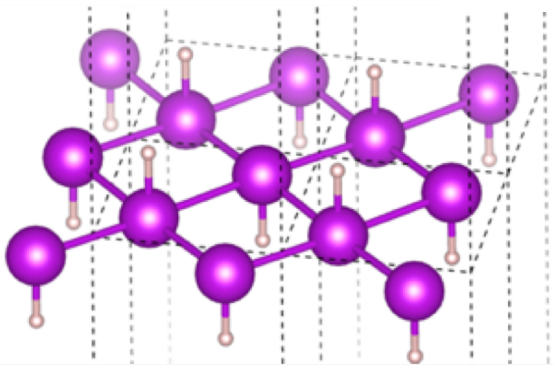
Square nets of electron doped Bi











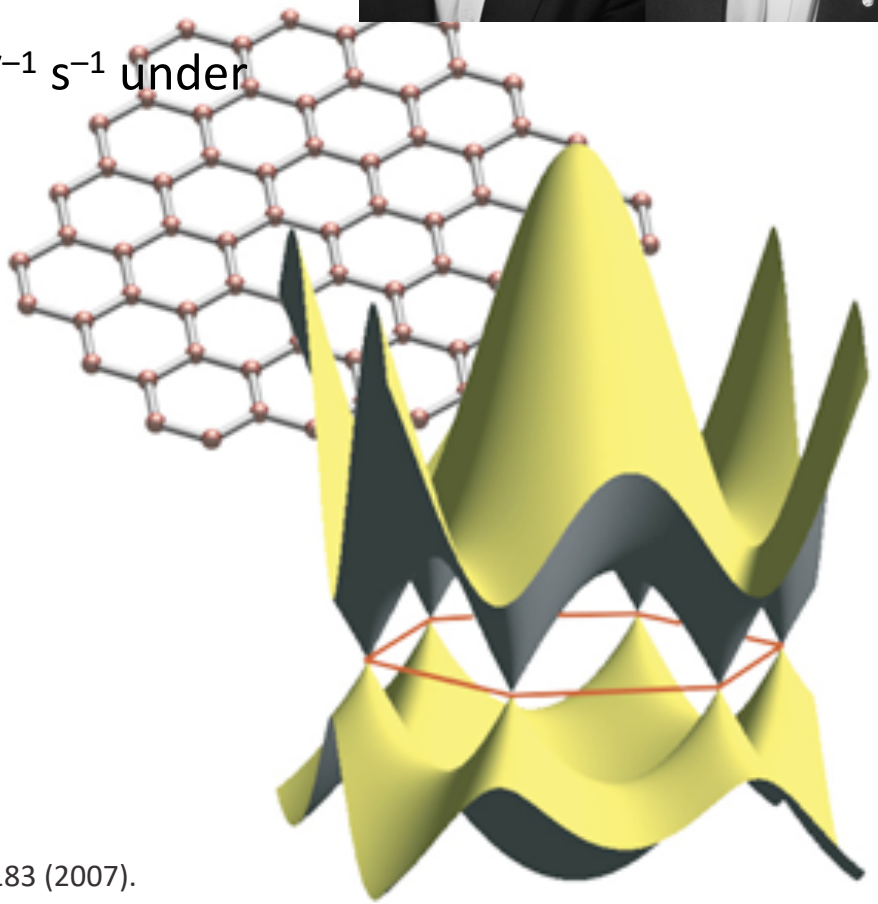
- Neither the valence nor conduction bands form a band representation -> topological (in this case, 2d QSH)

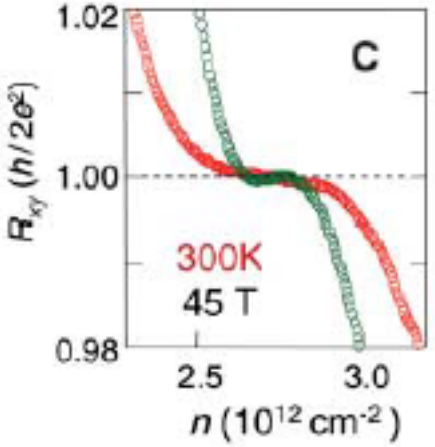
- Group 129, 139

Barry Bradlyn, L. Elcoro, Jennifer Cano, M. G. Vergniory, Zhijun Wang, C. Felser, M. I. Aroyo, B. Andrei Bernevig, Nature (2017)

Graphene

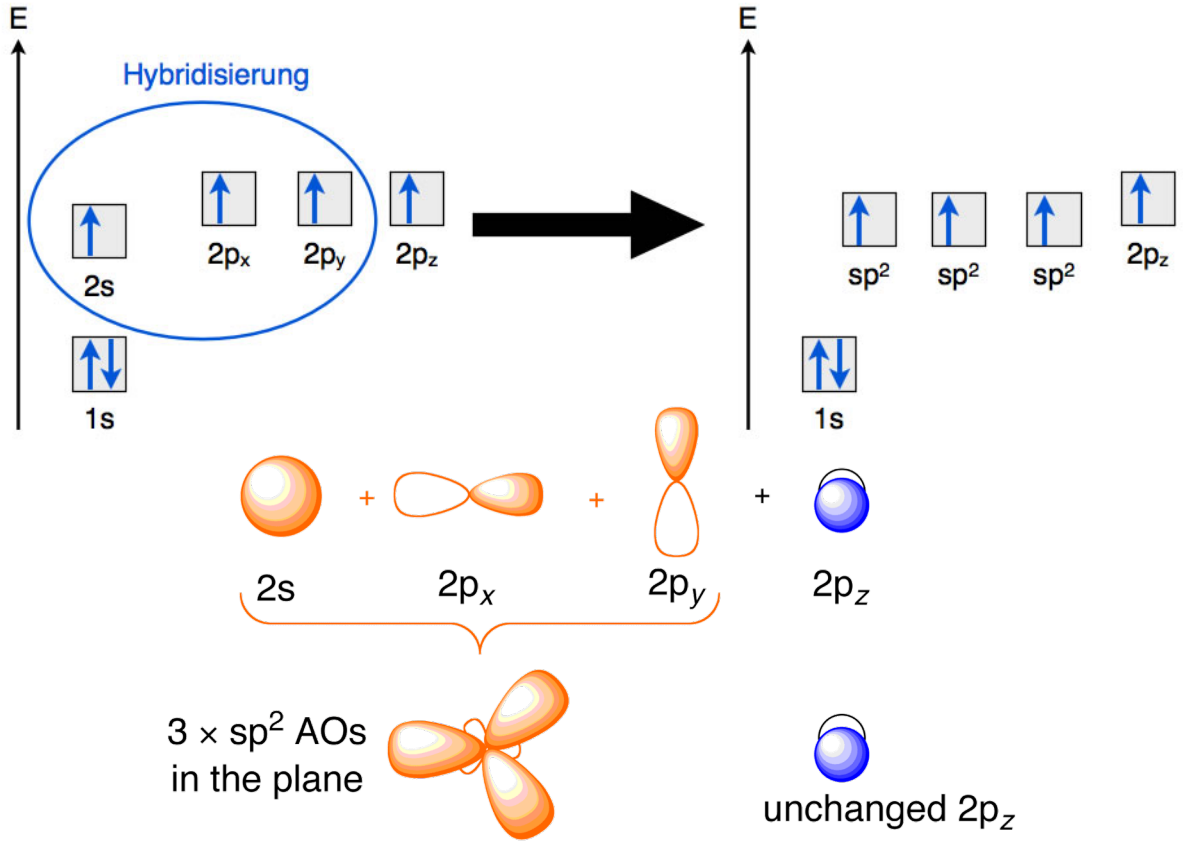
- Graphene's conductivity exhibits values close to the conductivity quantum e2/h per carrier type
- Graphene's charge carriers can be tuned continuously between electrons and holes in concentrations n = 10^{13} cm^{-2}
- Mobilities μ can exceed 15,000 cm^2 V^{-1} s^{-1} under ambient conditions
- InSb has μ ≈77,000 cm^2 V^{-1} s^{-1}

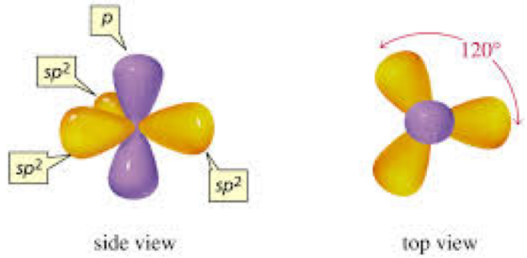


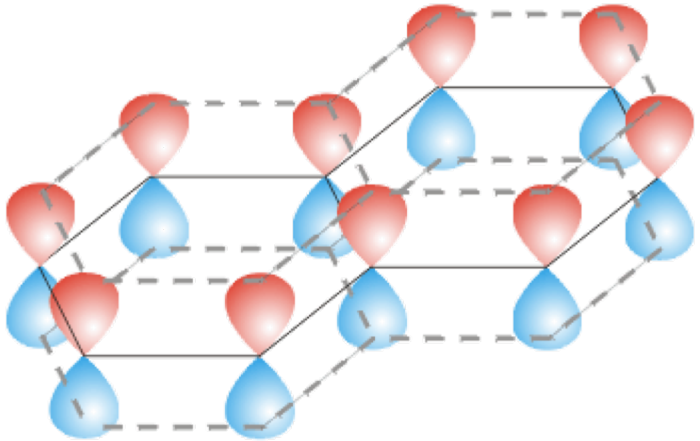


Geim, A. K. & Novoselov, K. S. The rise of graphene. Nature Mater. 6, 183 (2007).

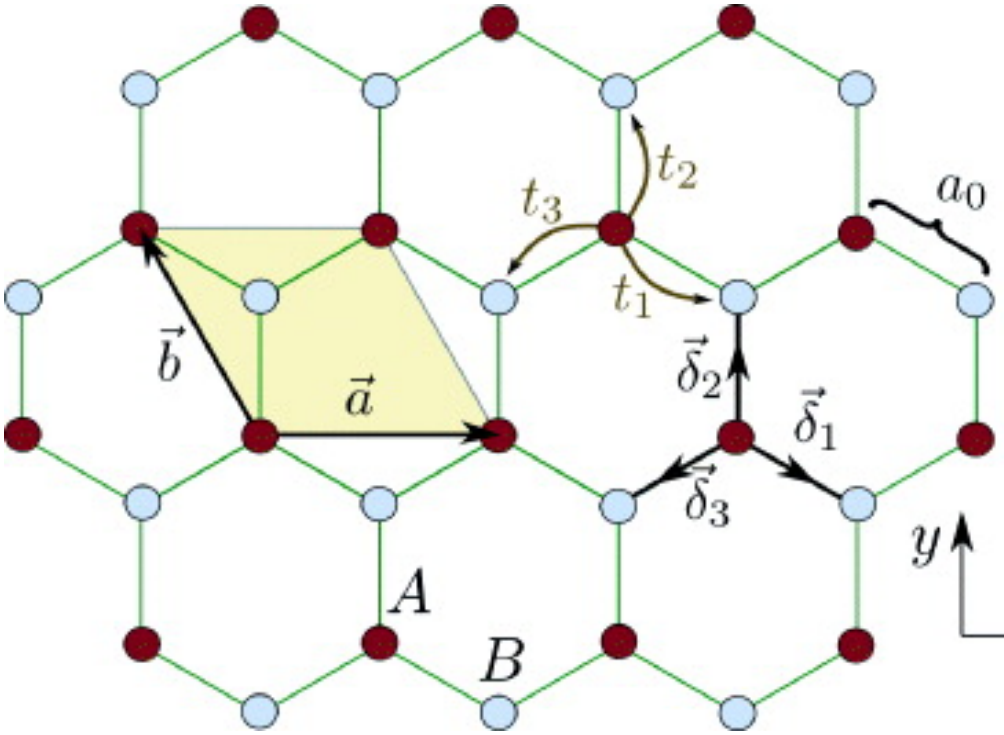
sp^2-Hybrid

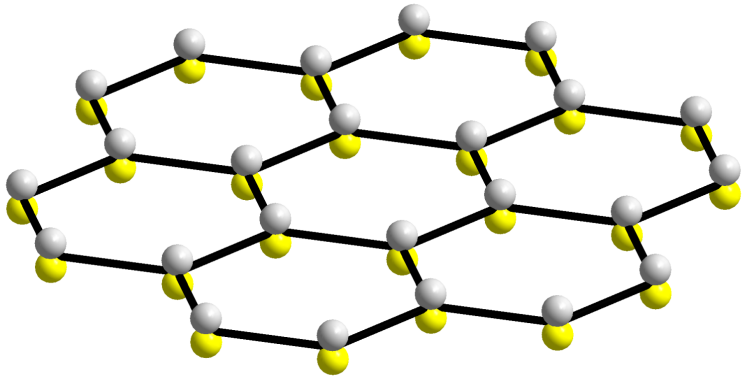


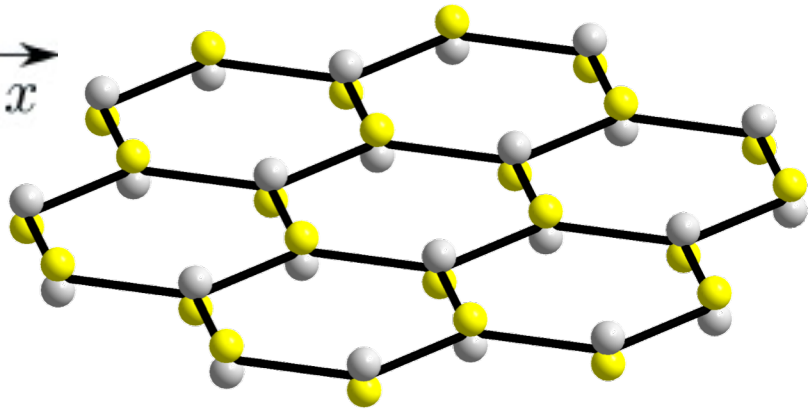




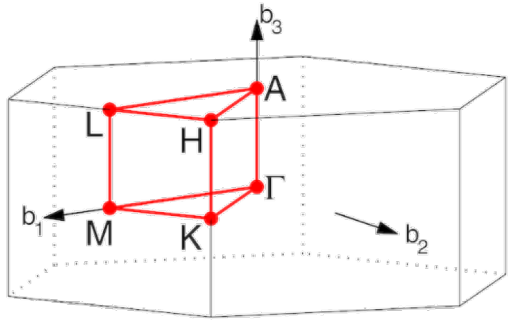
Graphene

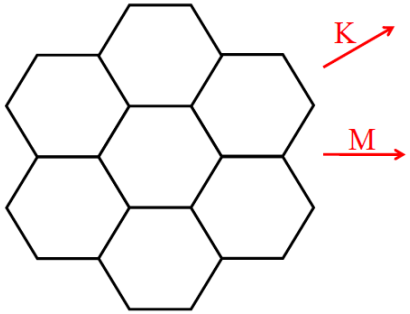

t_2
t_3
a_0
t_1
$\vec{b}$
$\vec{a}$
$\vec{\delta}_2$
$\vec{\delta}_1$
$\vec{\delta}_3$
y
x
A
B





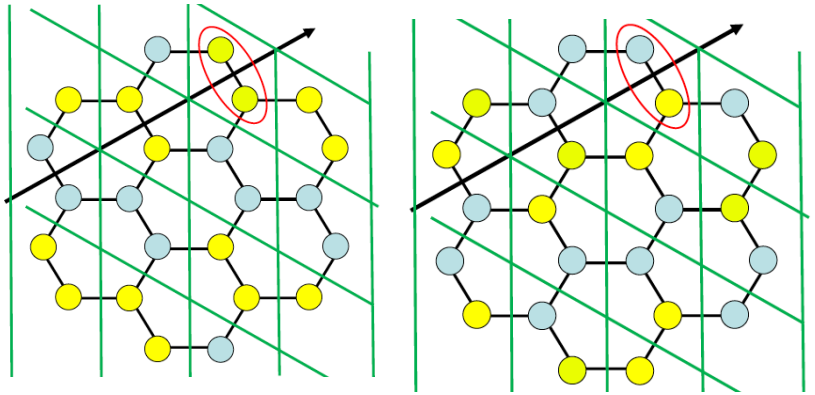
Graphene





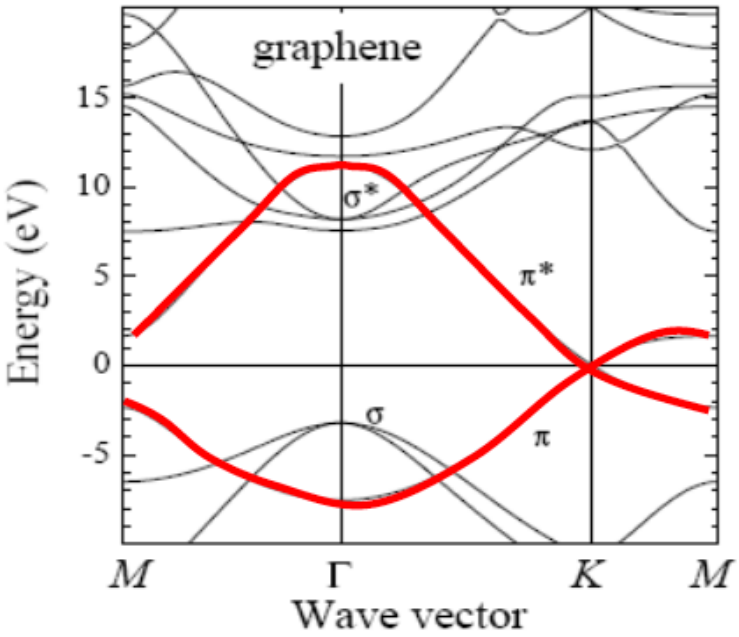
pz, π, K: non-bonding

pz, π*, K: non-bonding

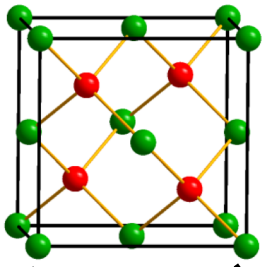


pz, π, M: bonding

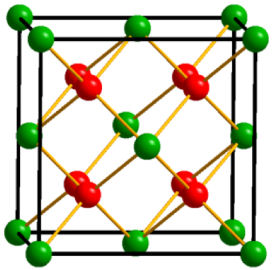
pz, π, M*: anti-bonding



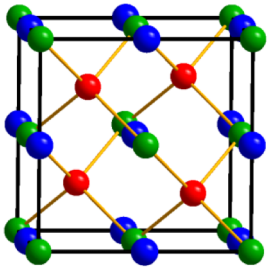
Structure to Property



HgTe

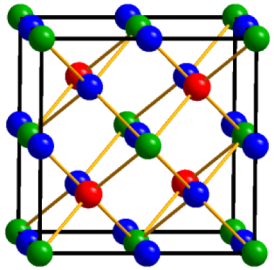


α Ag_2Te

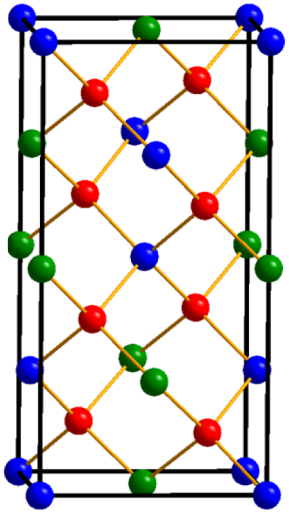


LaPtBi

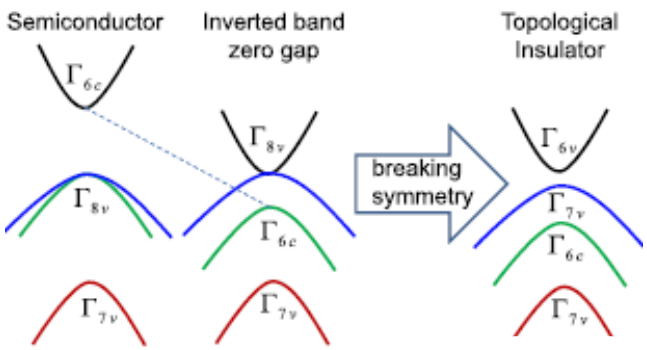
β Ag_2Te

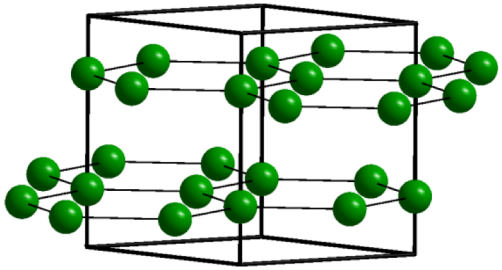


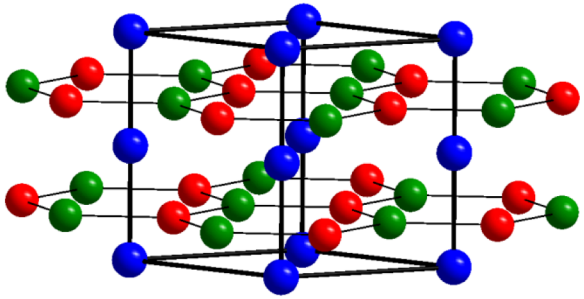
Li_2AgSb



$AuTlS_2$





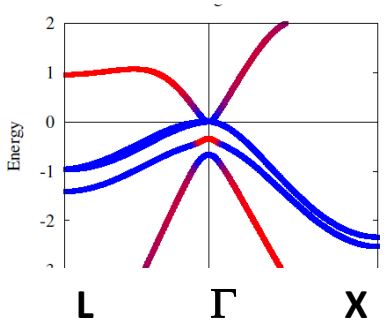


KHgSb

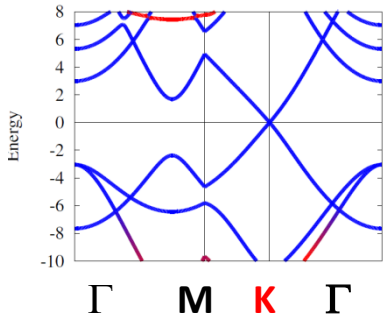
Müchler, et al., Angewandte Chemie 51 (2012) 7221.

Struktur und elektronische Struktur

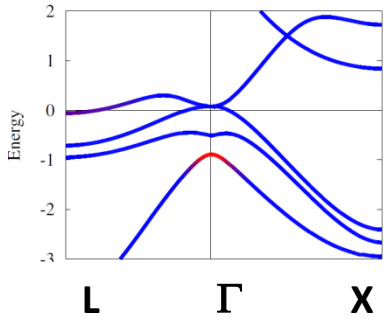
HgTe



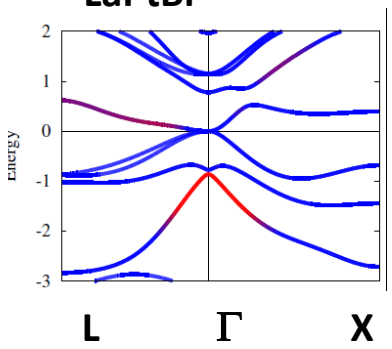
Graphite



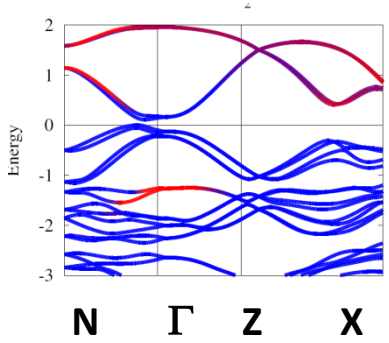
α Ag_2Te



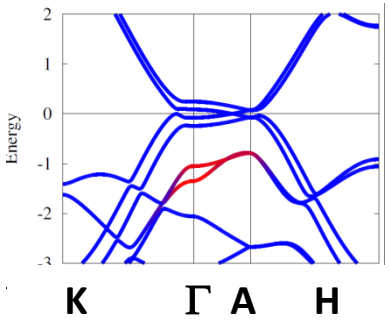
LaPtBi



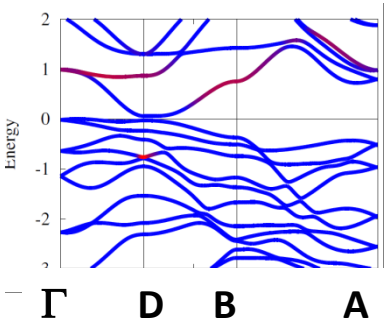
$AuTlTe_2$



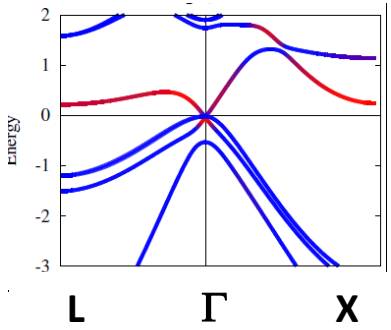
LiAuTe



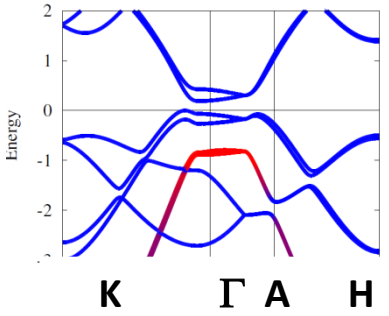
β Ag_2Te



Li_2AgSb



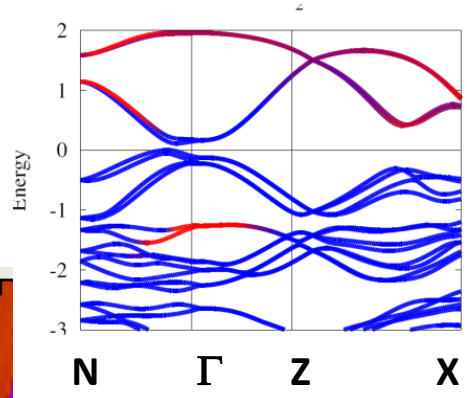
KHgSb

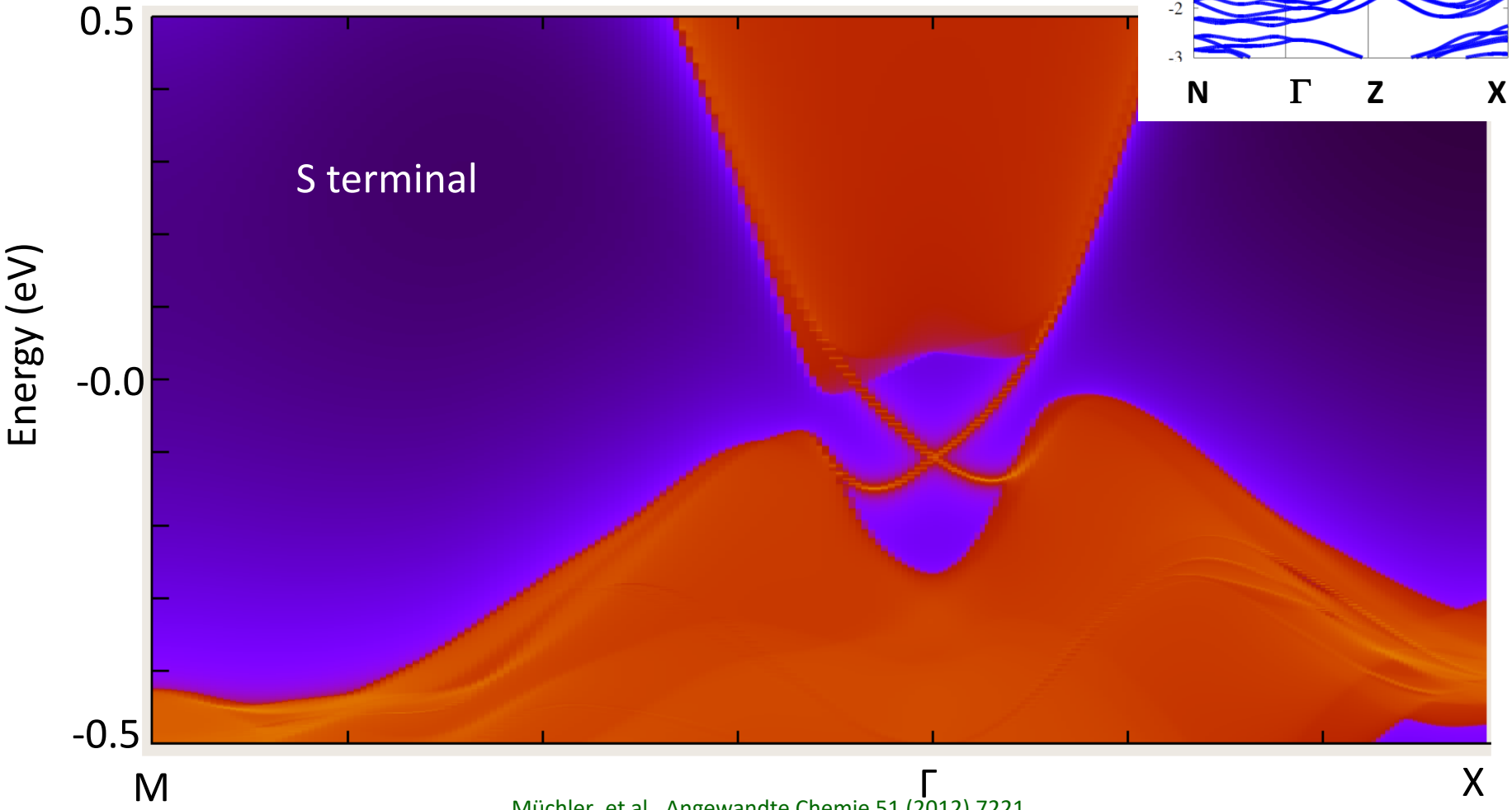


Müchler, et al., Angewandte Chemie 51 (2012) 7221.

Structure and electronic structure

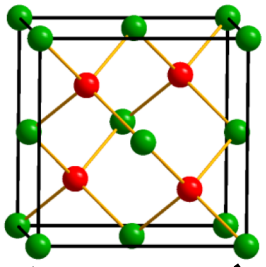
$AuTlTe_2$



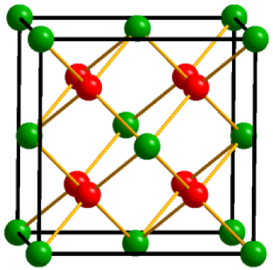


Müchler, et al., Angewandte Chemie 51 (2012) 7221.

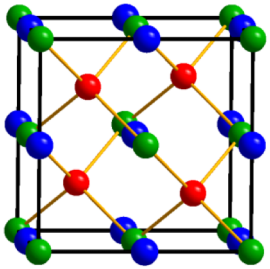
Structure to Property



HgTe

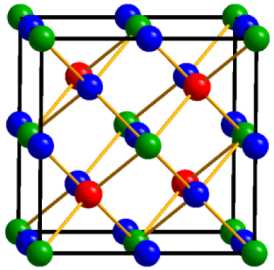


α Ag_2Te

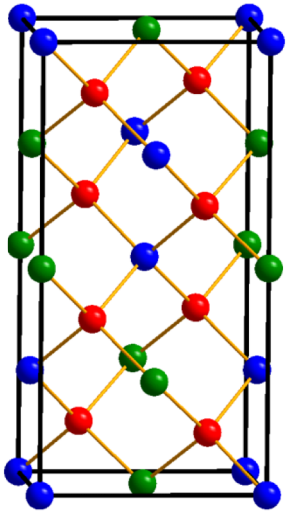


LaPtBi

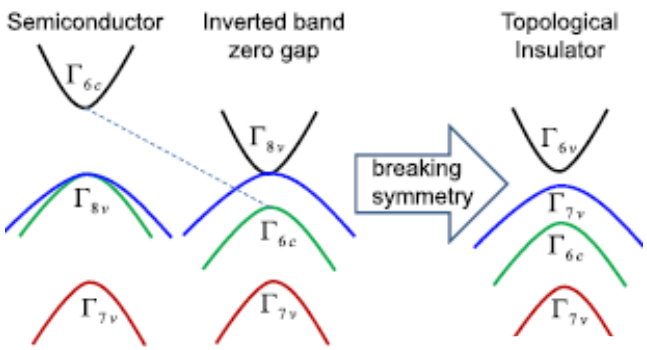
β Ag_2Te

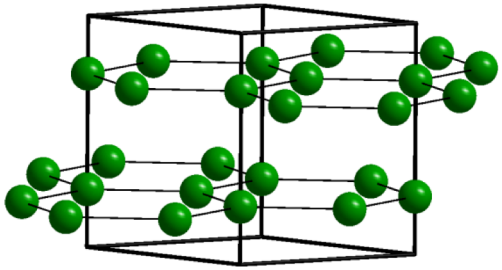


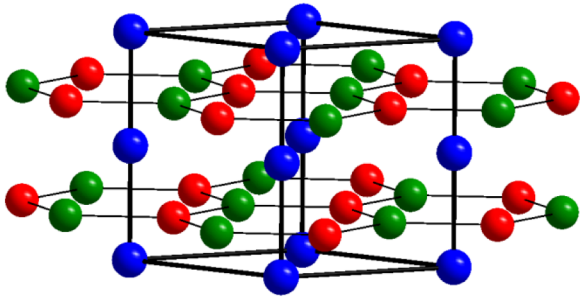
Li_2AgSb



$AuTlS_2$



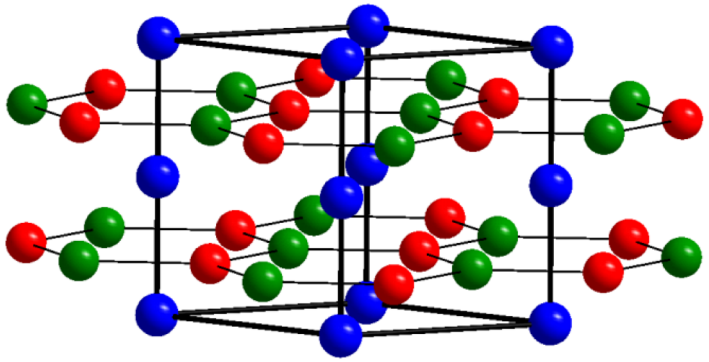


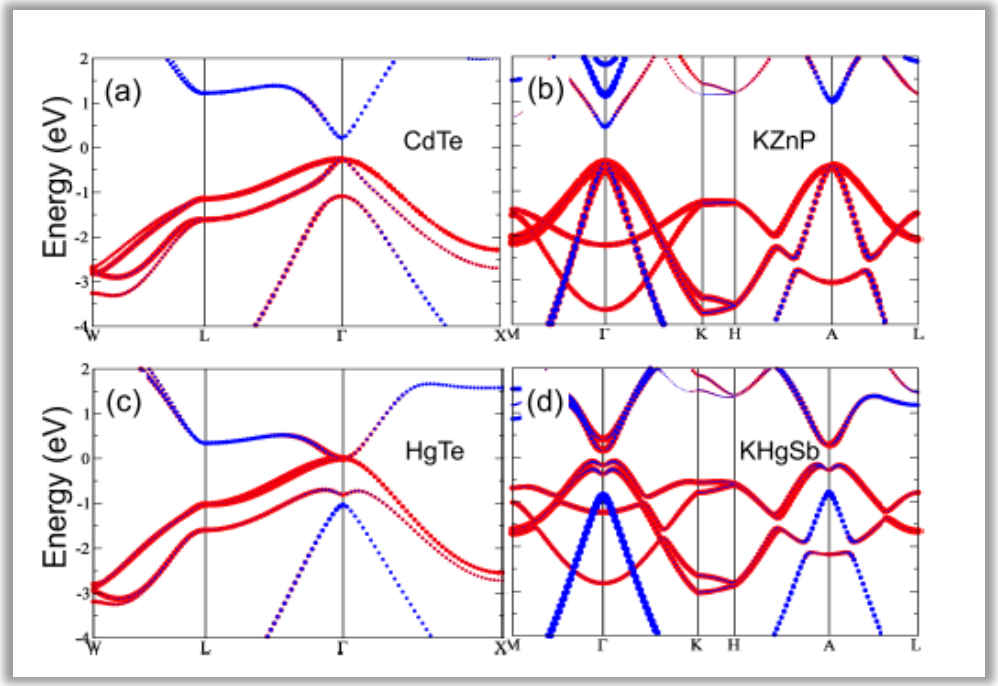


KHgSb

Müchler, et al., Angewandte Chemie 51 (2012) 7221.

Honeycomb from sp^3 to sp^2

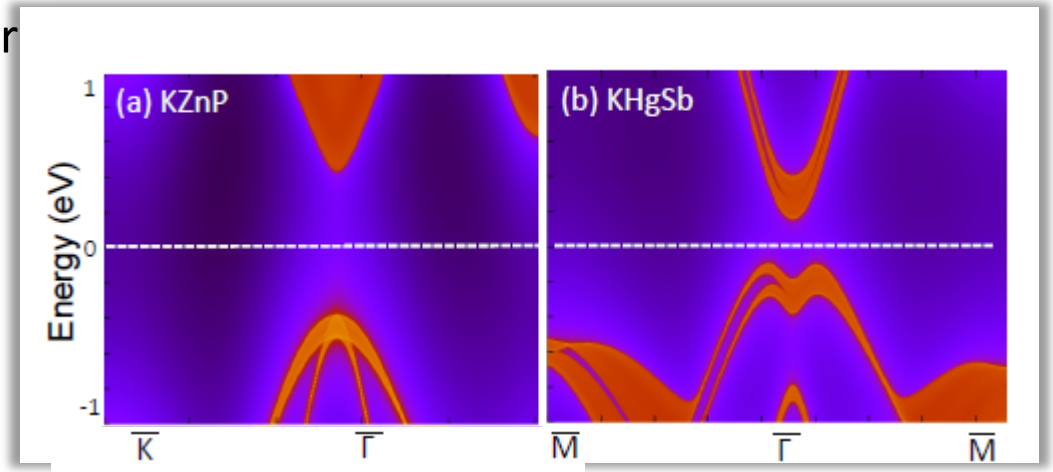




Band inversion is found in the heavier compounds

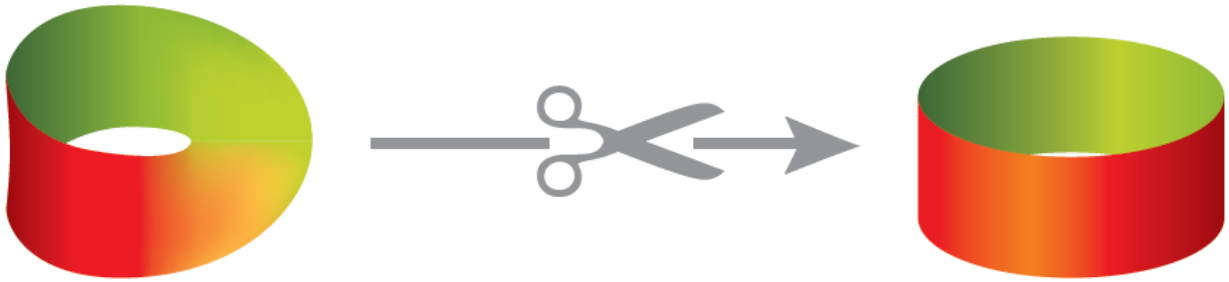
No surface state? Why ?

➡ Interaction between the two layers in the unit cell and two Dirac Cones

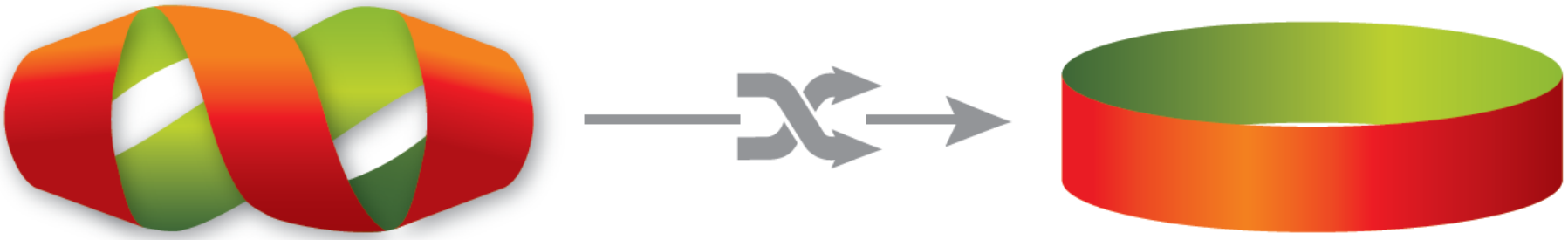


Zhang, Chadov, Müchler, Yan, Qi, Kübler, Zhang, Felser, Phys. Rev. Lett. 106 (2011) 156402 arXiv:1010.2195v1

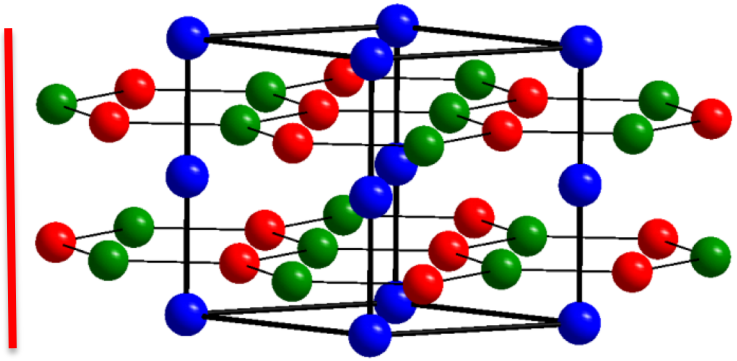
a)

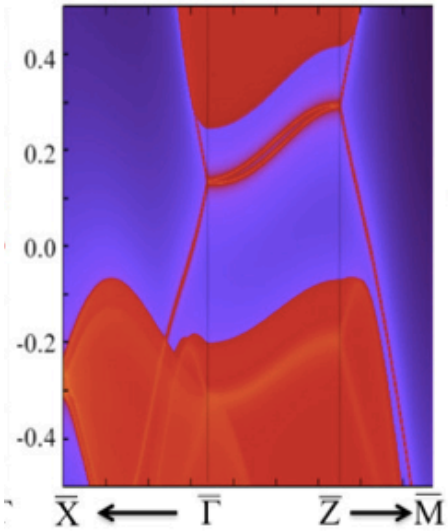


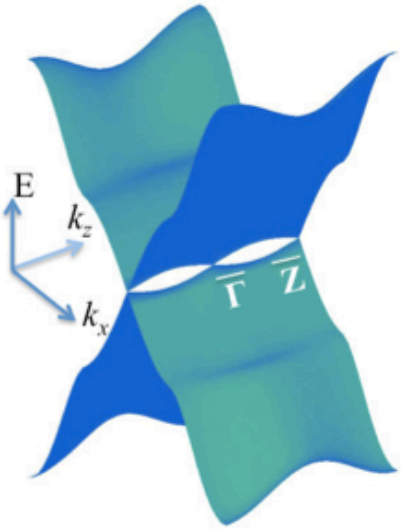
b)

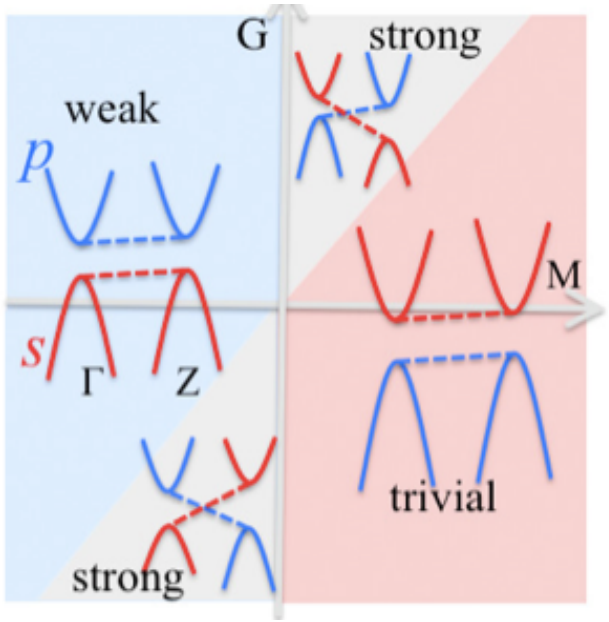


Honeycomb: Weak TI









KHgSb	KHgAs	KHgP
NaHgSb	NaHgAs	NaHgP
LiHgSb	LiHgAs	LiHgP
KCdSb	KCdAs	KCdP
NaCdSb	NaCdAs	NaCdP
LiCdSb	LiCdAs	LiCdP

KAuTe	KAuSe
NaAuTe	NaAuSe
LiAuTe	LiAuSe
KAgTe	KAgSe
NaAgTe	NaAgSe
LiAgTe	LiAgSe

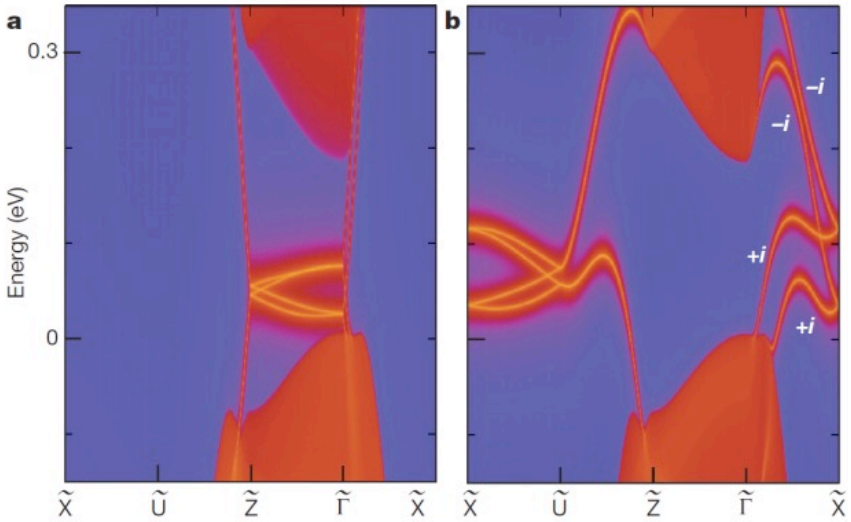
Yan, Müchler, Felser, Physical Review Lett. 109 (2012) 116406

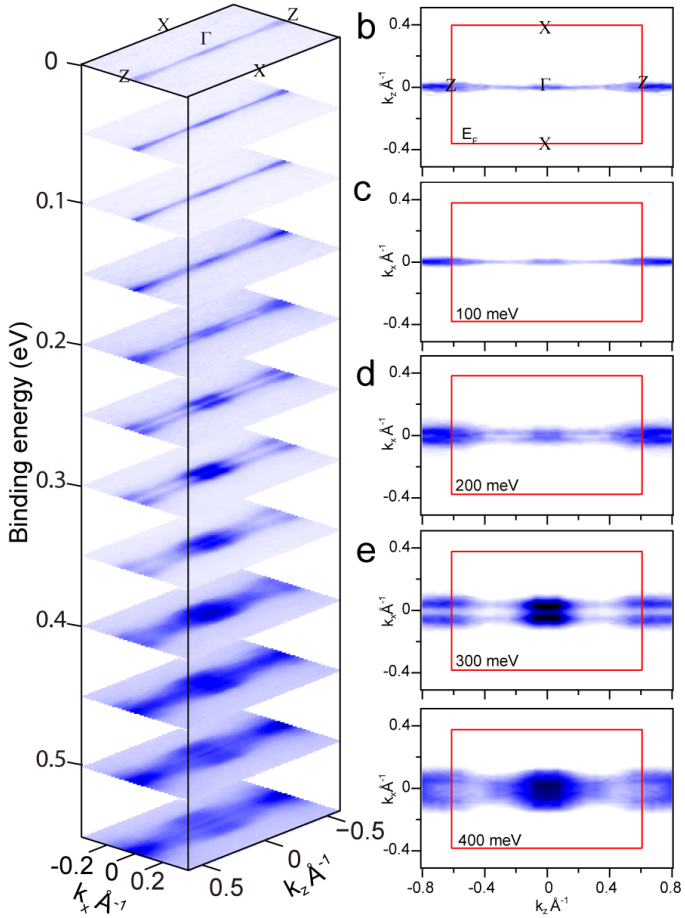
Hourglass

ARTICLE

Hourglass fermions

Zhijun Wang[1]*, A. Alexandradinata[1,2]*, R. J. Cava[3] & B. Andrei Bernevig[1]





Wang et al. Nature 2016

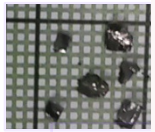
unpublished results

Topology – interdisciplinary

Chemistry

Real space - local

Crystals



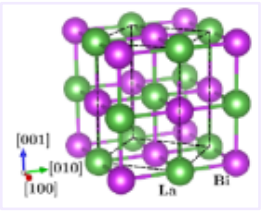
LaBi

Physics

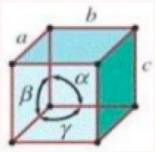
Recipro. space - delocalized

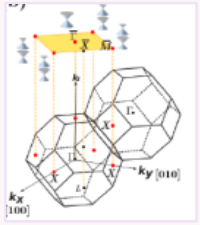
Brillouin zone

Crystal structure

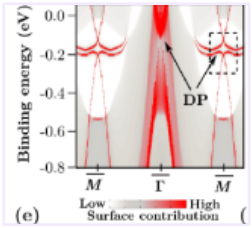


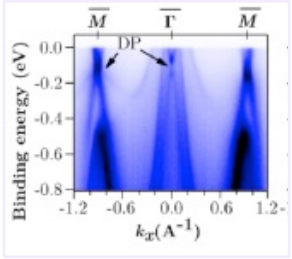
Symmetry





Electronic structure

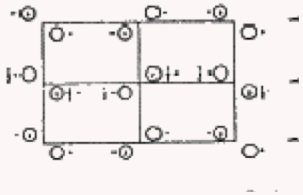




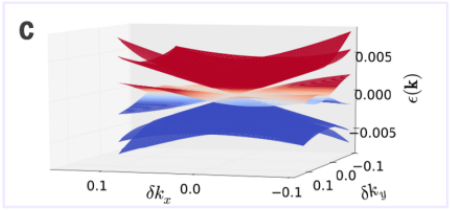
Position of the atoms

Check	WP	Representative
☐	8g	x,y,z
☐	4f	x,1/2,z
☐	4e	x,0,z
☑	4d	x,x,z
☑	2c	1/2,0,z
☐	1b	1/2,1/2,z
☑	1a	0,0,z

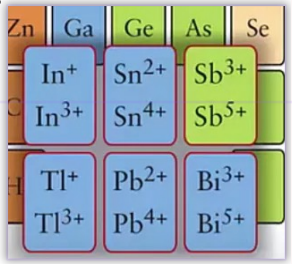
Local symmetry



Band connectivity



Inert pair effect



Relativistic effects

Dirac equation,Darwin term

$$H_{\text{Darwin}} = \frac{\hbar^2}{8m_e^2c^2}(\Delta V)$$

Barry Bradlyn, L. Elcoro, Jennifer Cano, M. G. Vergniory, Zhijun Wang, C. Felser, M. I. Aroyo, B. Andrei Bernevig, Nature (2017)

Topological Metals

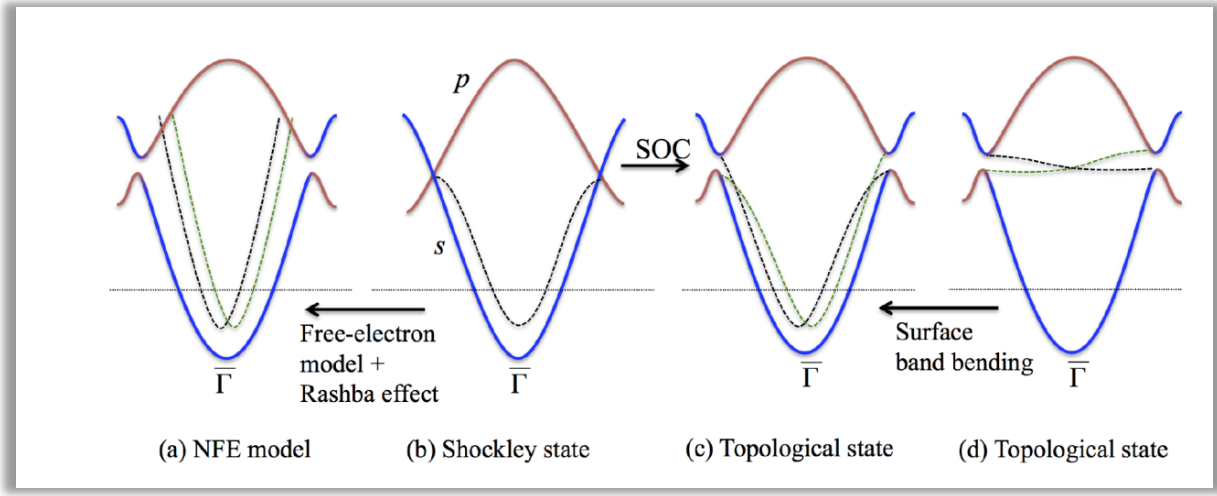
Rewriting the text book: Au

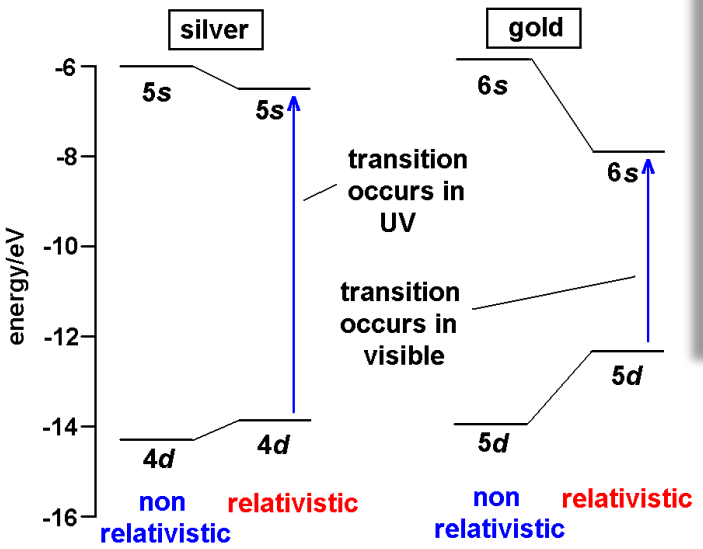
AUGUST 15, 1939 PHYSICAL REVIEW VOLUME 56

On the Surface States Associated with a Periodic Potential

WILLIAM SHOCKLEY
Bell Telephone Laboratories, New York, New York

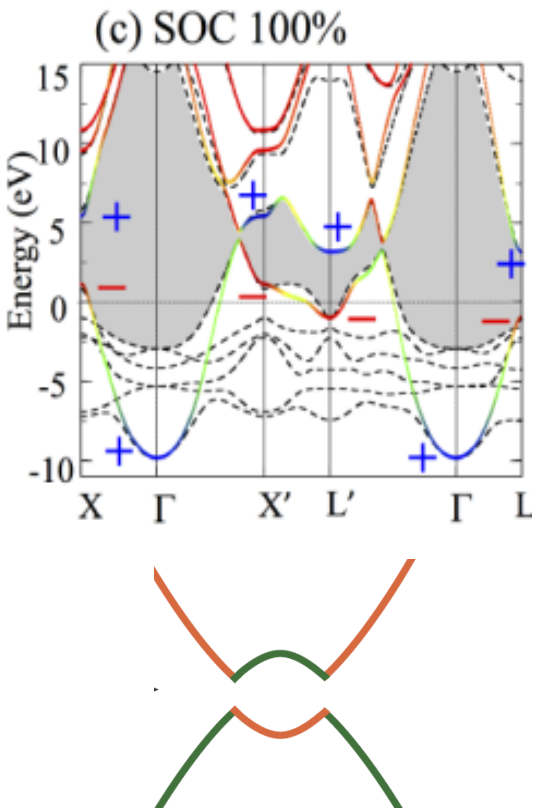
(Received June 19, 1939)

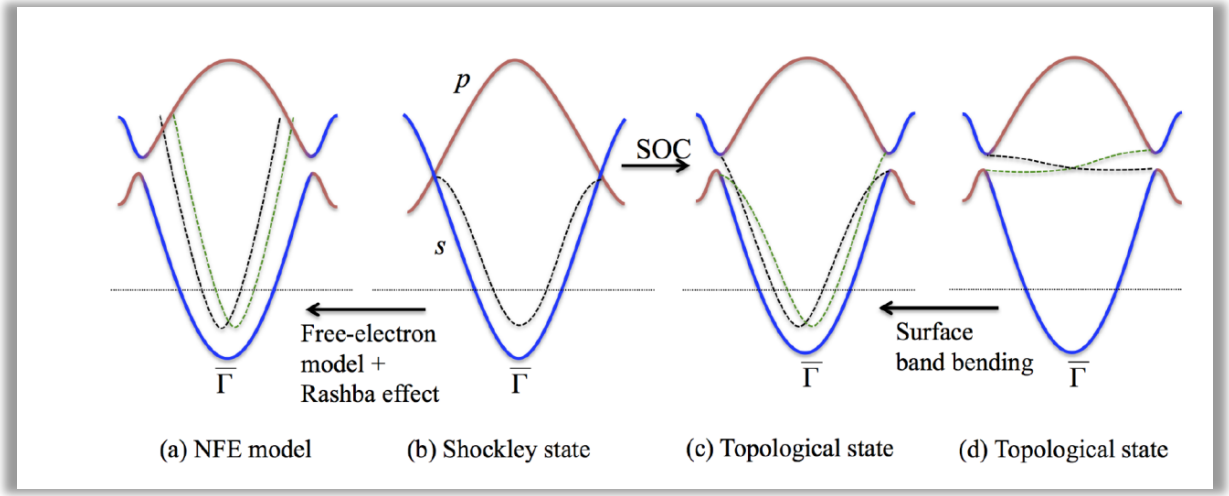


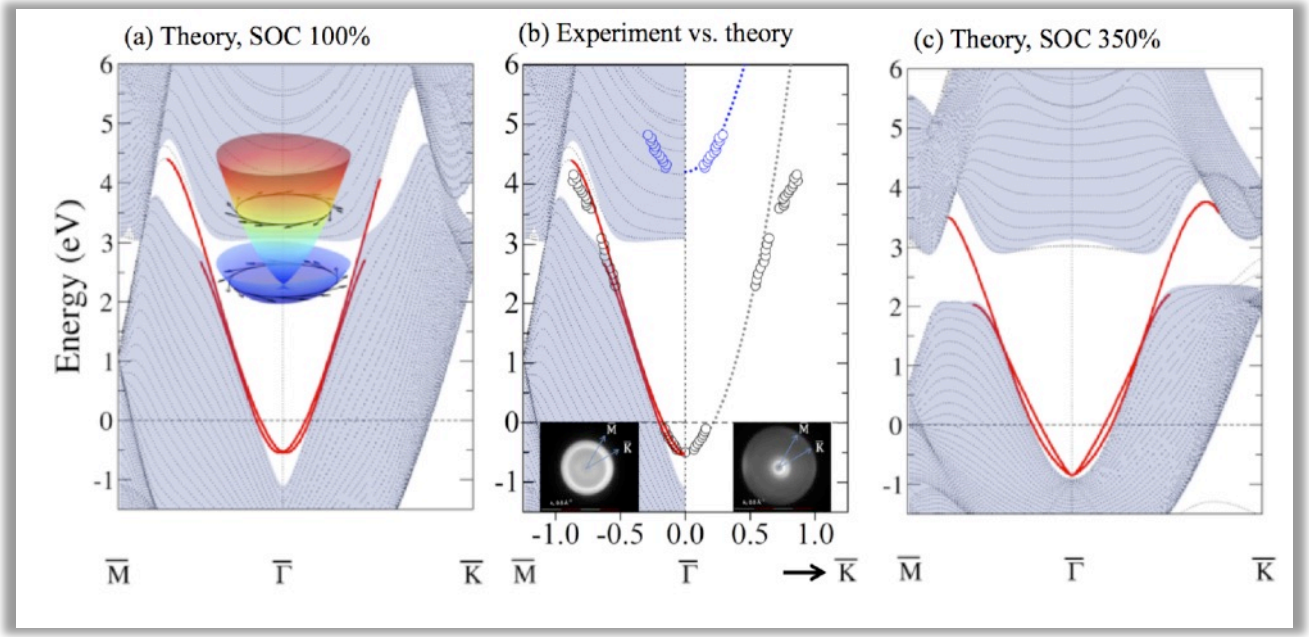


Binghai Yan at al., Nature Communication 6 (2015) 10167

Rewriting the text book: Au







$Cs^{+}Au^{-}$

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

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†

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

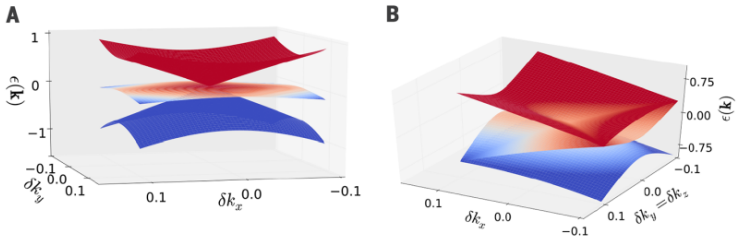
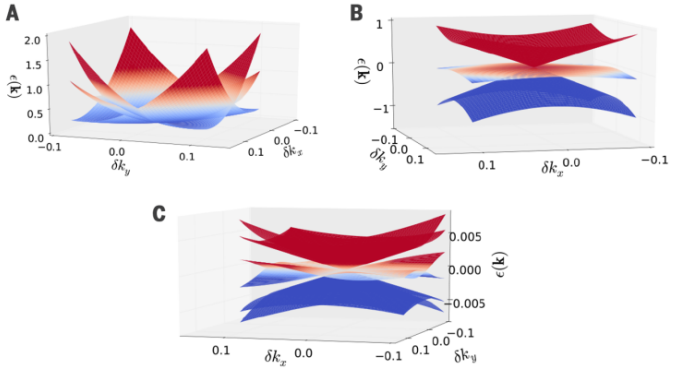
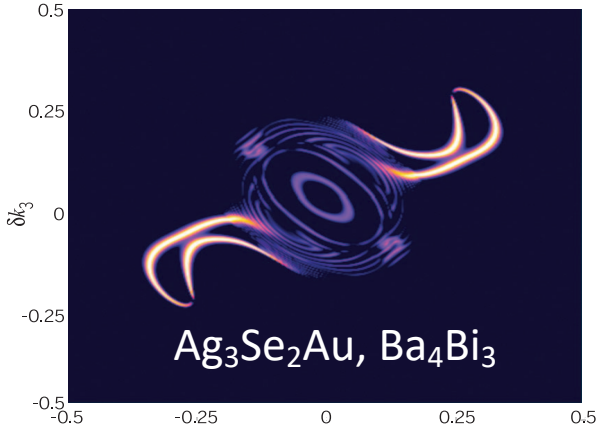


Fig. 1. Energy dispersion near a threefold degeneracy at the *P* point. (**A** and **B**) Shown are threefold degenerate points in (A) SGs 199 and 214 and (B) SG 220. In the latter case, pairs of bands remain degenerate in energy along the high-symmetry lines $|\delta k_x| = |\delta k_y| = |\delta k_z|$.





Science, 353, 6299, (2016)

Universe – applying a lattice

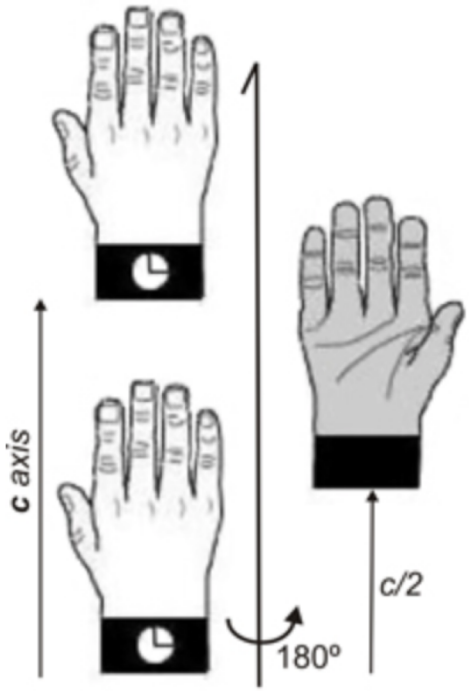
Bringing order to the expanding fermion zoo

Carlo Beenakker Commentary

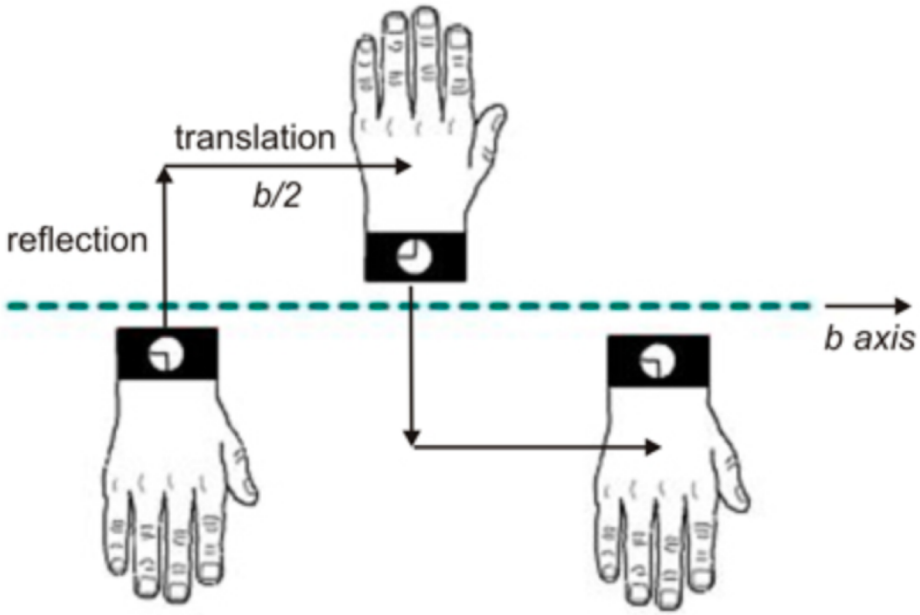
Heisenberg (1930): We observe space as a continuum, but we might entertain the thought that there is an underlying lattice and that space is actually a crystal. Which particles would inhabit such a lattice world? Werner Heisenberg *Gitterwelt* (lattice world) hosted electrons that could morph into protons,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

Non symmorphic crystal structures

•non-symmorphic: elements with *fractional lattice translations*

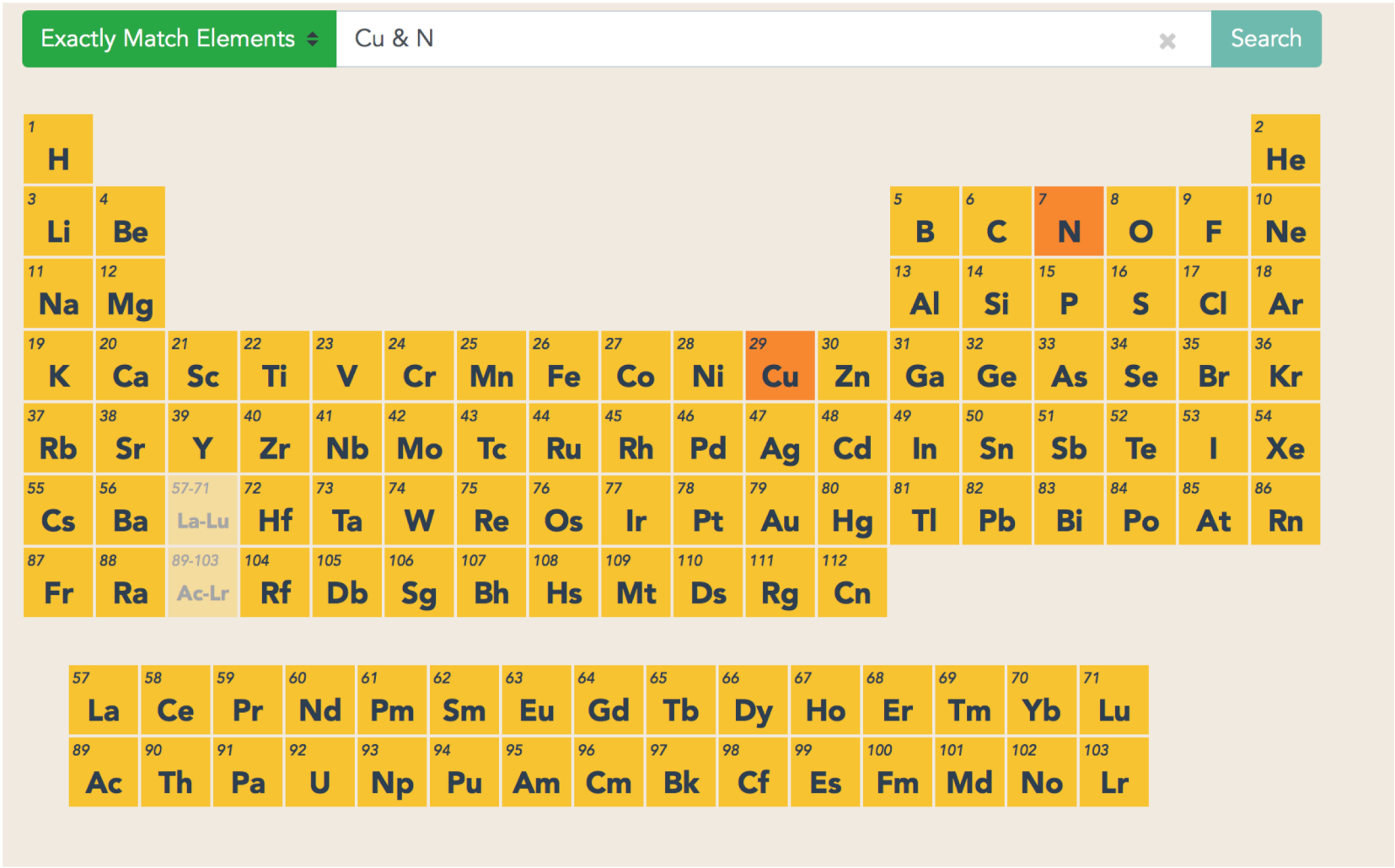


Twofold screw axis.
A screw axis consists of a rotation followed by a translation



Glide plane.
A glide plane consists of a reflection followed by a translation

http://materiae.iphy.ac.cn



Found 4 entries, showing 4

« ‹ 1 › »

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MAT00015330	$FeSi_2$	123	HSL_SM	TCI	0	0	View Details
MAT00022653	Fe_5Si_3	193	HSP_SM	HSL_SM	0	0	View Details
MAT00023895	FeSi	198	Triv_Ins	Triv_Ins	N/A	N/A	View Details