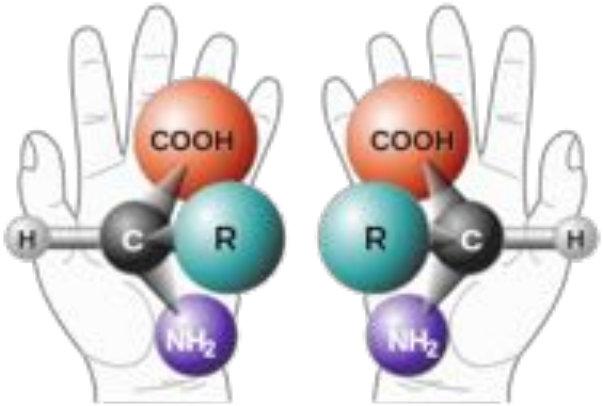
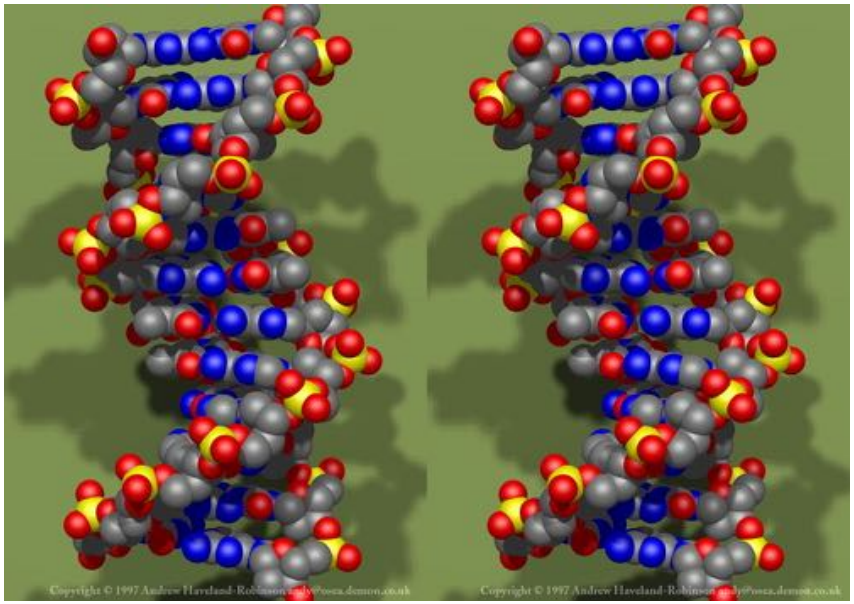
Topology: crystal structure and bands

Claudia Felser

Topology in Chemistry

Molecules with different chiralities can have different physical and chemical properties

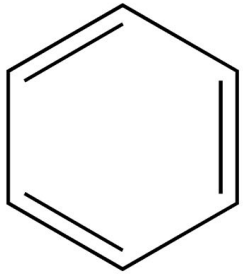


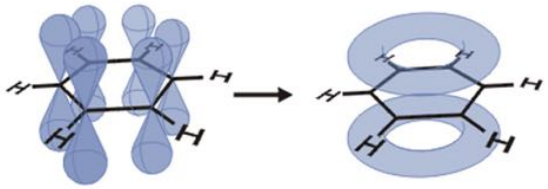


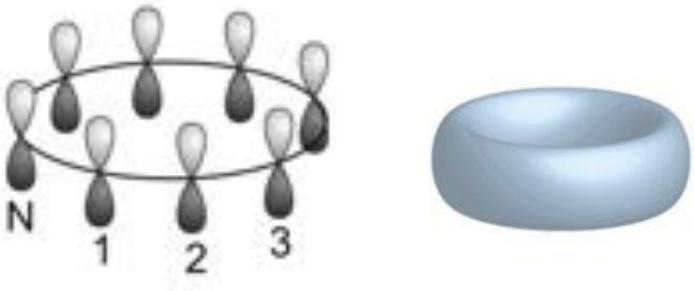
Topology in Chemistry

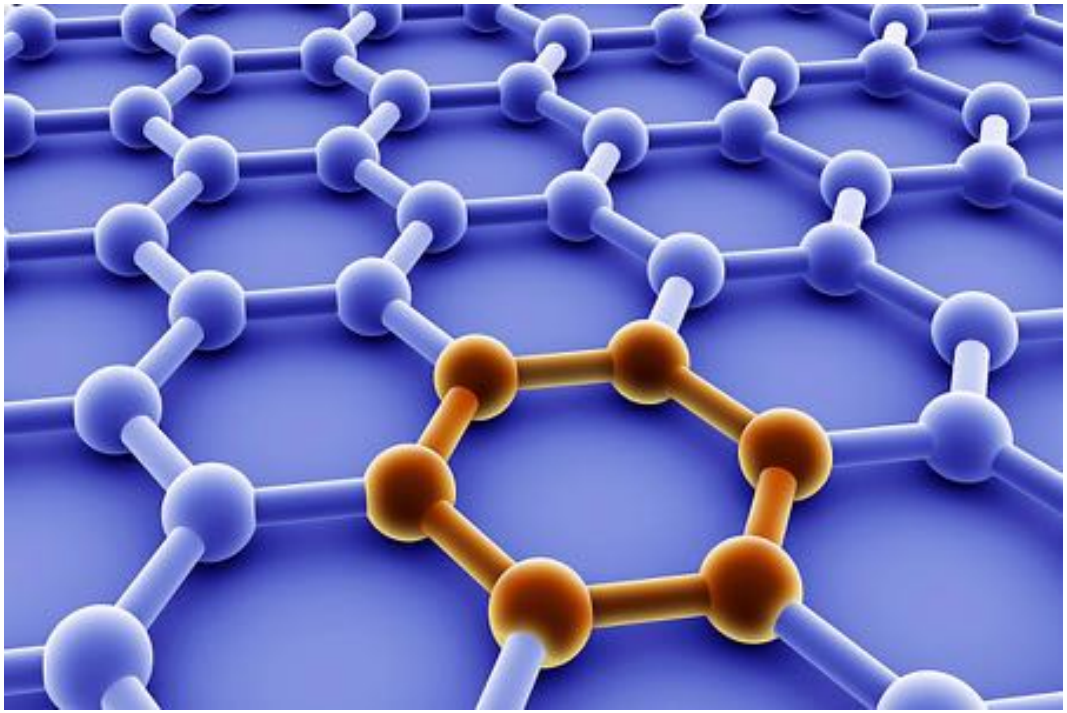
Aromatic compounds

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

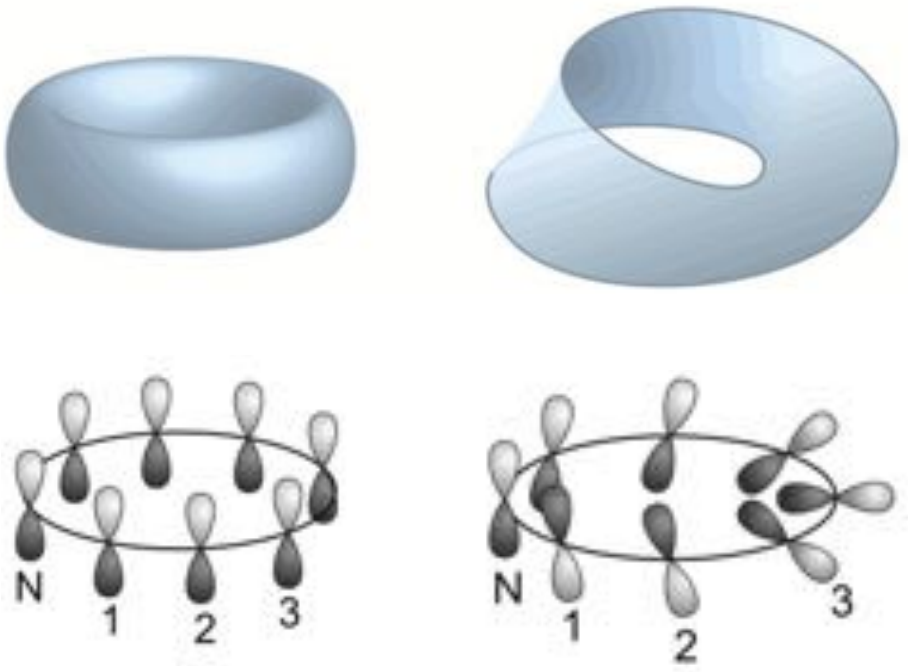








Topology in Chemistry

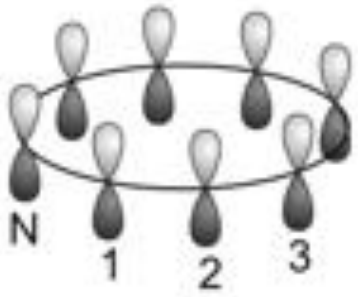


Magic electron numbers of π-electrons

Hückel:
4n+2 aromatic
4n antiaromatic

Möbius
4n aromatic
4n+2 antiaromatic

Hückel and Möbius Aromaticity



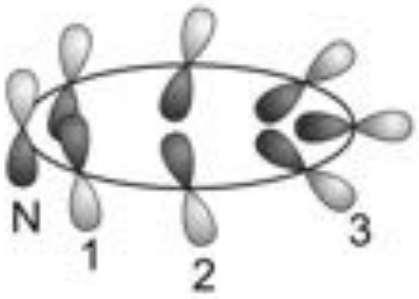
ORGANIC CHEMISTRY

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.

Möbius Annulenes



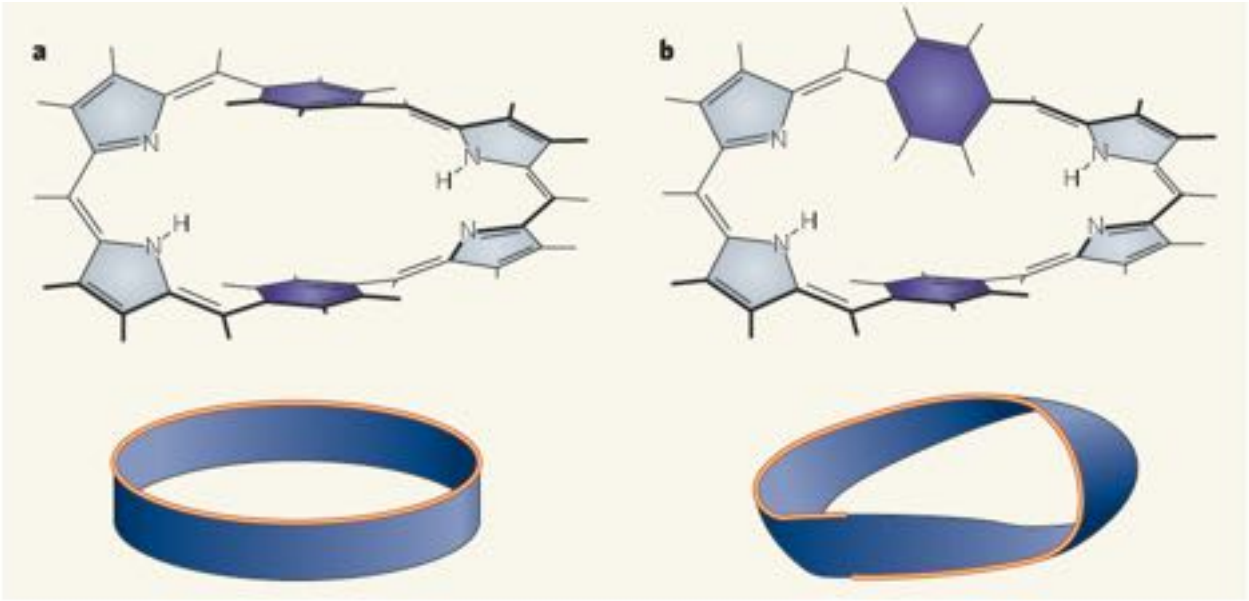
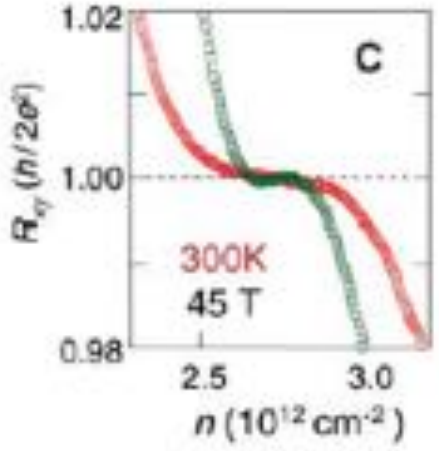
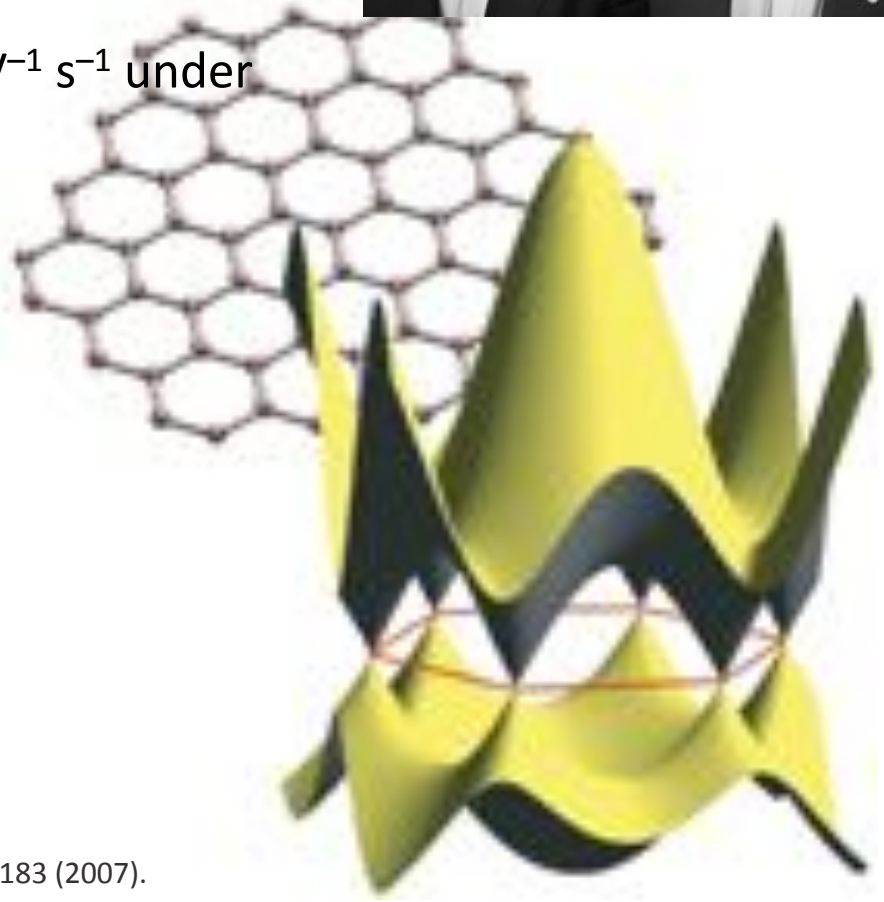


Figure 2 | A molecular topological switch. Latos-Grażyński and colleagues[1] have made a compound that is antiaromatic in nonpolar solvents, but not in polar solvents. **a**, In nonpolar solvents, the two benzene rings (purple) in the molecule are parallel, and the molecule is a two-sided, non-twisted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

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).

Topology – interdisciplinary

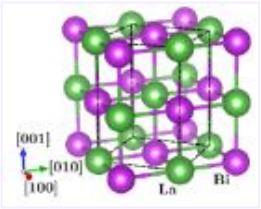
Chemistry

Real space - local

Crystals

LaBi

Crystal structure

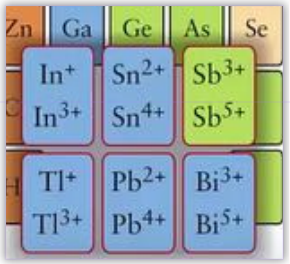


Position of the atoms

Orbitals

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

Inert pair effect

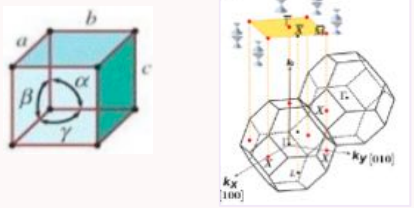


Physics

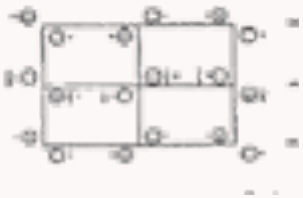
Recipro. space - delocalized

Brillouin zone

Symmetry

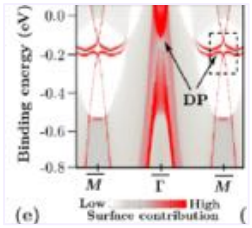


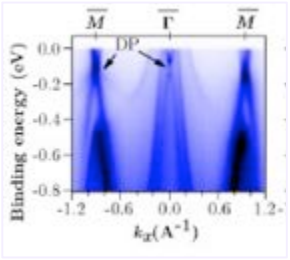
Local symmetry



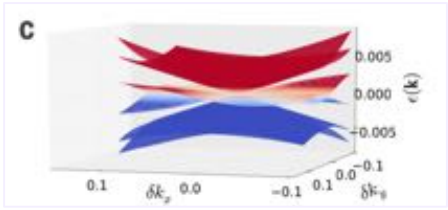
Relativistic effects

Electronic structure





Band connectivity

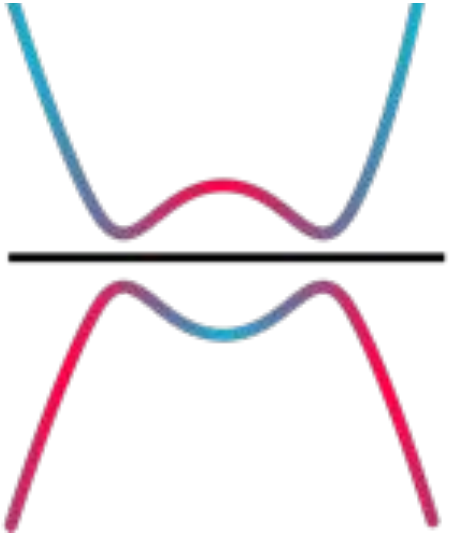


Darwin term

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

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

Topological Insulators

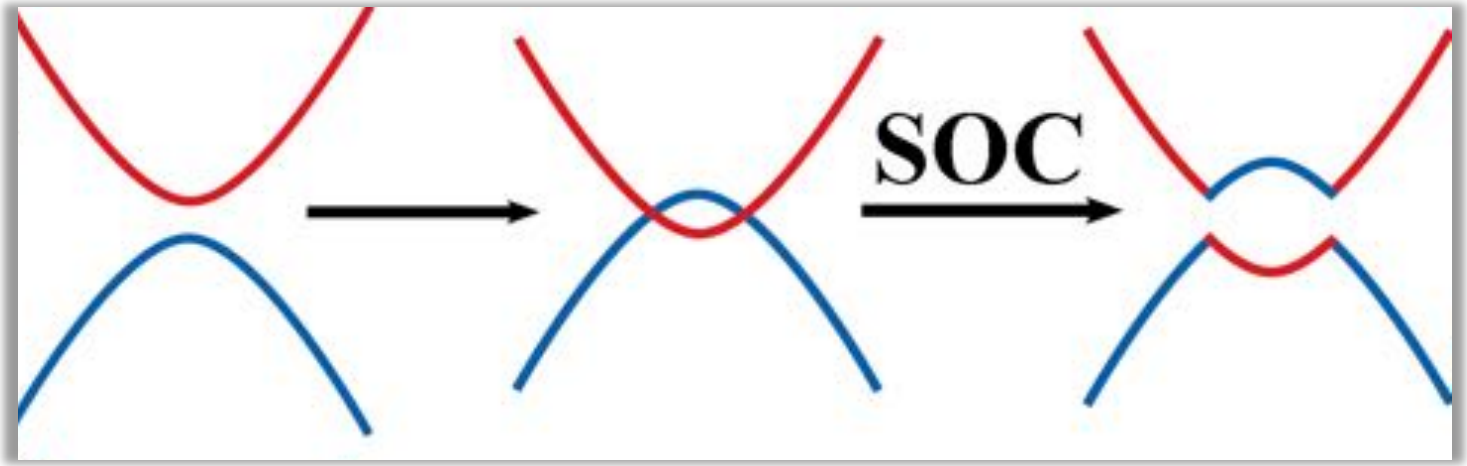


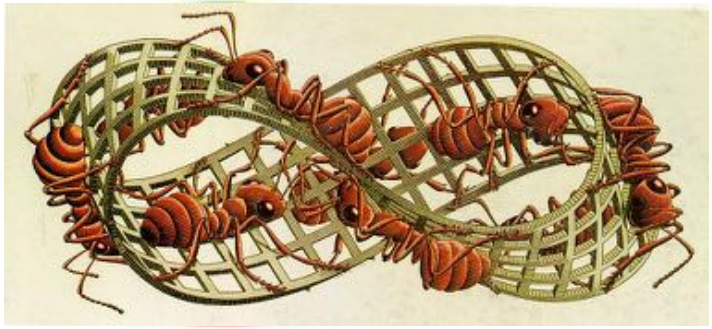
Trivial and Topological Insulators

Trivial semiconductor
CdS

Topological Insulator
Without spin orbit coupling

Topological Insulator
Withspin orbit coupling





M. C. Escher

Topological Insulators

Z_2 Topological Order and the Quantum Spin Hall Effect

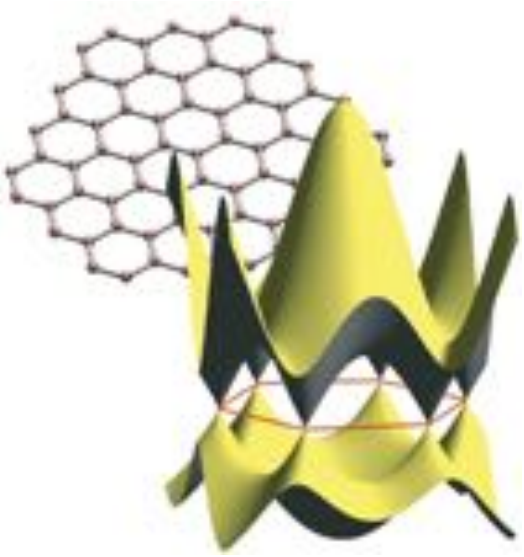
C. L. Kane and E. J. Mele

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



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?

No insulating element

Lets take 2 Elements

Topological Insulators

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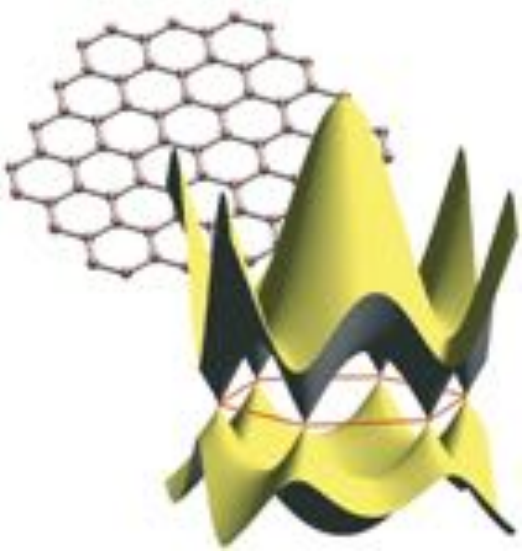
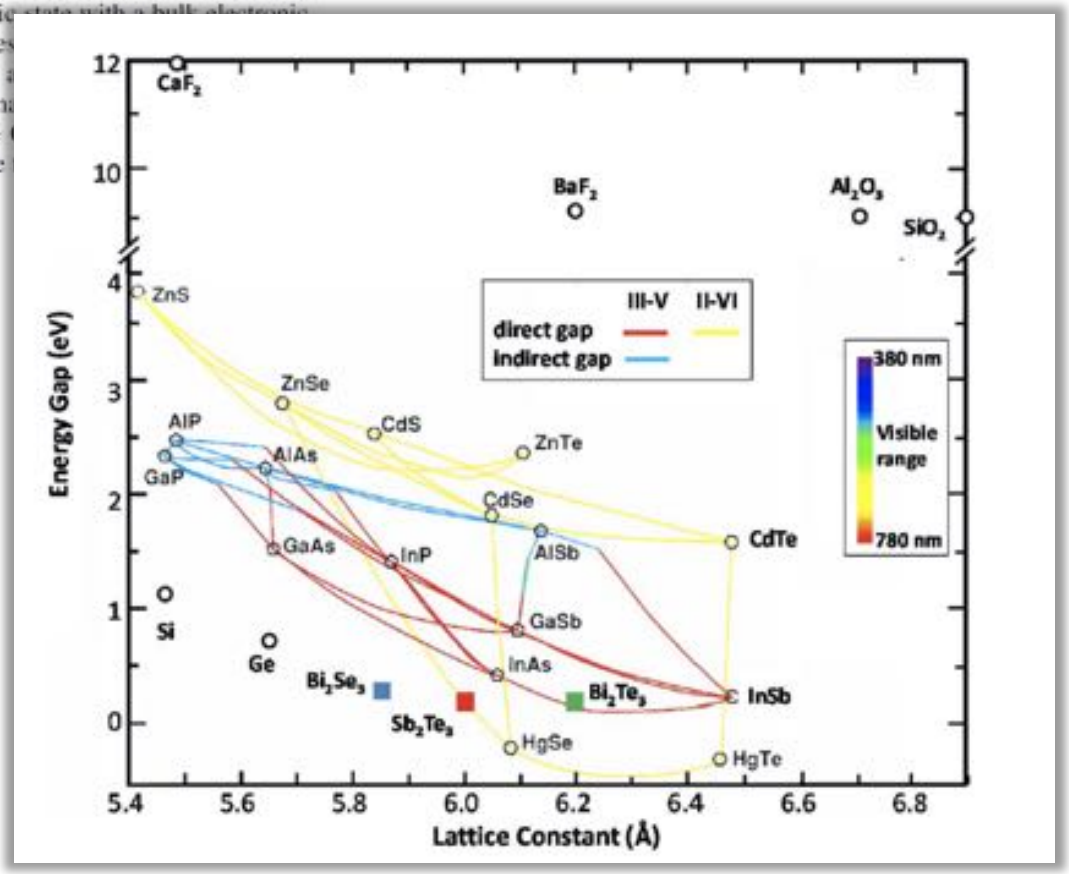


First prediction in graphene by Kane

Heavy insulating binaries

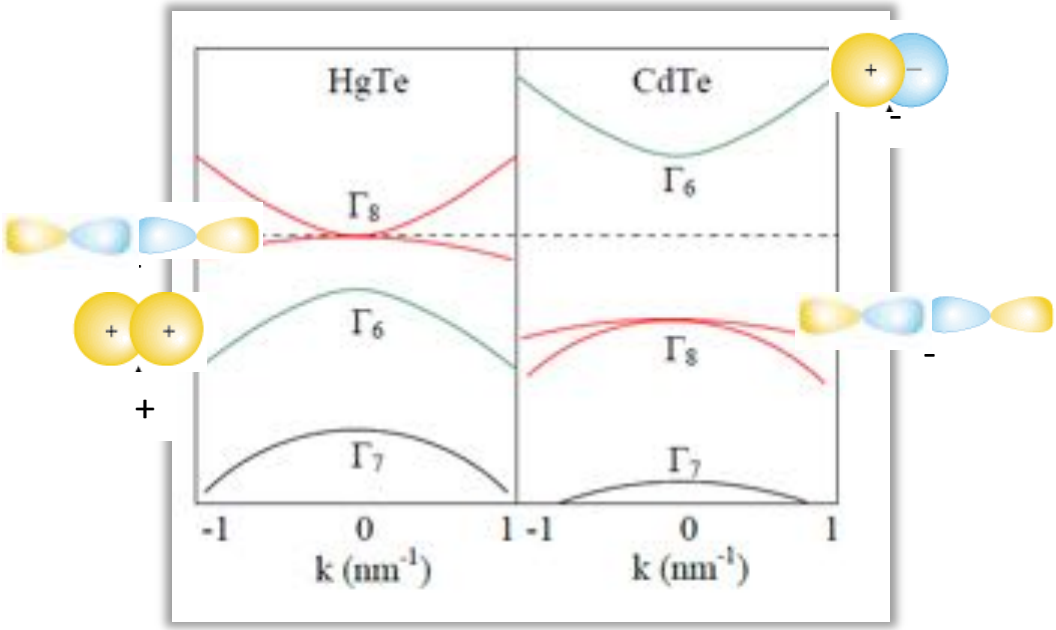


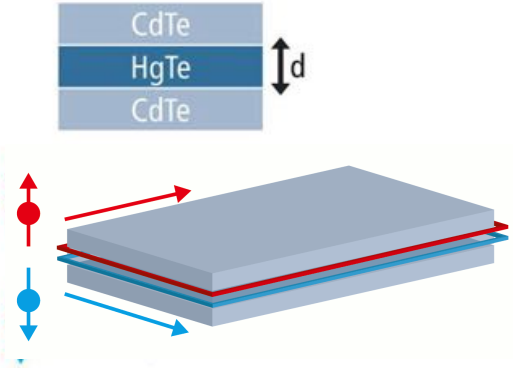
Kane and Mele, PRL 95, 146802 (2005)
Bernevig, et al., Science 314, 1757 (2006)
Bernevig, S.C. Zhang, PRL 96, 106802 (2006)
König, et al. Science 318, 766 (2007)

Quantum Spin Hall

Science
AAAS

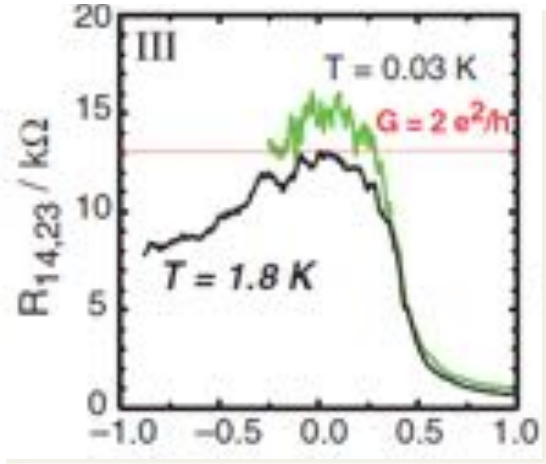
Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells
B. Andrei Bernevig, *et al.*
Science **314**, 1757 (2006);
DOI: 10.1126/science.1133734





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

Inert pair effect

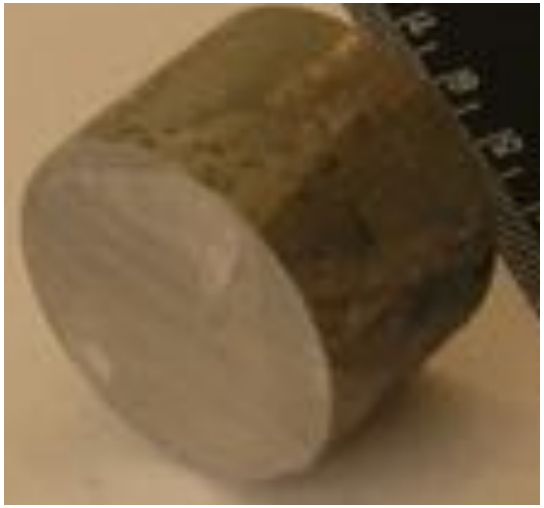


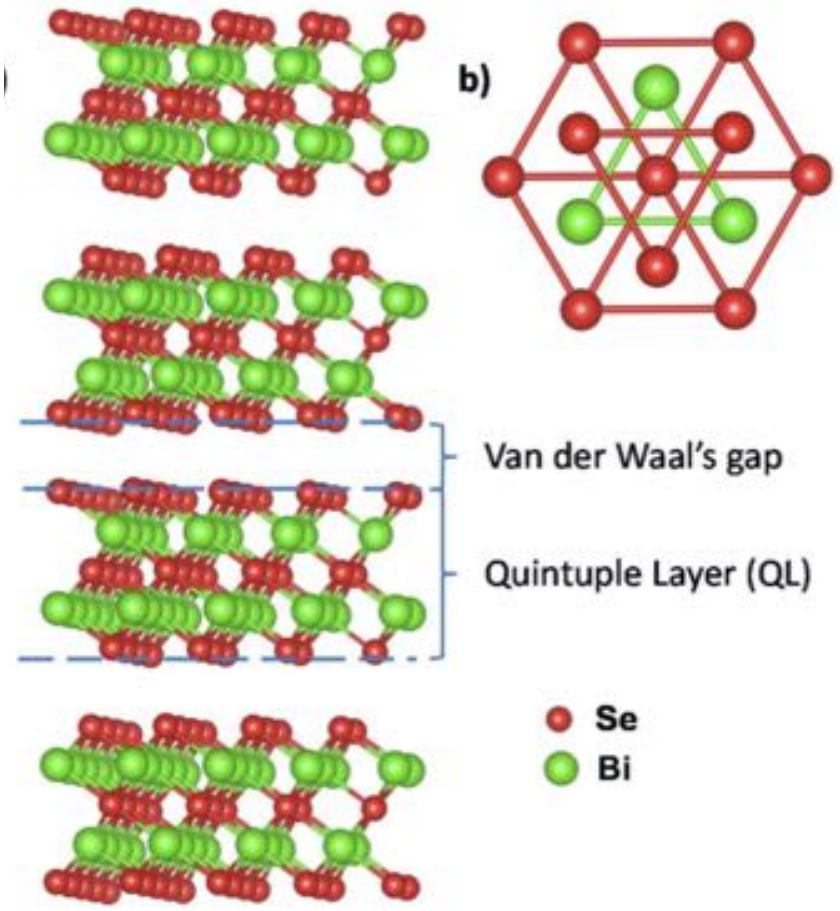
Bernevig,et al., Science 314, 1757 (2006)
Bernevig, S.C. Zhang, PRL 96, 106802 (2006)
König, et al. Science 318, 766 (2007)

Topologische Isolatoren

Bi-Sb Legierungen

Bi_2Se_3 und verwandte Strukturen



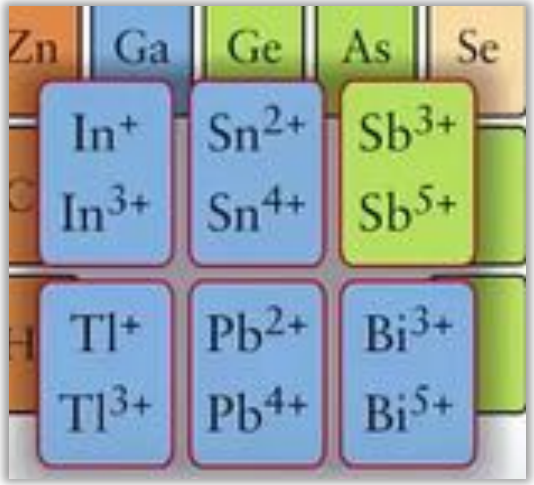


Moore and Balents, PRB 75, 121306(R) (2007)
Fu and Kane, PRB 76, 045302 (2007)
Murakami, New J. Phys. 9, 356 (2007)
Hsieh, et al., Science 323, 919 (2009)
Xia, et al., Nature Phys. 5, 398 (2009); Zhang, et al., Nature Phys. 5, 438 (2009)

Materials

Table I. Proposed topological insulator materials grouped into several different material classes.[4,12,13,18,23–29]

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	



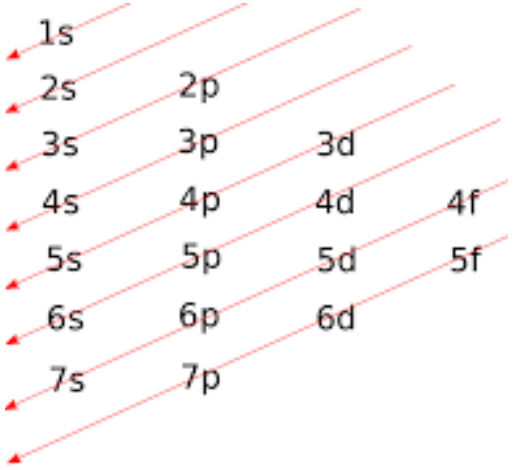
Claudia Felser and Xiao-Liang Qi , Guest Editors, MRS Bull. 39 (2014) 843.

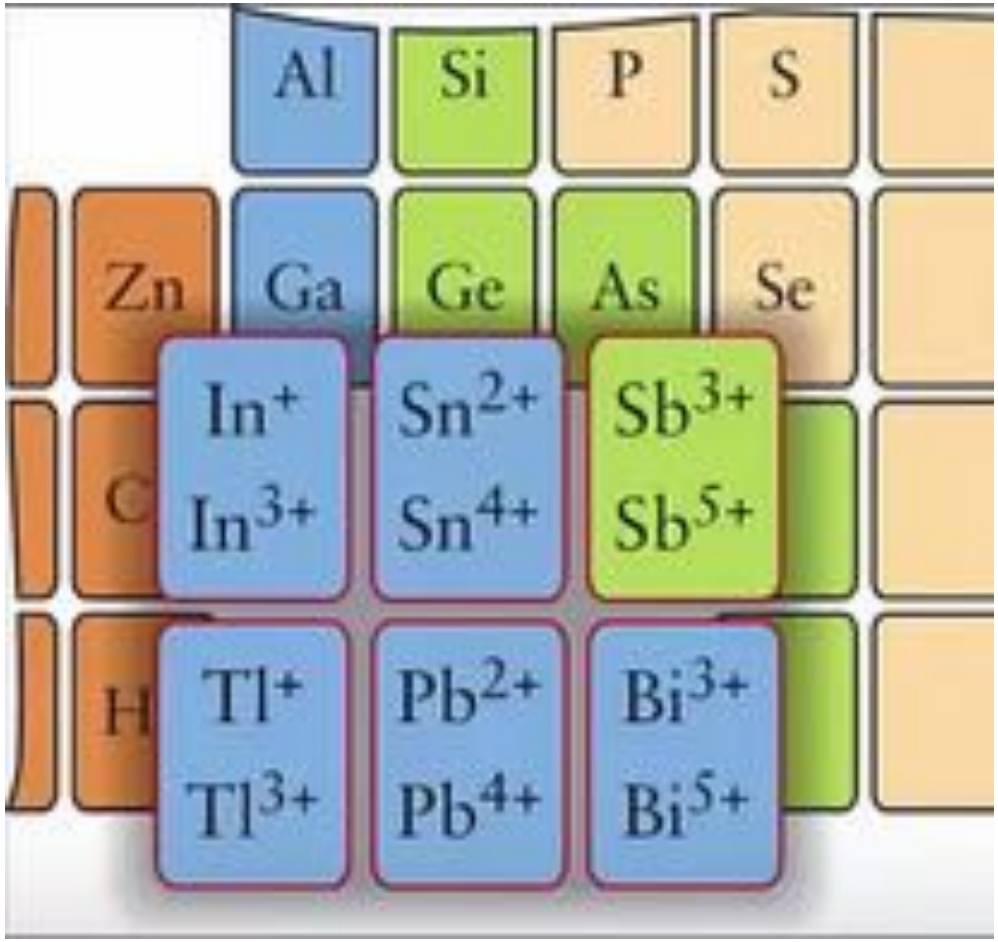
$Tl^{+1}\ Sn^{2+}\ Bi^{+3}$

Inert pair effect

Inert pair effect

- 1s electrons of heavier elements move at speeds ~ speed of light.
- electron mass ~ 1/orbital radius
- contraction of the 1s orbital = decreased of shielding for the outer s electrons
- valence s electrons behave like core electrons
- harder to remove via ionization
- Al(III) Al(III) is preferred over Al(I) Al(I), but Tl(I) Tl(I) is preferred over Tl(III)





Topology – interdisciplinary

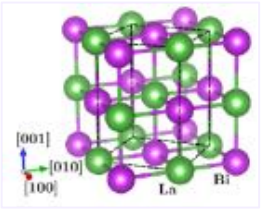
Chemistry

Real space - local

Crystals

LaBi

Crystal structure

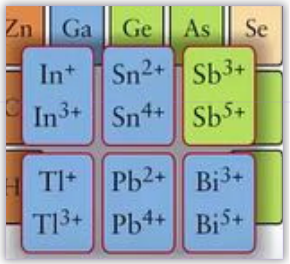


Position of the atoms

Orbitals

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

Inert pair effect

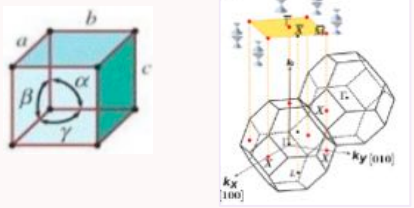


Physics

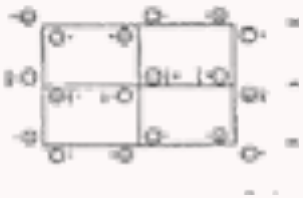
Recipro. space - delocalized

Brillouin zone

Symmetry

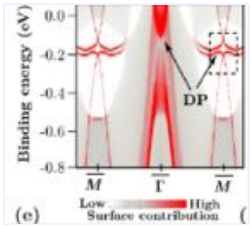


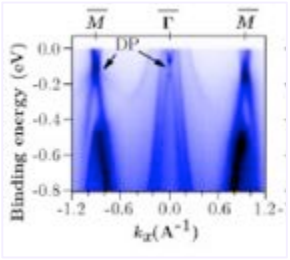
Local symmetry



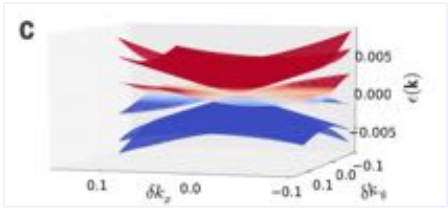
Relativistic effects

Electronic structure





Band connectivity



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)

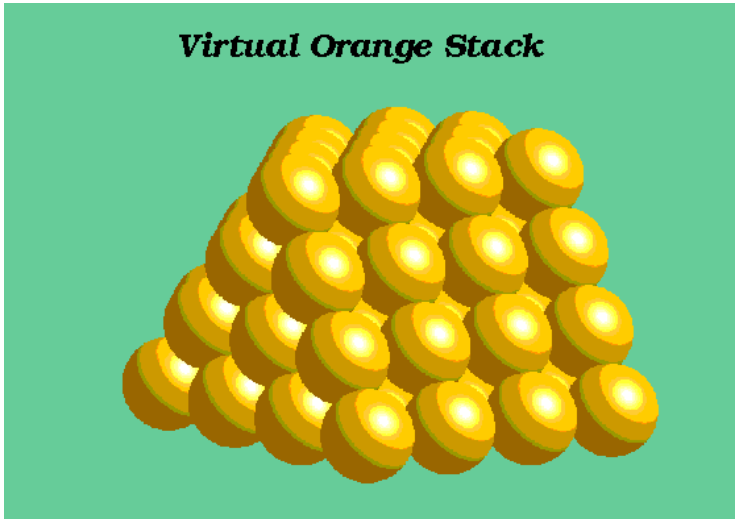
Crystal structure

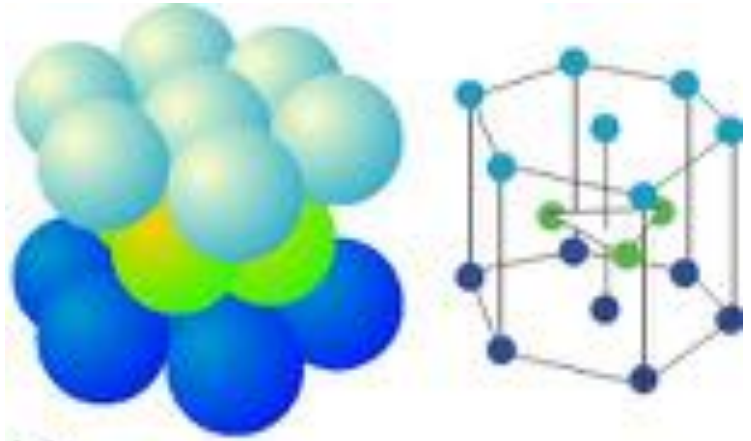
- Closed packed structures
  - Cubic
  - Hexagonal

How structures are made

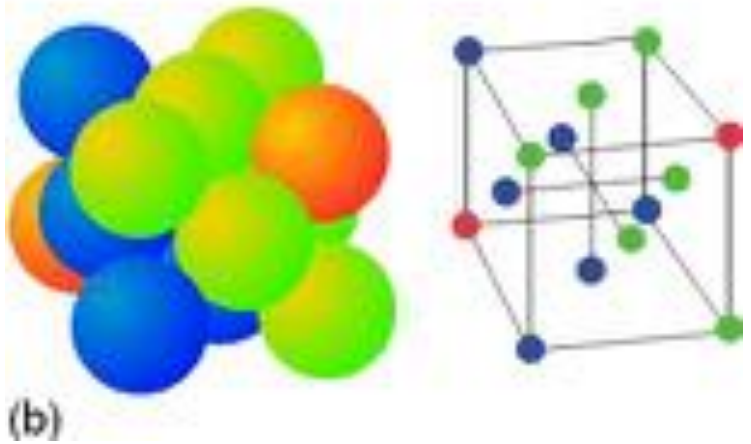
Anions always are the largest spheres, they build a closed packed lattice

In oxides: O^{2-}





hexagonal close packing

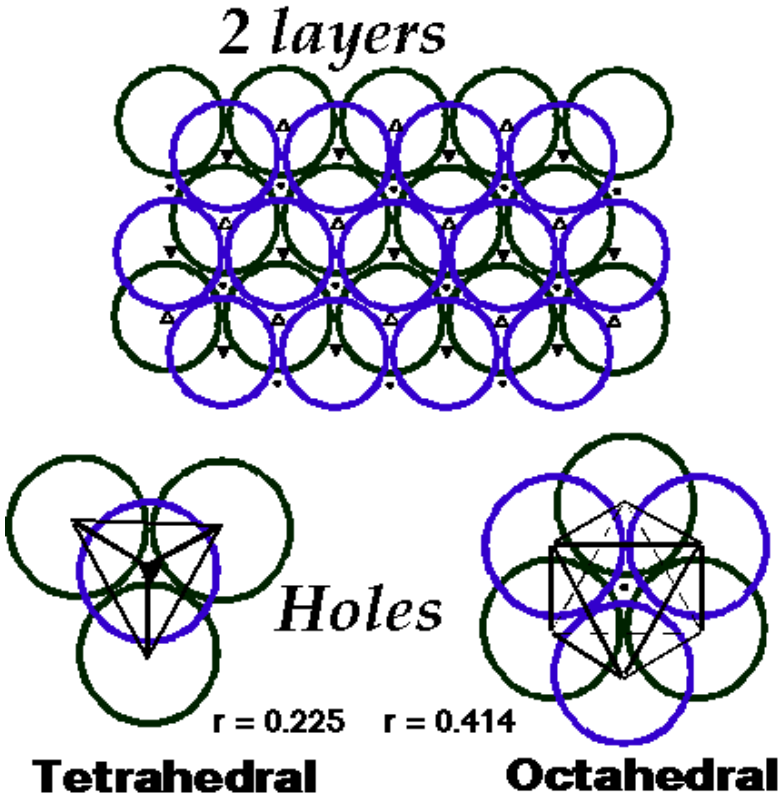


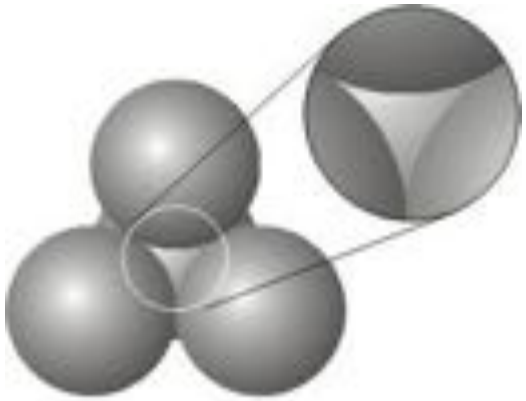
cubic close packing

How structures are made: holes

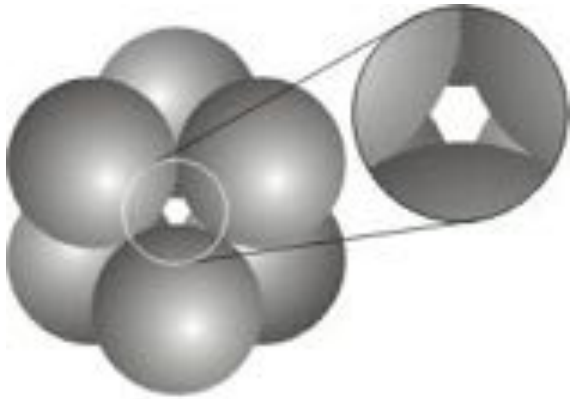
Anions always are the largest spheres, they build a closed packed lattice

Cations are stuffed in the holes



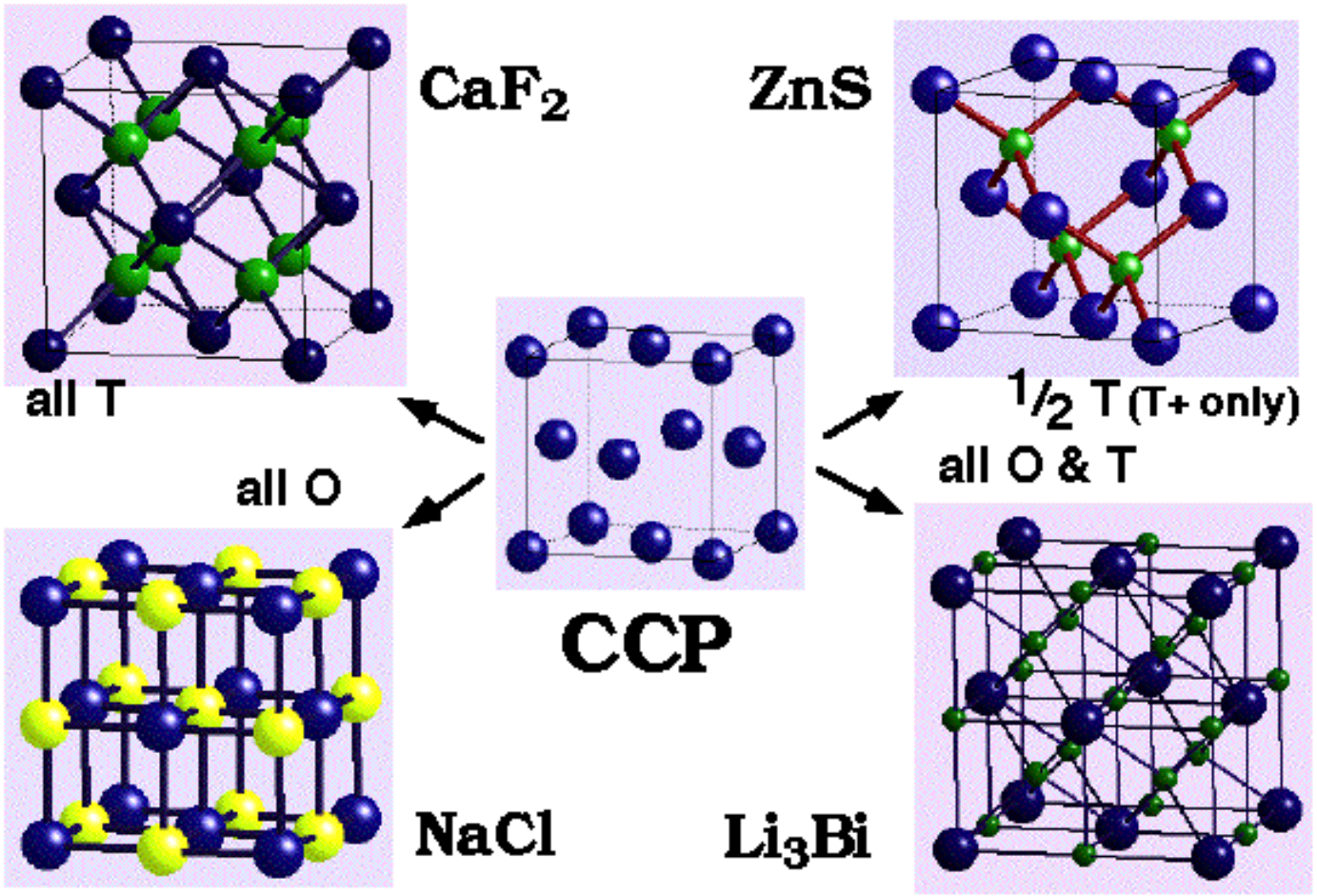


5 Tetrahedral hole

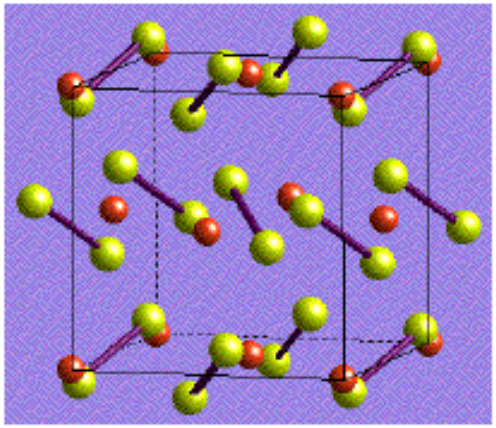


2 Octahedral hole

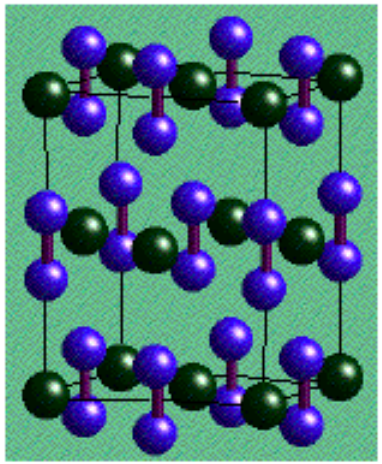
Simple ionic structures



NaCl Variants

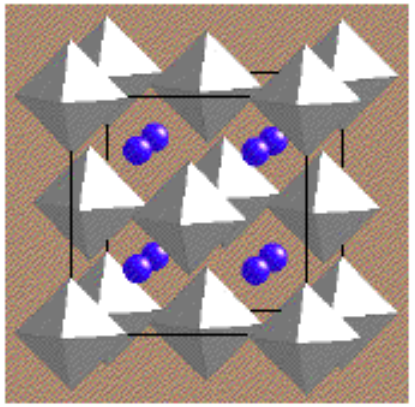


FeS_2 Pyrite

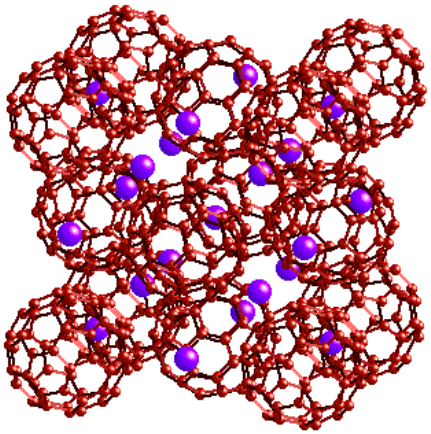


SrO_2

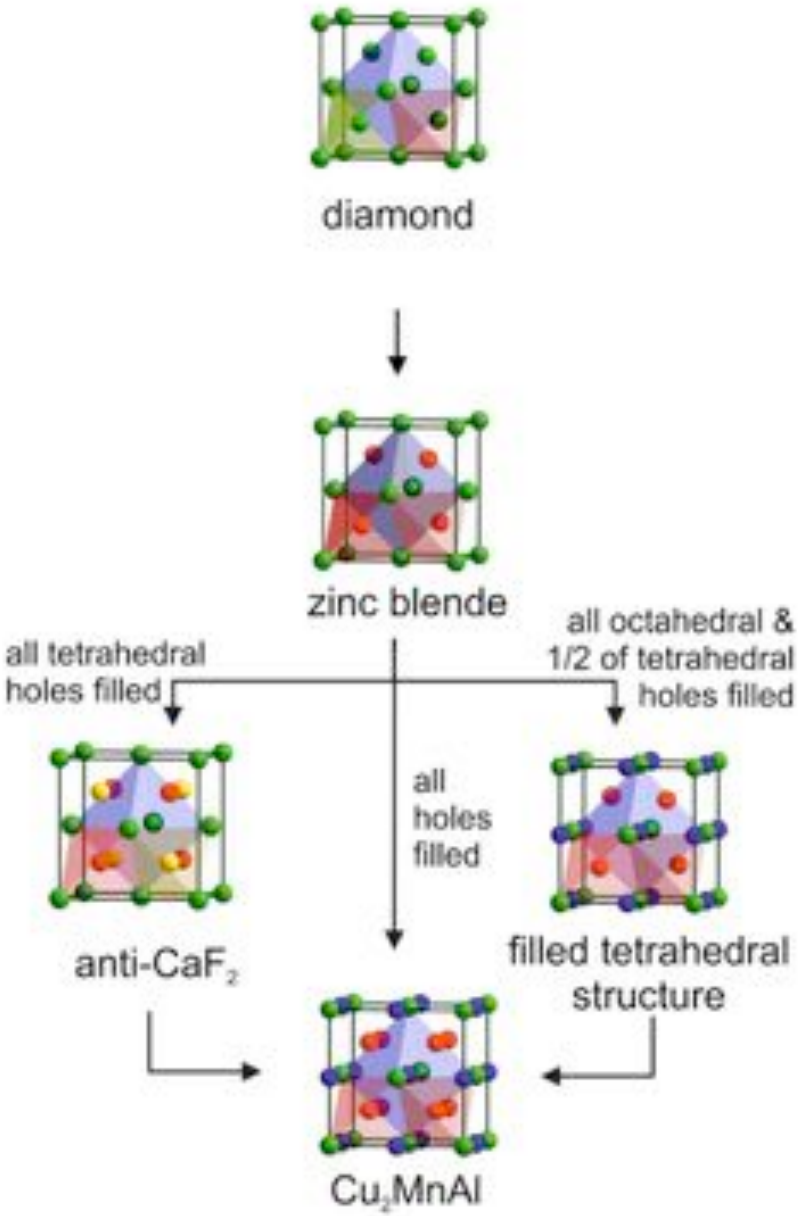
CaF_2 Variant

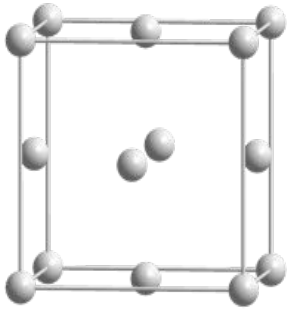


K_2PtCl_6

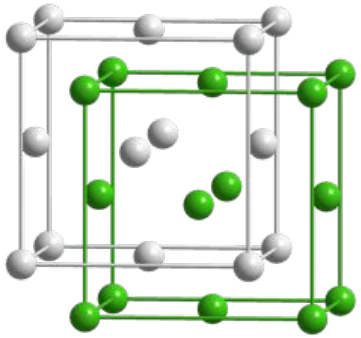


K_3C_{60}

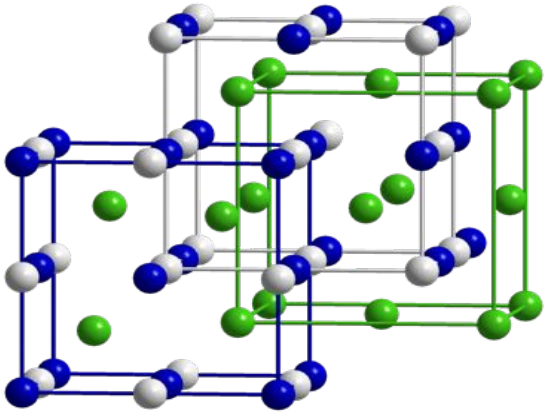

diamond
zinc blende
all tetrahedral holes filled
all octahedral & 1/2 of tetrahedral holes filled
all holes filled
anti-CaF2
filled tetrahedral structure
Cu2MnAl



fcc - lattice

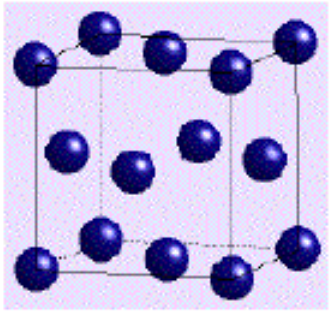


2 fcc – lattices
Zincblend structure

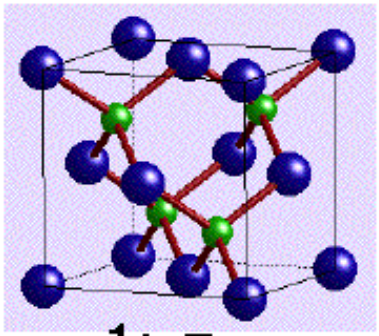


3 fcc – lattices
MgAgAs structure
(F-43m, $C1_b$)

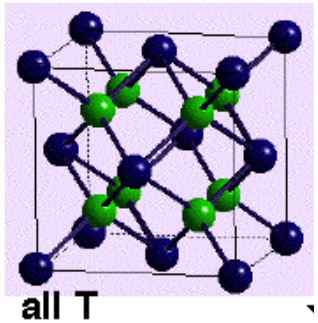
Heusler compounds



CCP

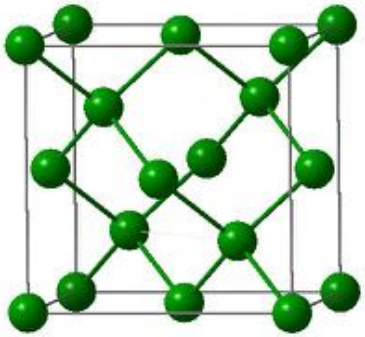


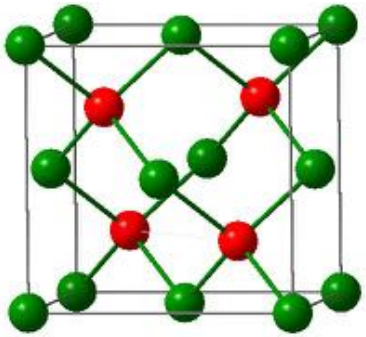
1/2 T (T+ only)



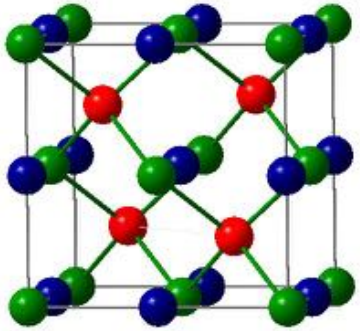
all T

Diamond **ZnS** **Heusler XYZ $C1_b$** **X_2YZ $L2_1$**

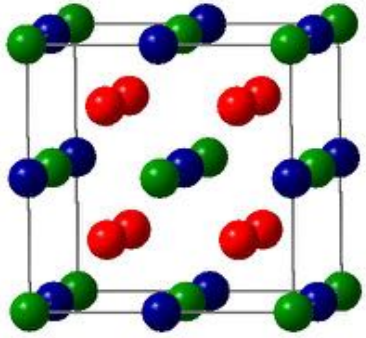




2 interpenetrating fcc
with half of the tetrahedral
sites filled



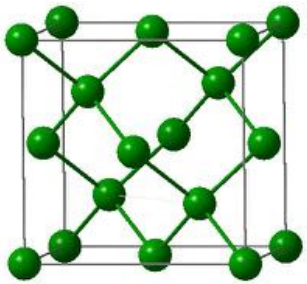
3 interpenetrating fcc
half of the tetrahedral sites
and the octahedral sites



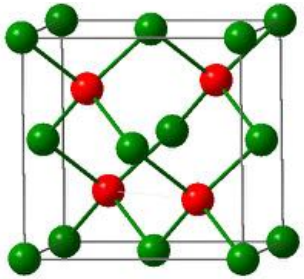
4 interpenetrating fcc
all tetrahedral sites filled
and the octahedral sites

Heusler compounds

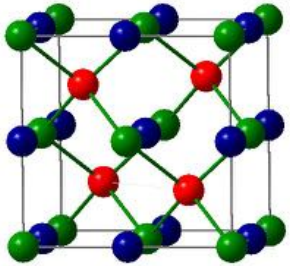
Diamond

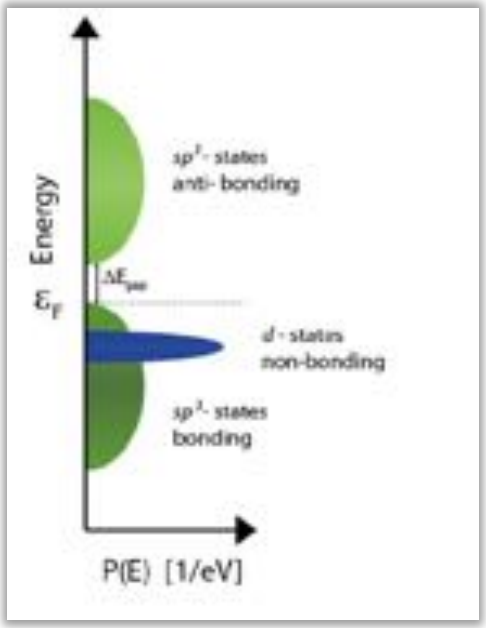


ZnS



Heusler XYZ $C1_b$





Cd Se

2 + 6 = 8

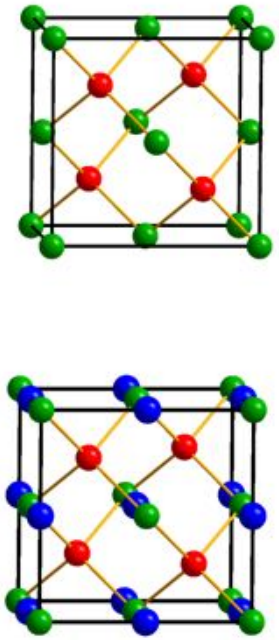
Li Zn Sb

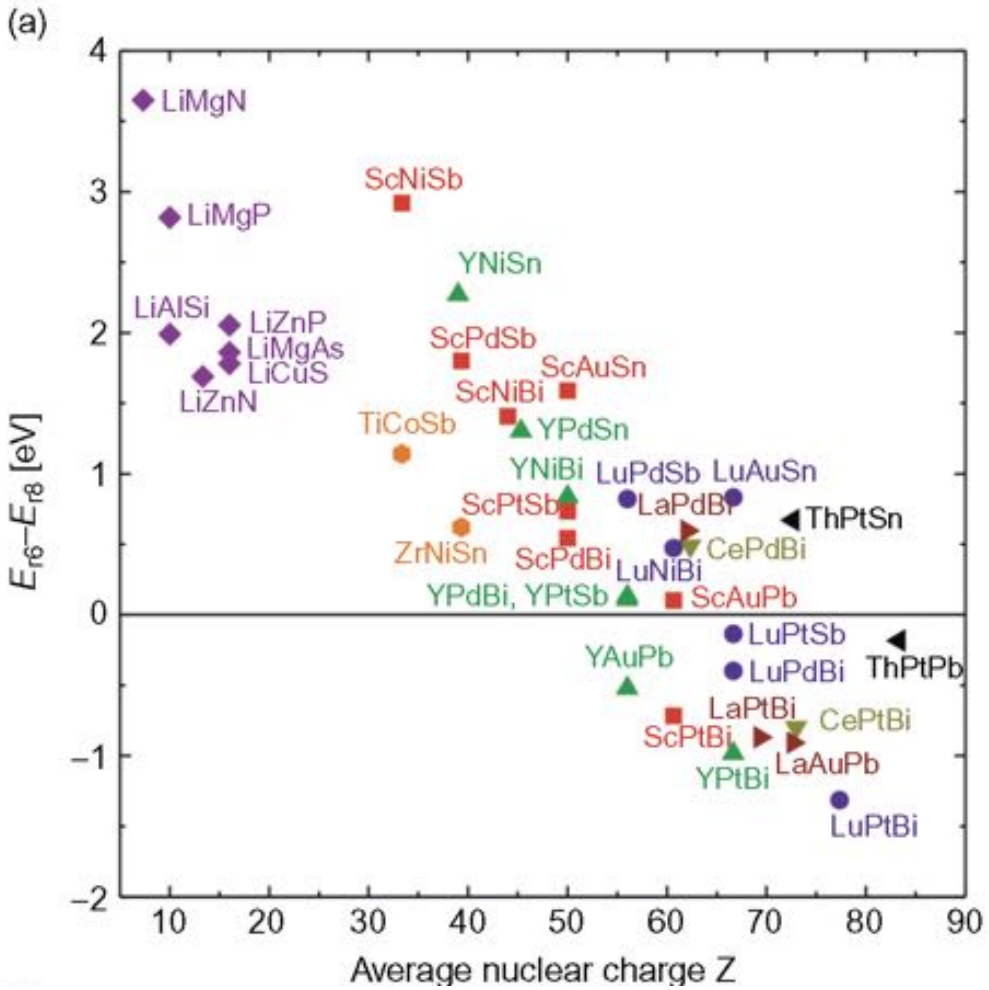
1 + 2 + 5 = 8

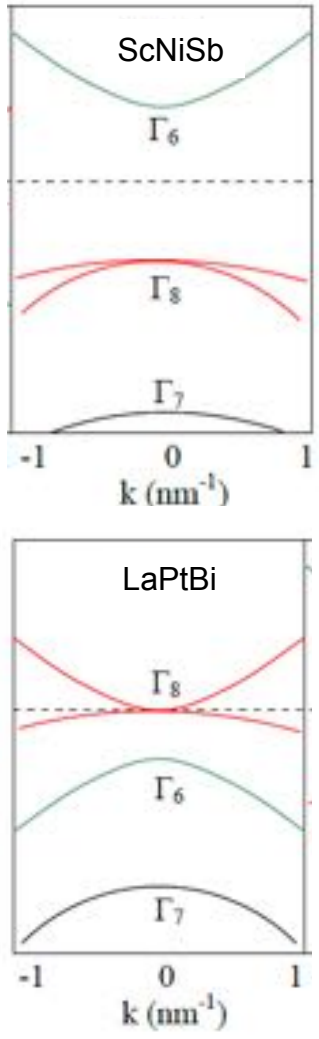
RE Pt Bi

3 + 10 + 5 = 18

Predicting topological insulators





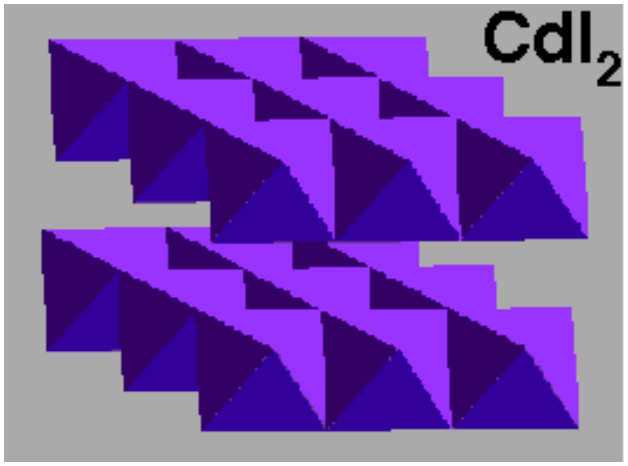


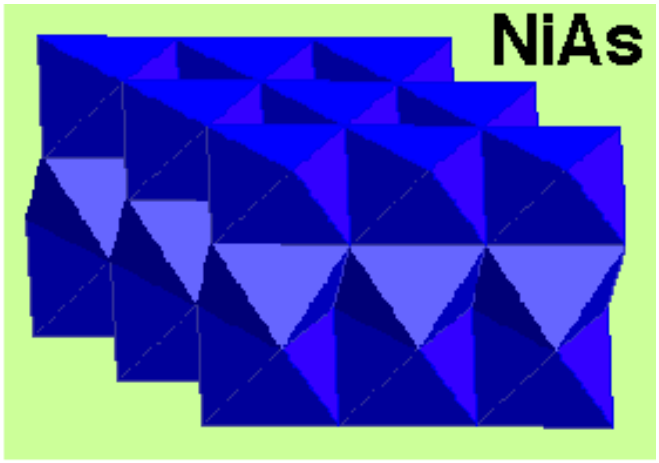
S. Chadov et al., Nat. Mater. **9** 541 (2010).
H. Lin et al., Nat. Mater. **9** 546 (2010).

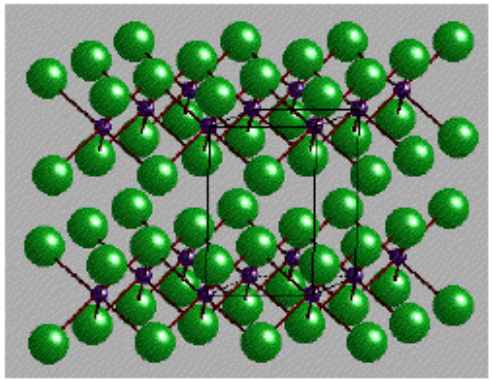
Formula	Type/fraction of sites occ.	HCP	CCP
AB	All octahedral	NiAs Nickel Arsenide	NaCl Rock Salt
	Half tetrahedral	ZnS Wurtzite	ZnS Zinc Blende
A_2B	All tetrahedral	Not known	CaF_2/Mg_2Si (Fluorite/Anti-Fluorite)
A_3B	All octahedral & tetrahedral	Not known	Li_3Bi

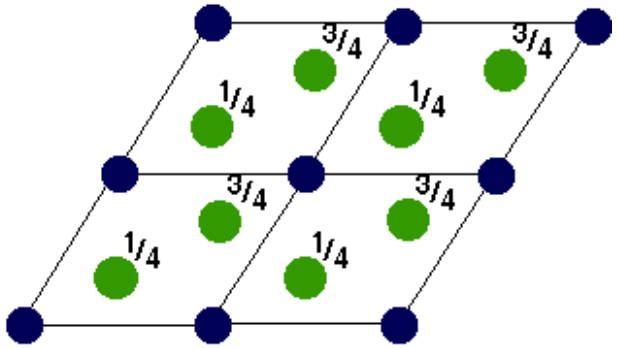
- Layered structure
  - Removing one layer
  - Anisotropic bonding − lone pairs − inert pair

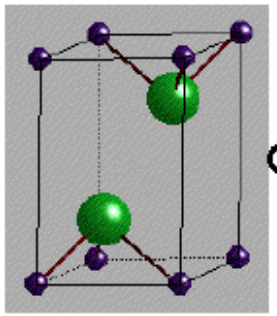
Layered structure





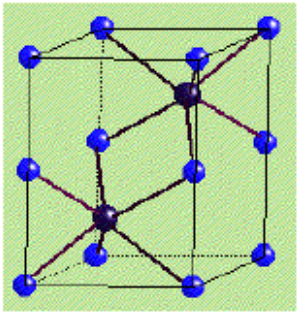




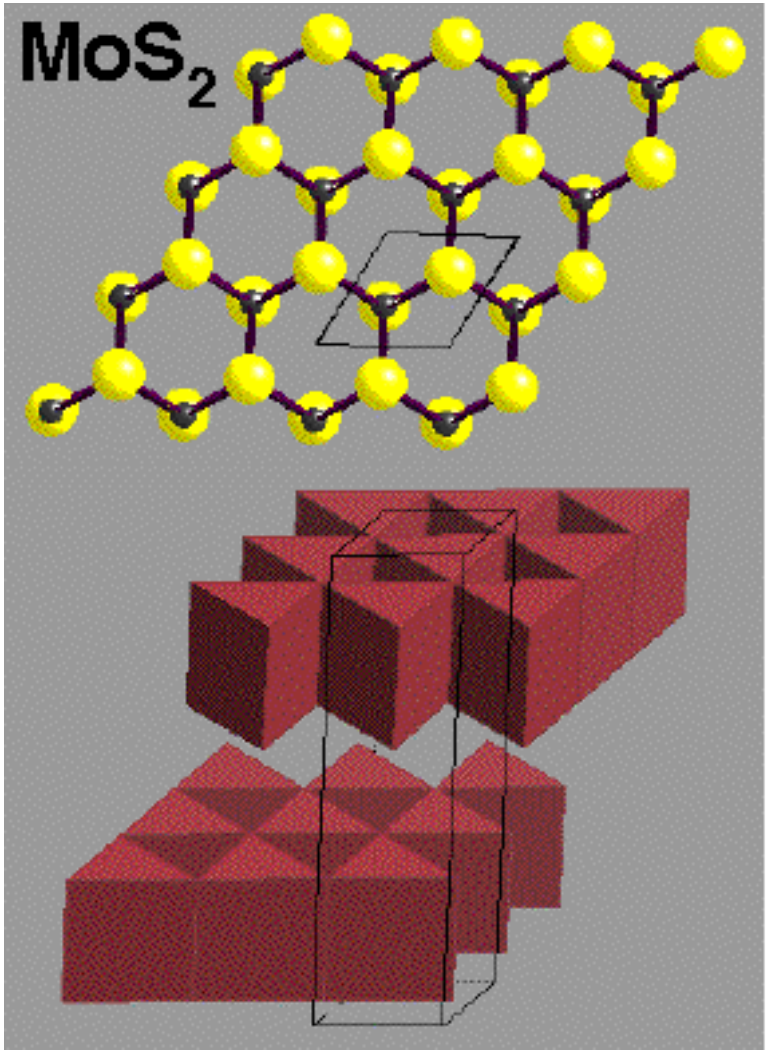


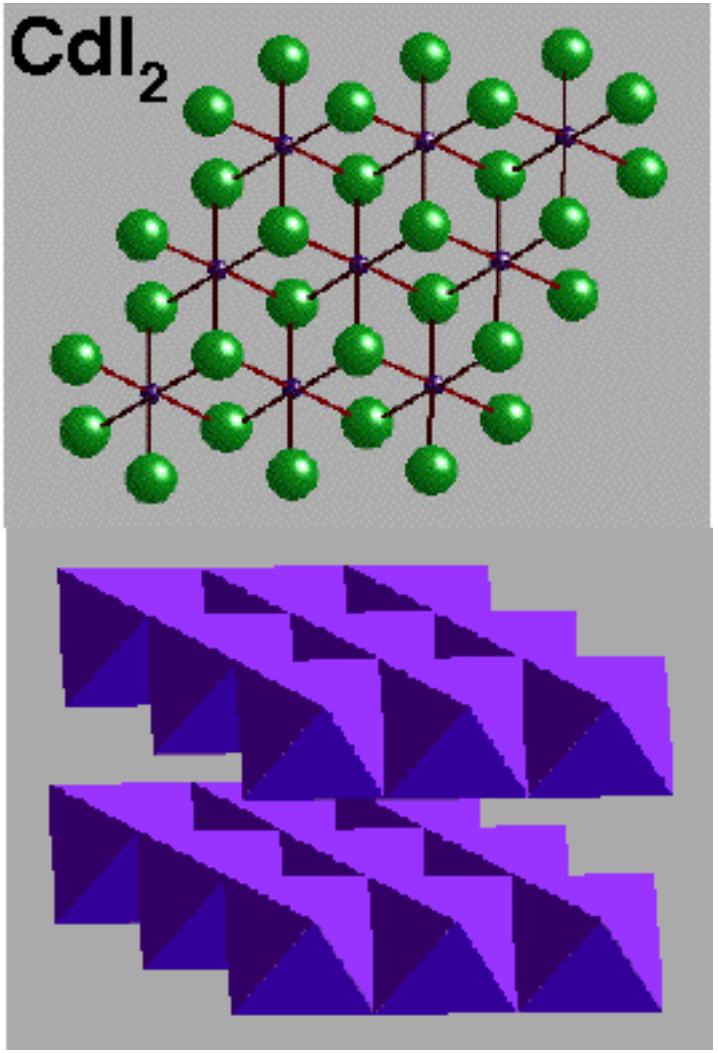
Comparison

CdI_2 *vs* NiAs



Layered structure



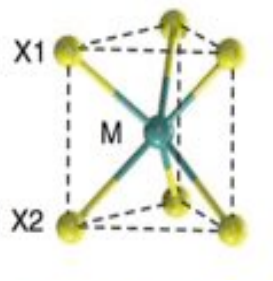


MoS_2 : crystal field

Mo^{4+} (d^2)

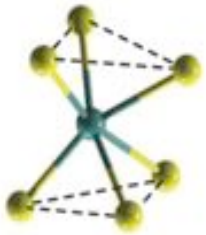
S^{2-} (s^2p^6)

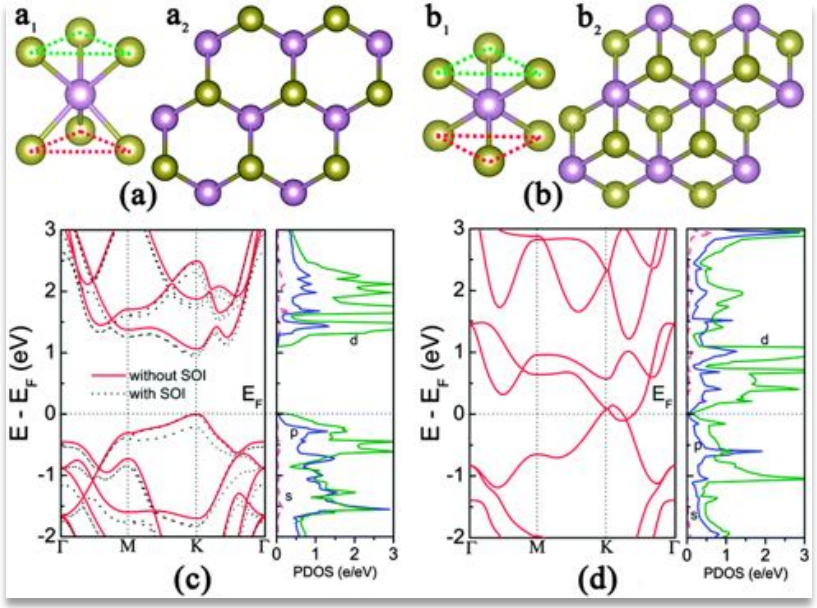
2 H



1T

1T', Td





dxz, dyz

dxy, dx^2-y^2

dz^2

Semiconductor

dz^2, dx^2-y^2

dxy, dxz, dyz

Metal

dz^2

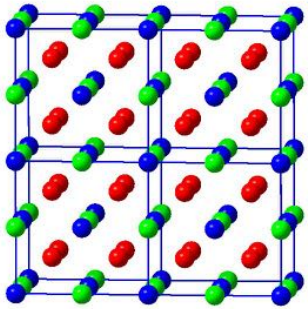
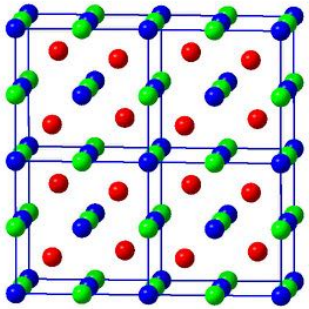
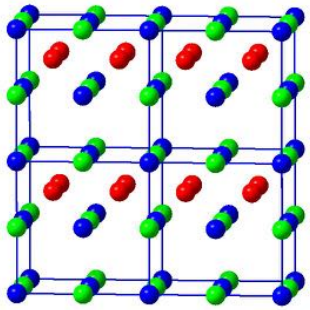
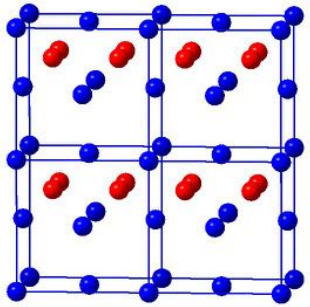
dx^2-y^2

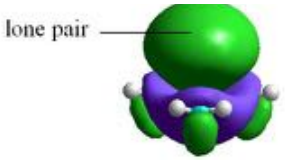
dxy

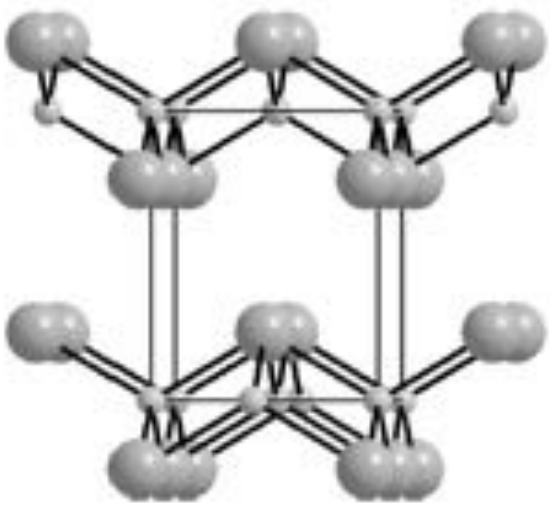
dxz, dyz

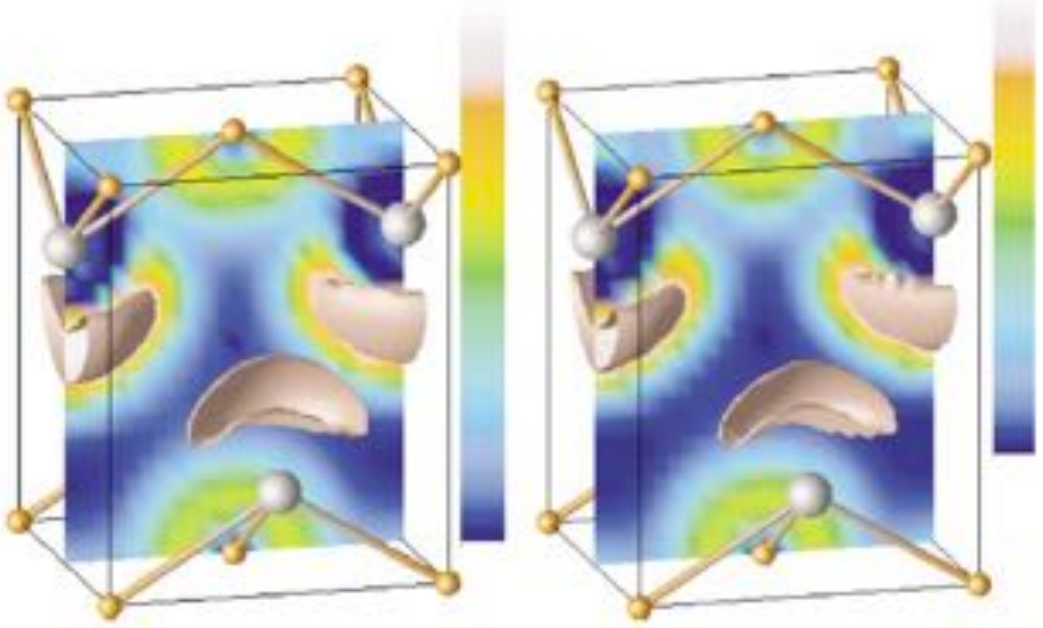
Semimetal

Heuslers go low dimensional

Semiconductor main group	Li_2MgSi	LiAlSi		
Semiconductor transition metal	Fe_2VAl	TiNiSn .	NaCuS	
Semiconductor heavy	Li2HgPb or Na Os_2ThPb ???	MgHgPb ??? LaPtBi topolo.	PbFCl	PbO
Superconductor main group	$ZrNi_2Ga$	No inversion	NaAlSi Tc=7K	
Superconductor transition metal	Pd_2ZrAl Tc=5K	LaPtBi Tc=0.6K	LiFeAs Tc=18	FeSe Tc=8K p=9GPa Tc=37K





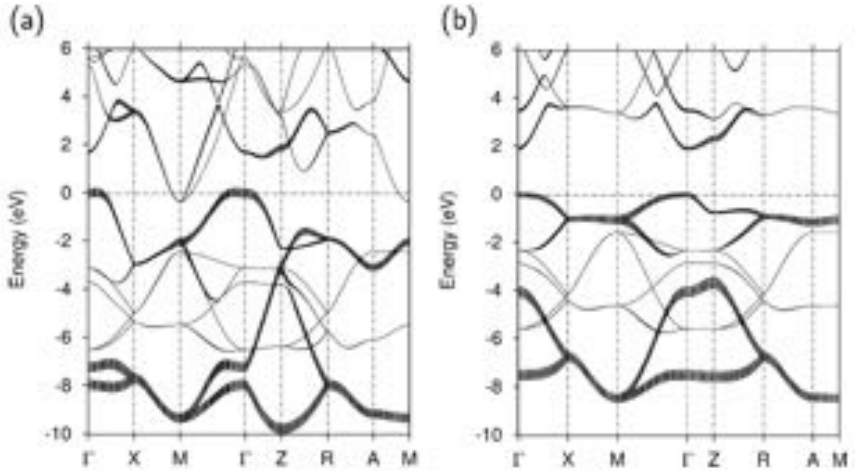
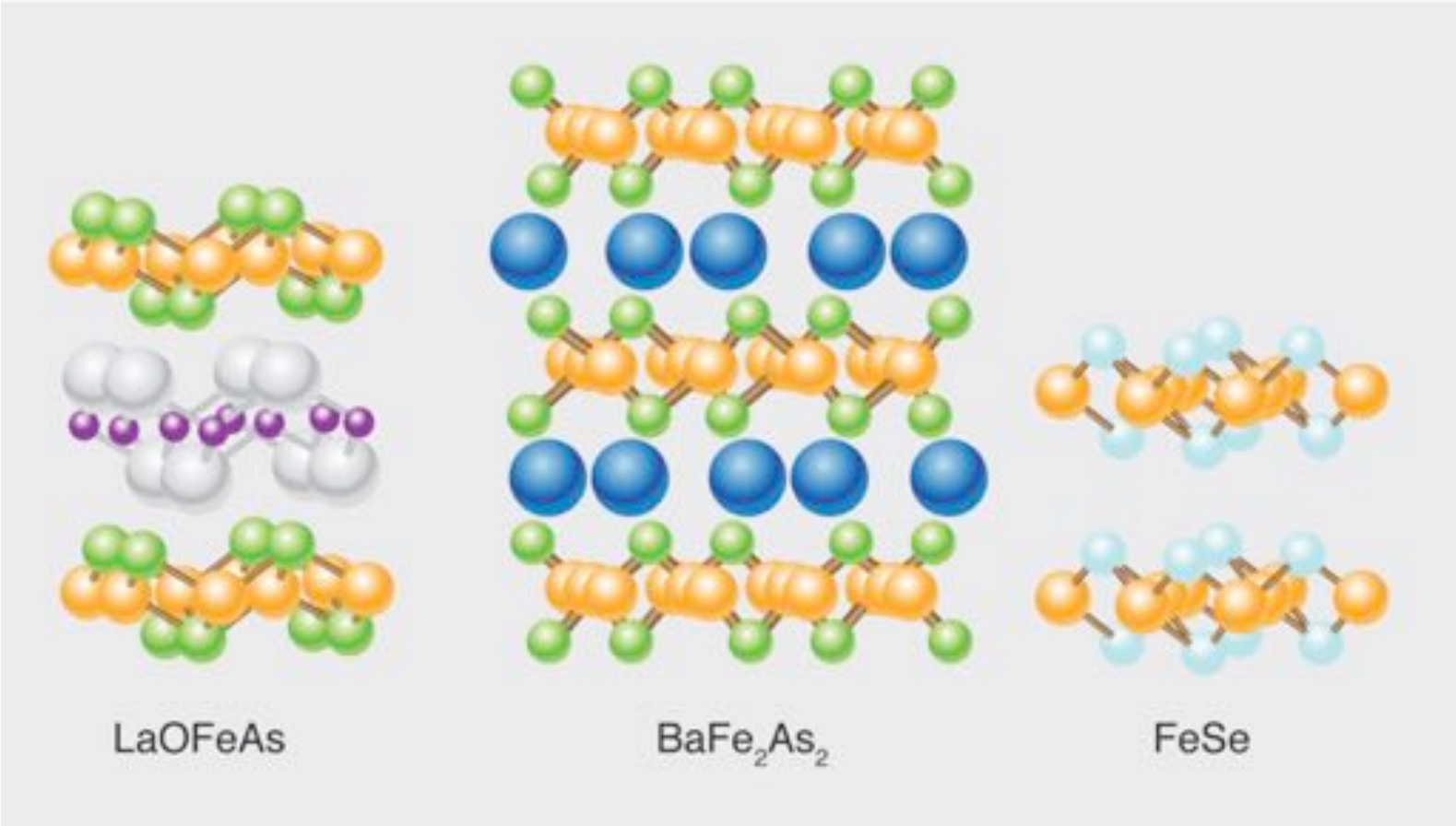


Fig. 8. Sn s fatband structure for (a) tetragonal SnO and (b) tetragonal SnO with an increased inter-slab separation.

Raulot et al., Solid State Sciences 4 (2002) 467

Fe-pnictides

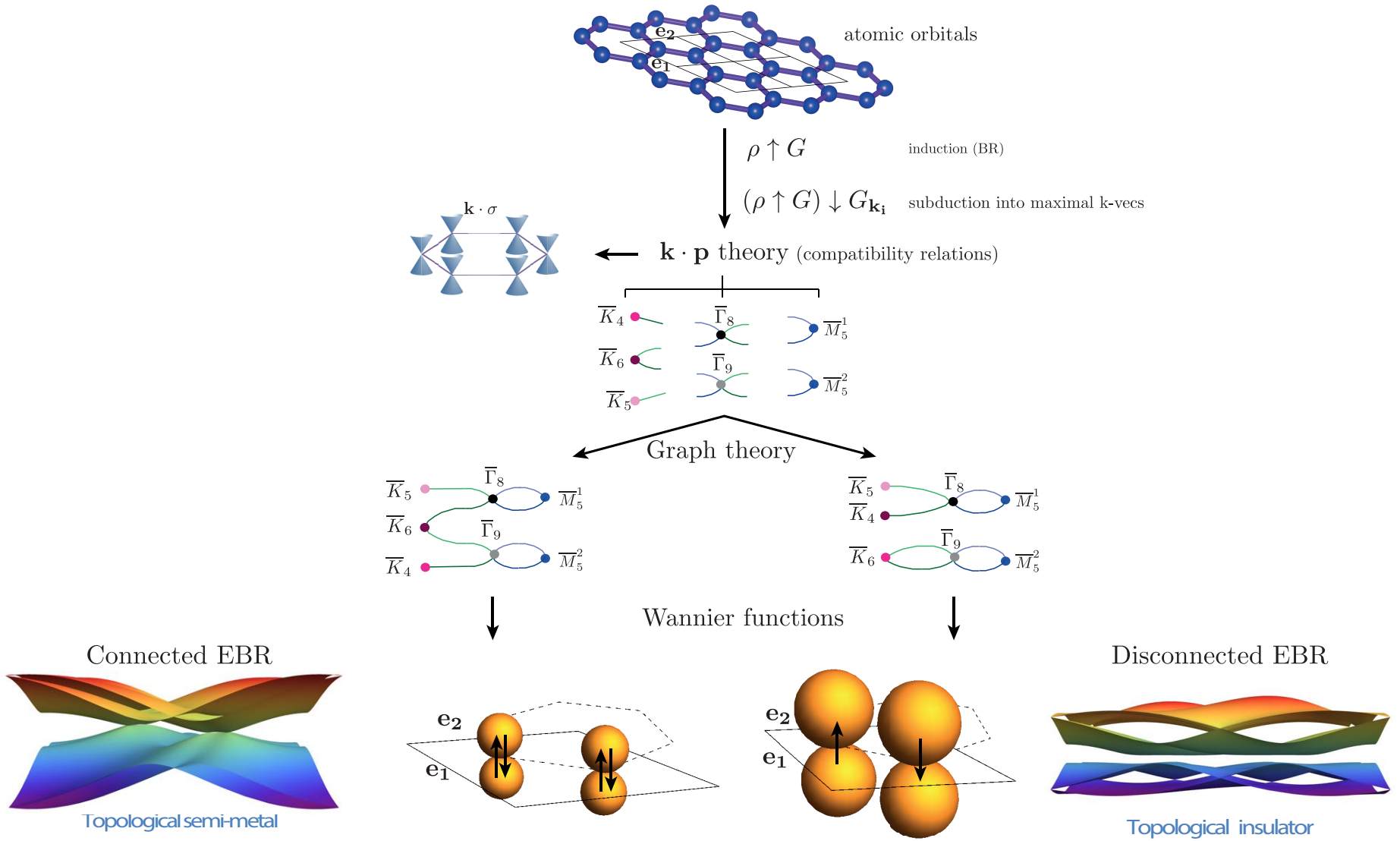


Formula	Type/fraction of sites occ.	HCP	CCP
AB	All octahedral	NiAs Nickel Arsenide	NaCl Rock Salt
	Half tetrahedral	ZnS Wurtzite	ZnS Zinc Blende
A_2B	All tetrahedral	Not known	CaF_2/Mg_2Si (Fluorite/Anti-Fluorite)
A_3B	All octahedral & tetrahedral	Not known	Li_3Bi
AB_2	Half octahedral (Alternate layers 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	

Electronic structure

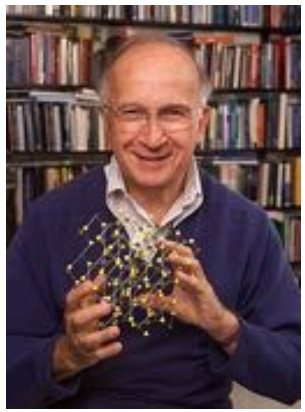
Translation

Barry, Andrei slide



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

From Orbitals to Bands



How Chemistry and Physics Meet in the Solid State

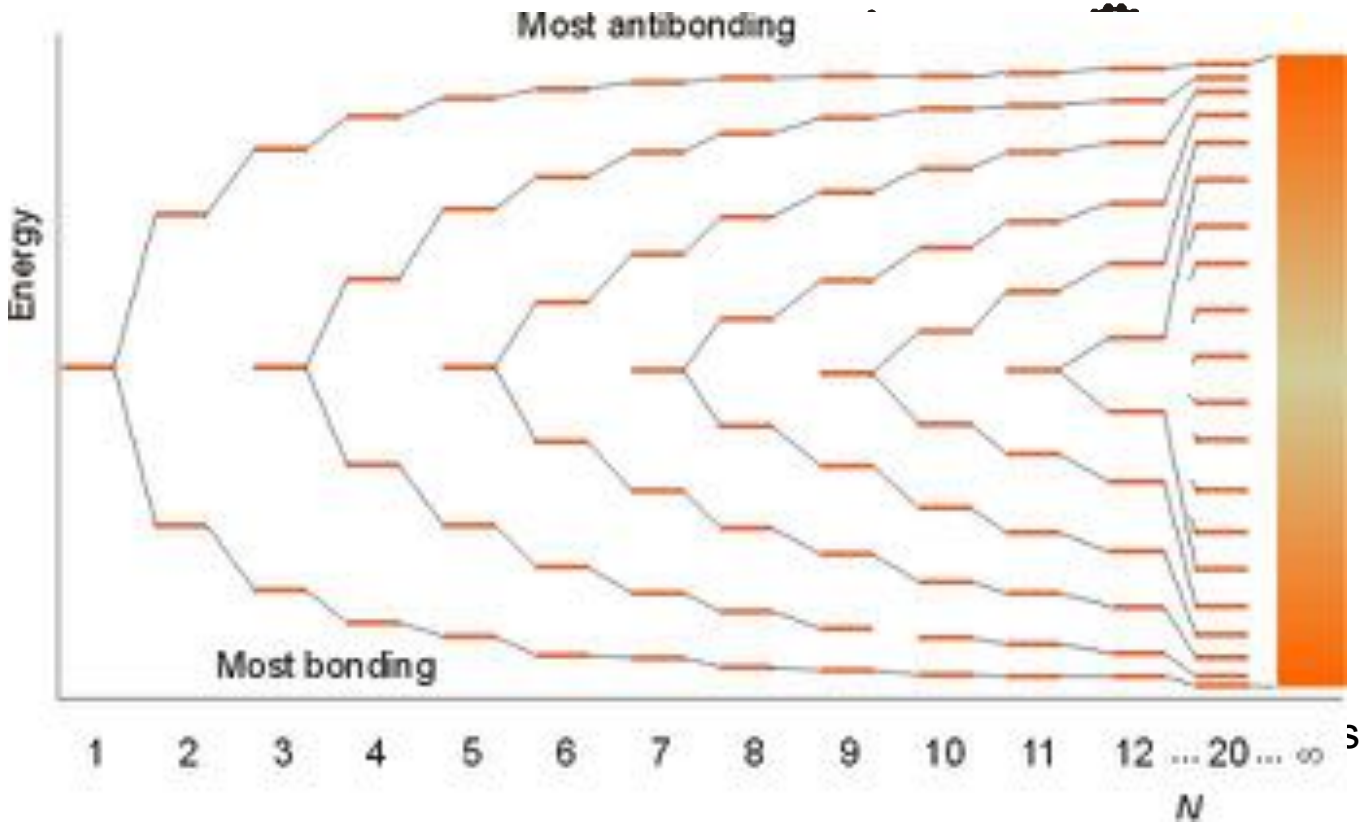
By Roald Hoffmann*

Hoffmann Angewandte. Chem. 26 (1987) 846

Energy bands in solids arise from overlapping atomic orbitals
⇒ crystal orbitals (which make up the bands)

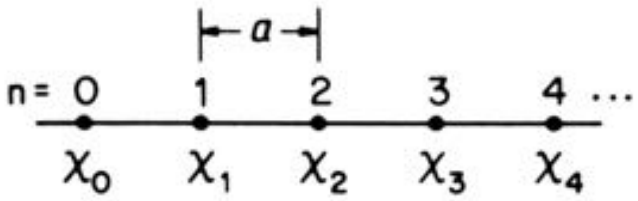
Recipe: use LCAO (tight binding) approach

Crystal = regular periodic array ⇒ translational symmetry



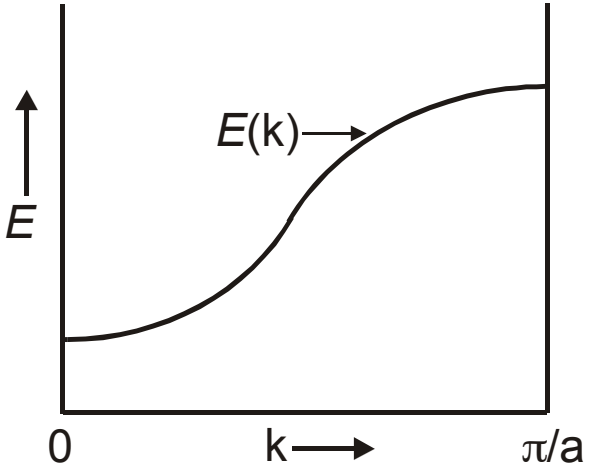
How to find a band structure

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



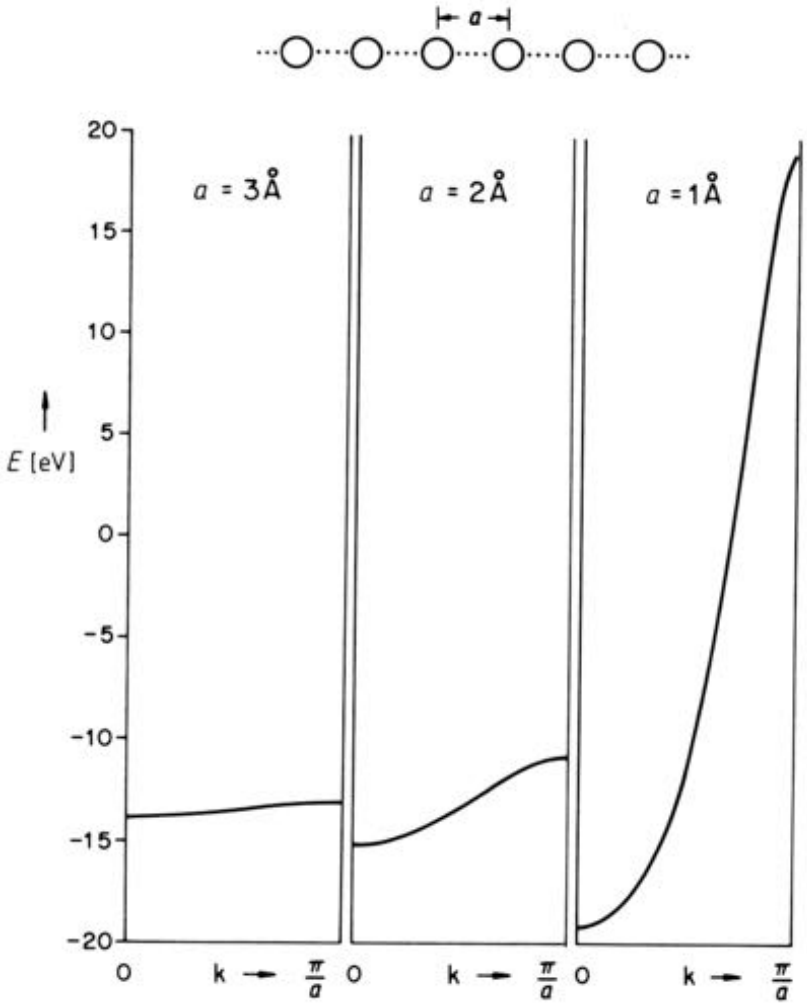
$k = 0 \qquad \Psi_0 = \sum_n e^0 \chi_n = \sum_n \chi_n = \chi_0 + \chi_1 + \chi_2 + \chi_3 \ldots\ldots$

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

Hoffmann Angewandte. Chem. 26 (1987) 846

Band Width

An important feature of a band is its bandwidth (dispersion), i.e. the difference between highest and lowest level.
The bandwidth is determined by the overlap between the interacting orbitals



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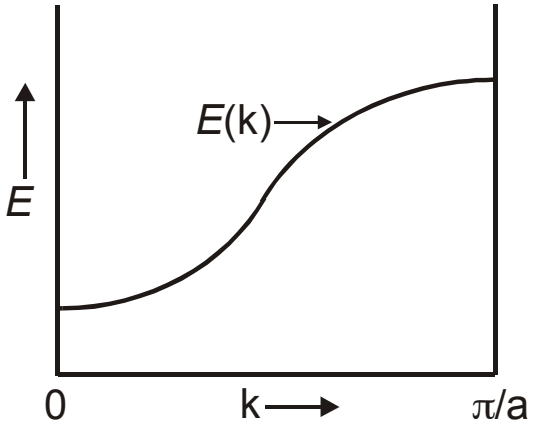
How to find a band structure

The topology of the orbital interaction determines how a band runs



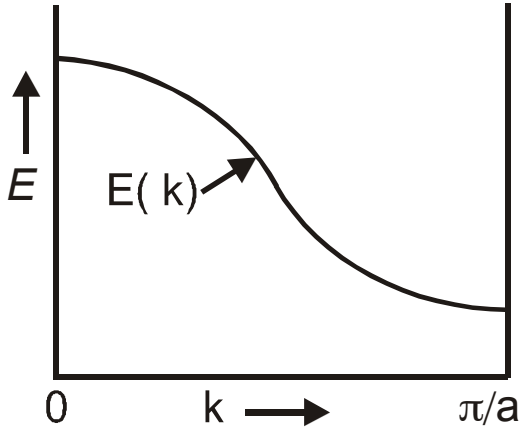
$k = 0 \quad \Psi_0 = \sum_n e^0 \chi_n = \sum_n \chi_n = \chi_0 + \chi_1 + \chi_2 + \chi_3 \ldots\ldots$

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

k = 0 bonding interaction ⇒ band runs „uphill“

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

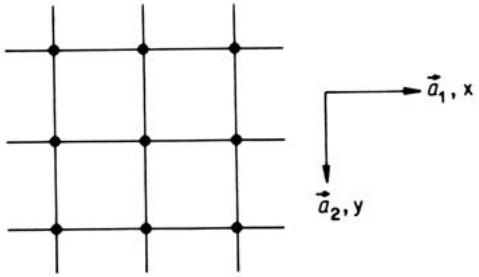
$\Psi_{\frac{\pi}{a}} = \chi_0 - \chi_1 + \chi_2 - \chi_3 + \ldots$



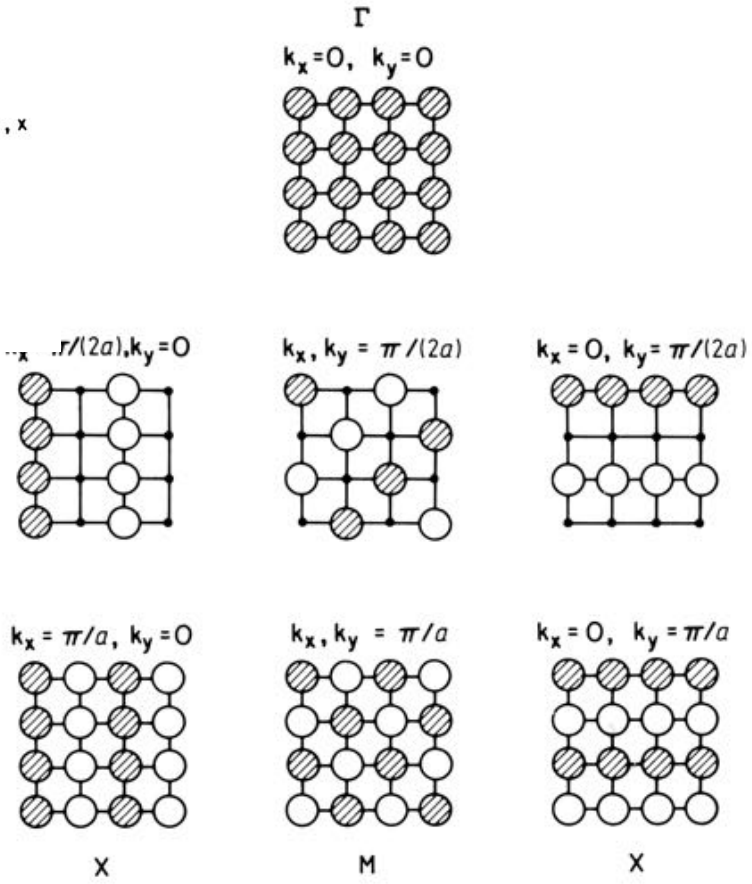
k = 0 antibonding interaction ⇒ band runs „downhill“

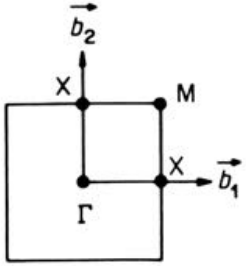
Hoffmann Angewandte. Chem. 26 (1987) 846

Square Lattice



Square lattice with one s basis orbital

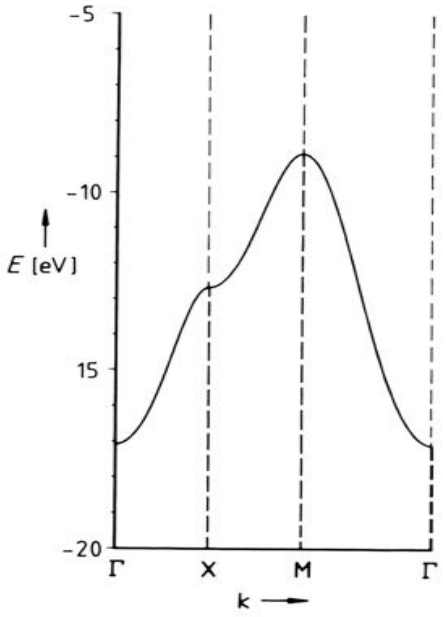




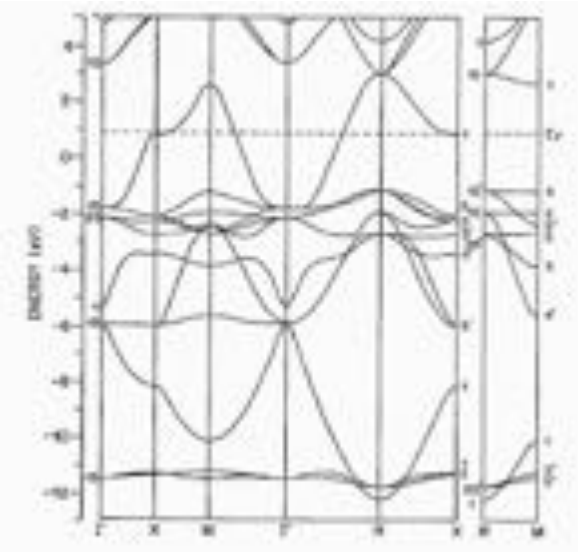
Corresponding lattice in reciprocal space

Edges of Brillouin zone:

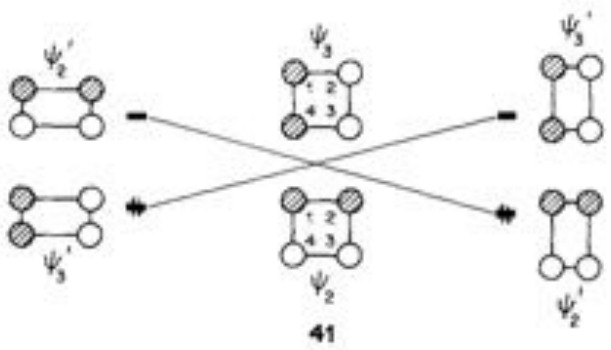
Special (high symmetry) k points

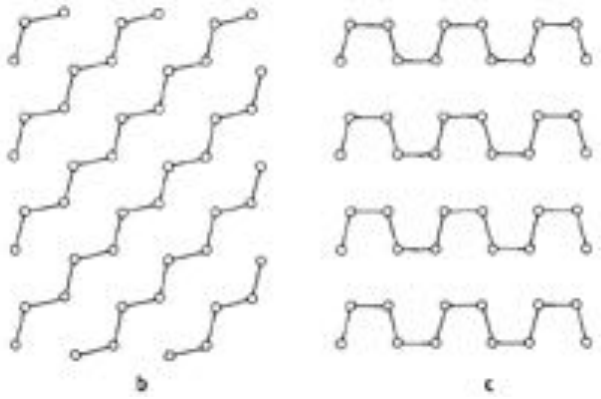


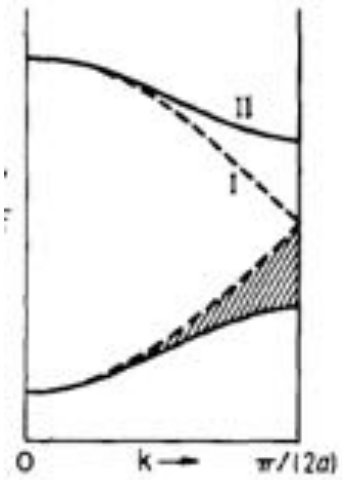
$BaBiO_3$

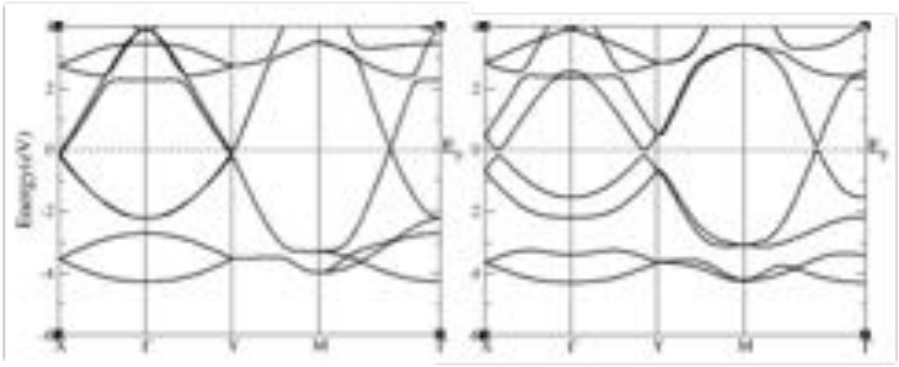


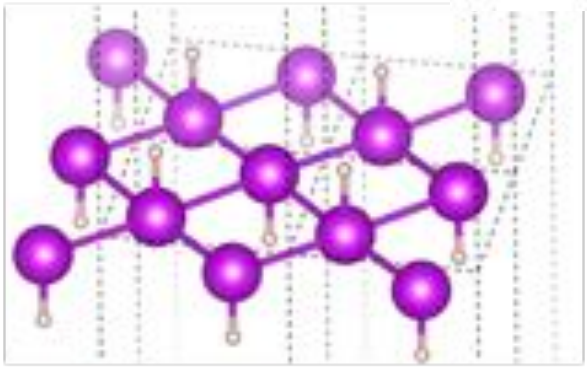
Square nets of electron doped Bi











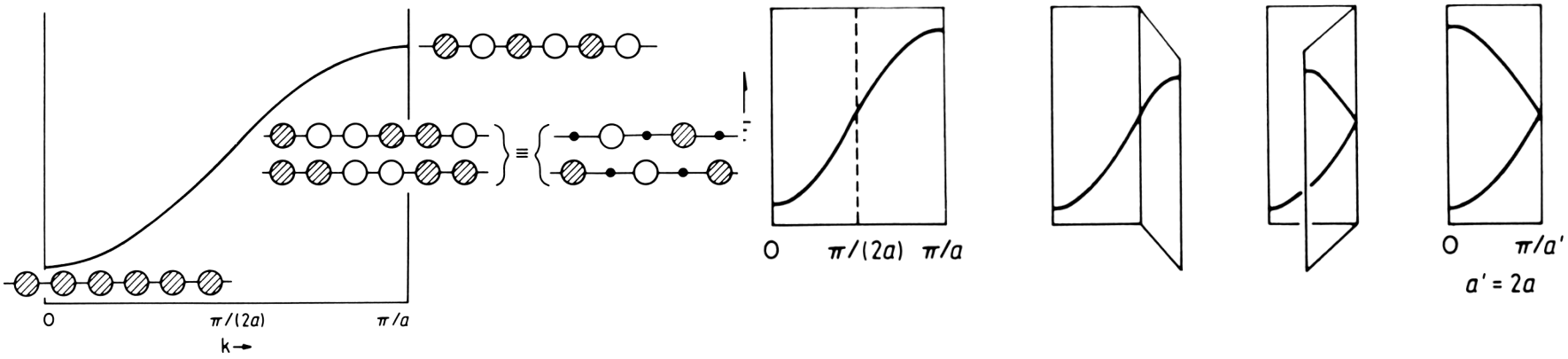
Square Nets of Main Group Elements in Solid-State Materials

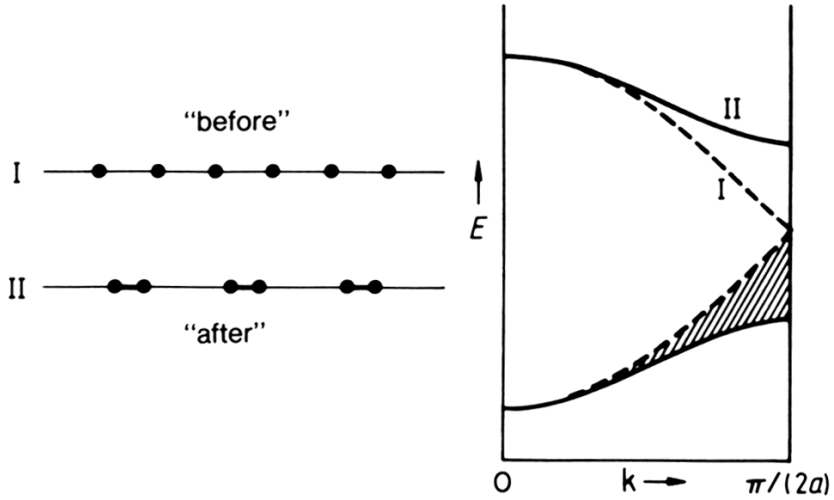
Wolfgang Tremel[1] and Roald Hoffmann*

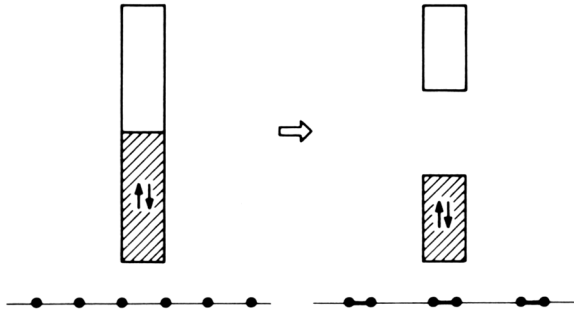
Contribution from the Department of Chemistry and Materials Science Center, Cornell University, Ithaca, New York 14853. *Received May 29, 1986*

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

Why is Hydrogen a molecule



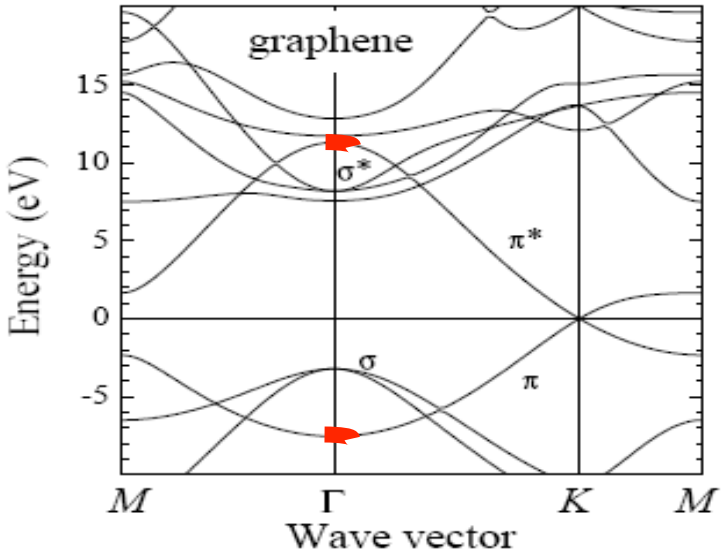


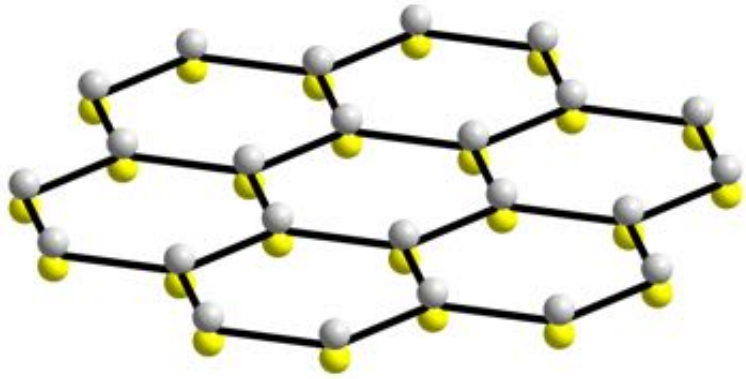


Peierls Distortion

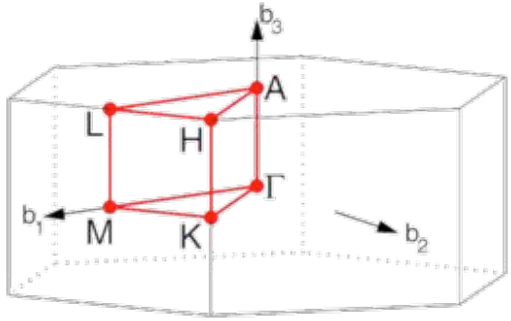
Hoffmann Angewandte. Chem. 26 (1987) 846

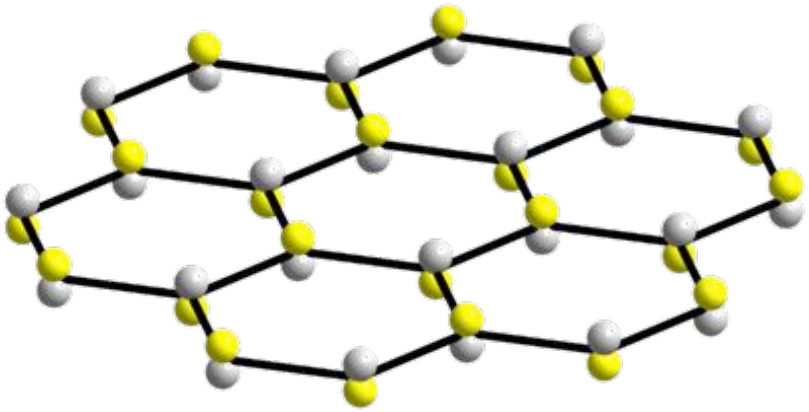
Graphene





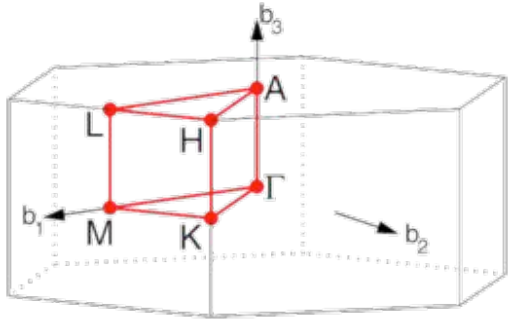
All P_z orbitals in-phase, Γ, Strongly π-bonding

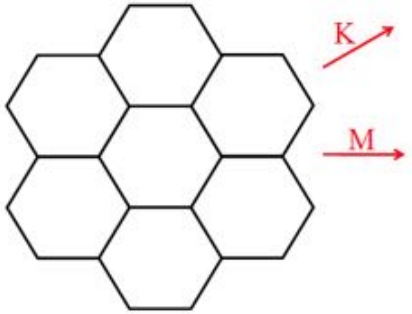




All P_z orbitals out-of-phase, Γ, Strongly anti π-bonding

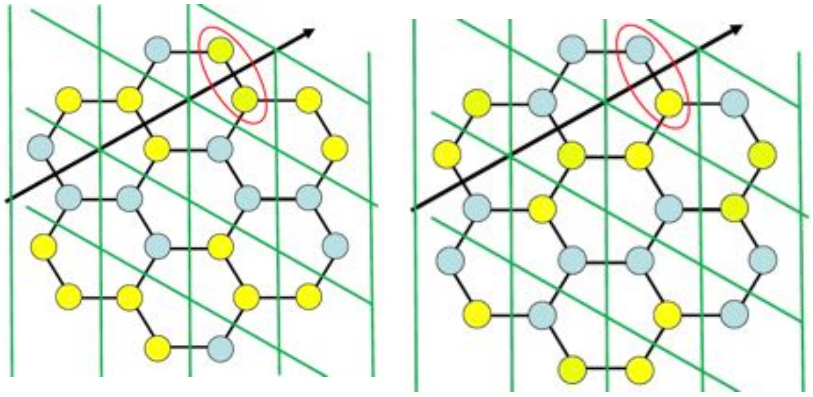
Graphene





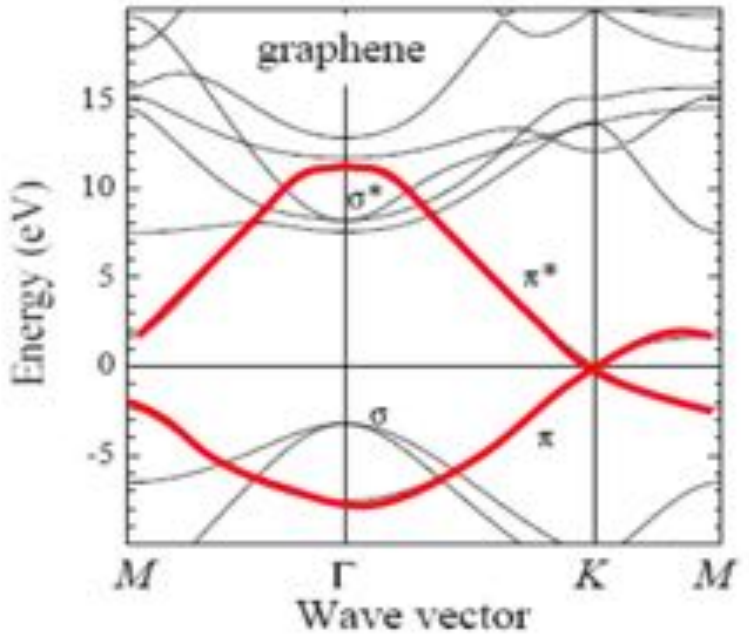
pz, π, K: non-bonding

pz, π*, K: non-bonding



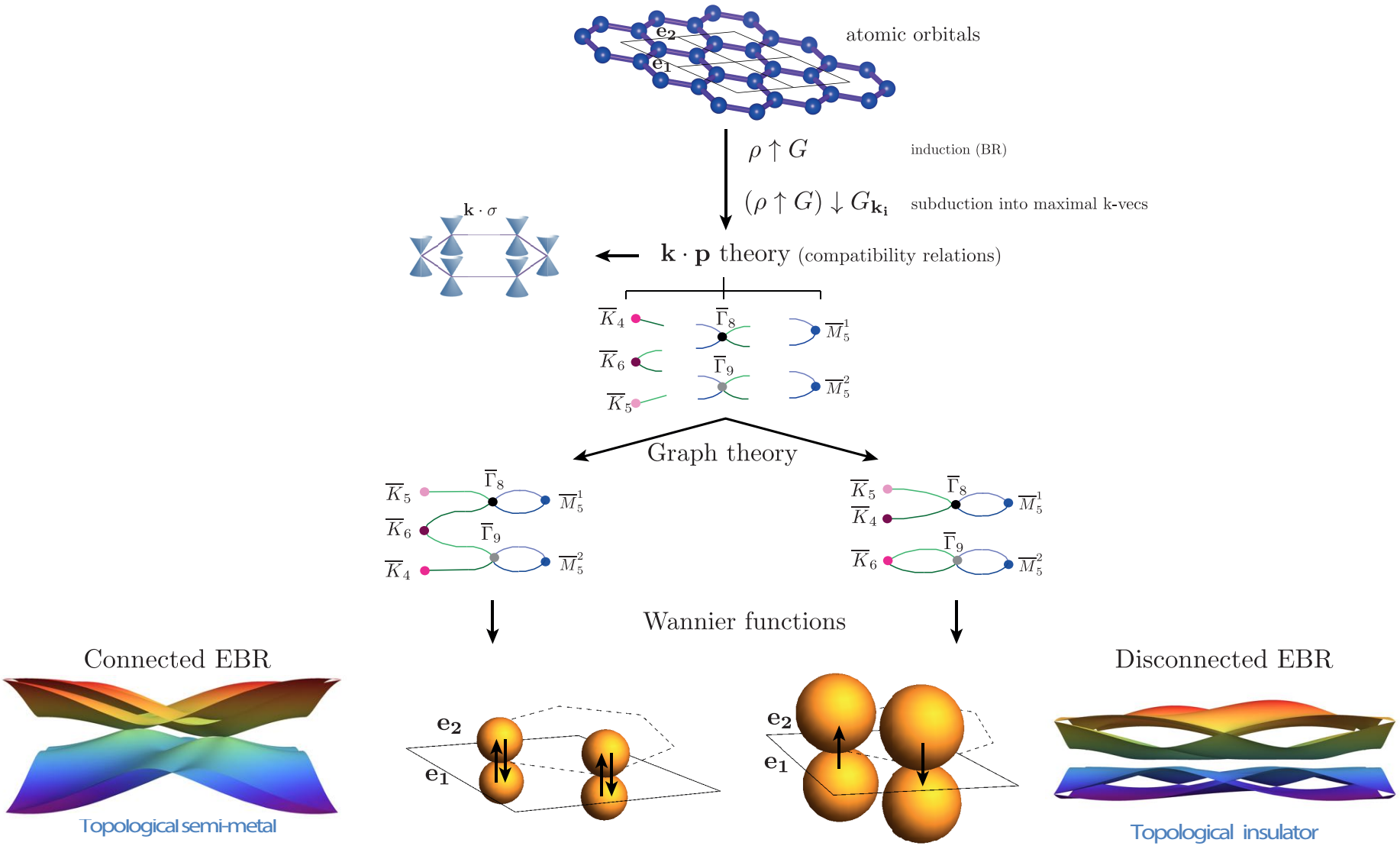
pz, π, M: bonding

pz, π, M*: anti-bonding



Translation

Barry, Andrei slide



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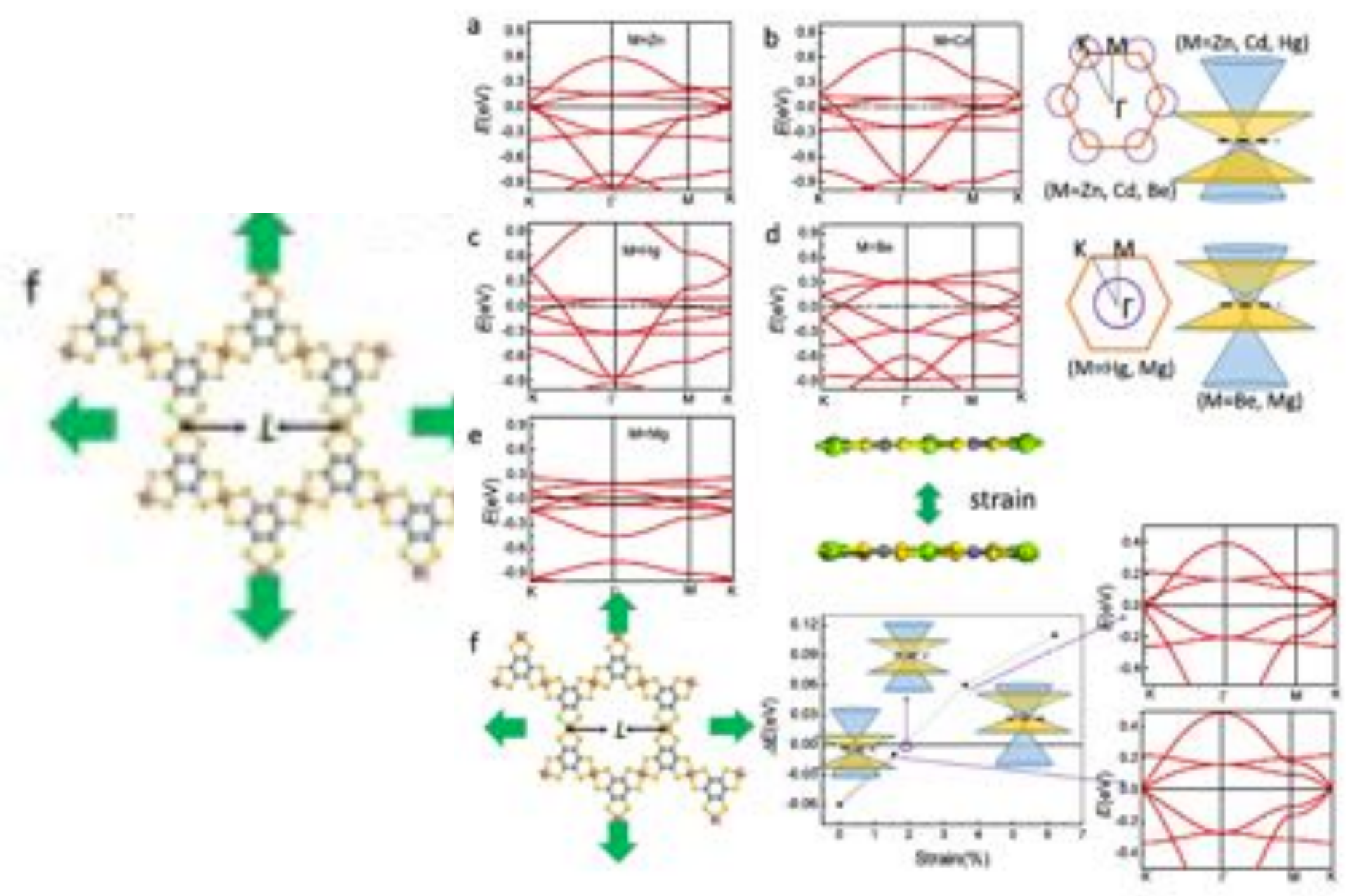
Conetronics in 2D Metal-Organic Frameworks



Wu et al. 2D Mater. 4 (2017) 015015 arXiv:1606.04094

Topology – interdisciplinary

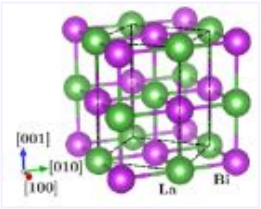
Chemistry

Real space - local

Crystals

LaBi

Crystal structure

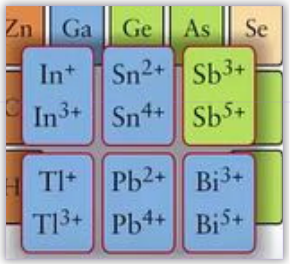


Position of the atoms

Orbitals

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

Inert pair effect

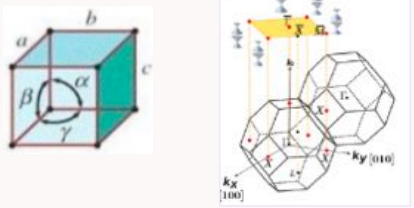


Physics

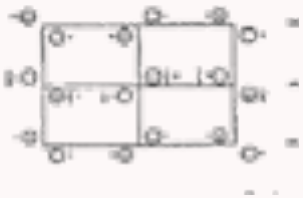
Recipro. space - delocalized

Brillouin zone

Symmetry

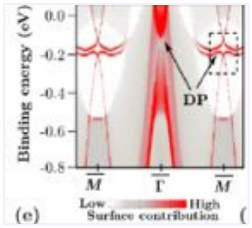


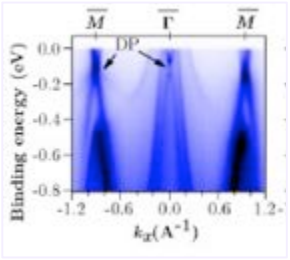
Local symmetry



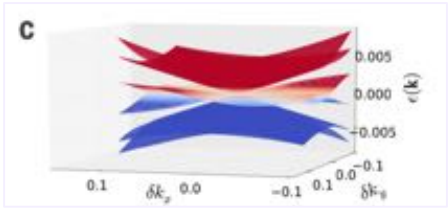
Relativistic effects

Electronic structure





Band connectivity

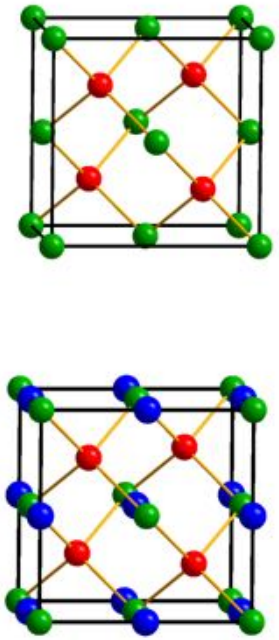


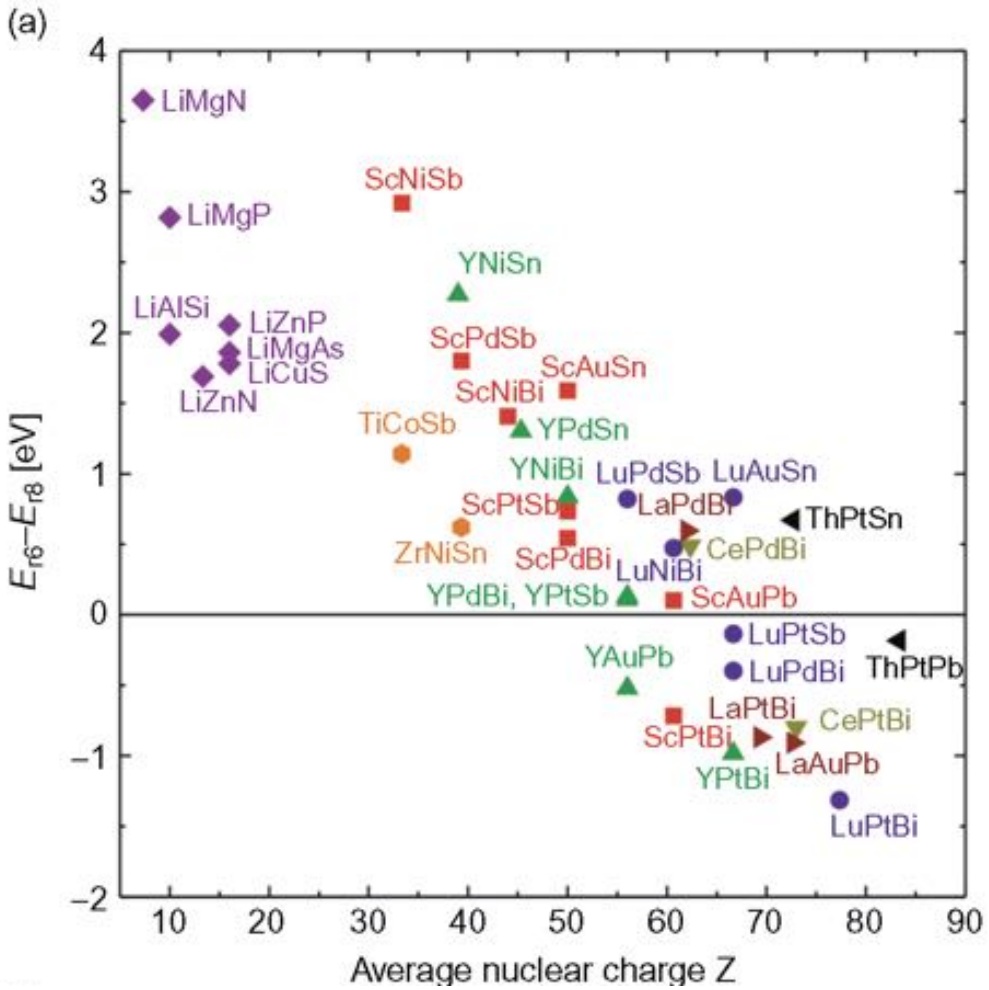
Darwin term

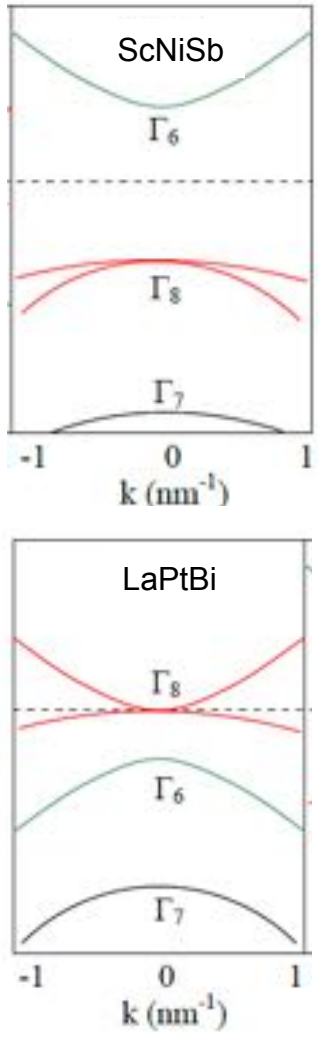
$$H_{\text{Darwin}} = \frac{\hbar^2}{8m_e^2c^2}(\Delta V)$$

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

Predicting topological insulators

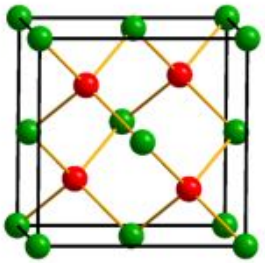




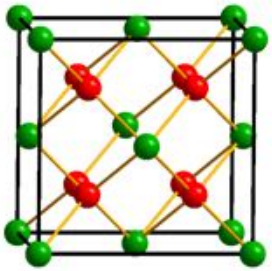


S. Chadov et al., Nat. Mater. **9** 541 (2010).
H. Lin et al., Nat. Mater. **9** 546 (2010).

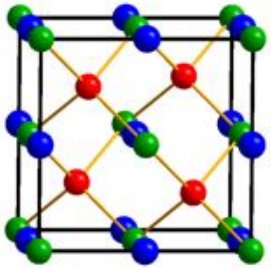
Structure to Property



HgTe

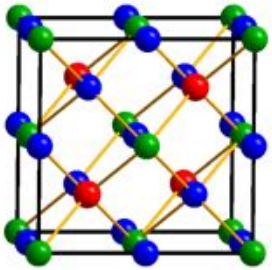


α Ag_2Te

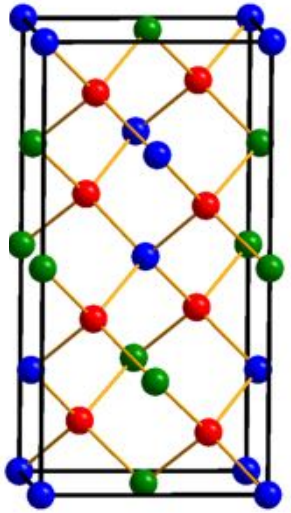


LaPtBi

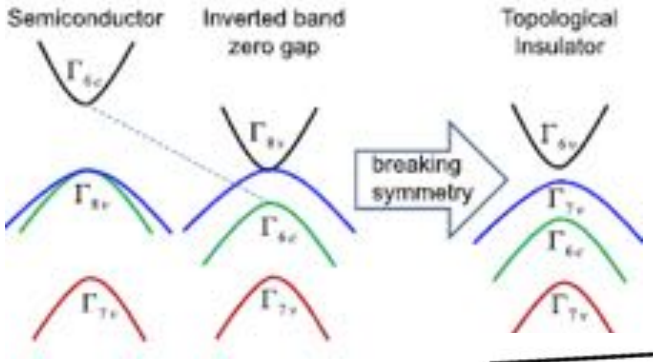
β Ag_2Te

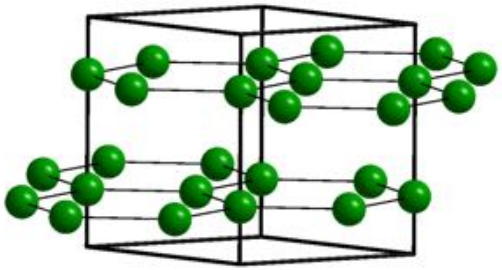


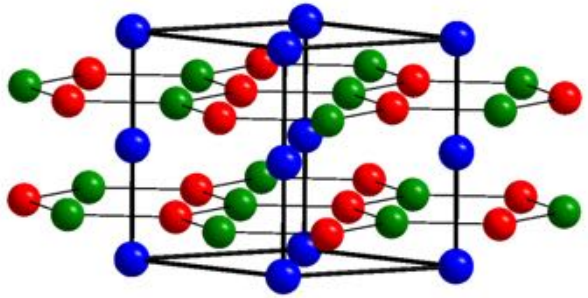
Li_2AgSb



$AuTlS_2$





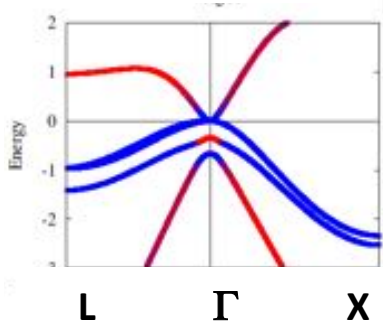


KHgSb

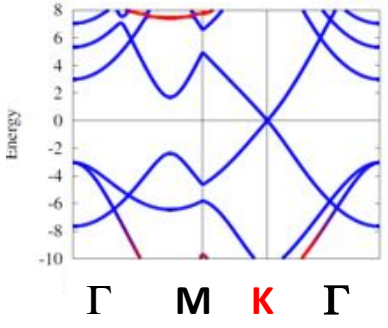
Müchler, et al., Angewandte Chemie 51 (2012) 7221.

Struktur und elektronische Struktur

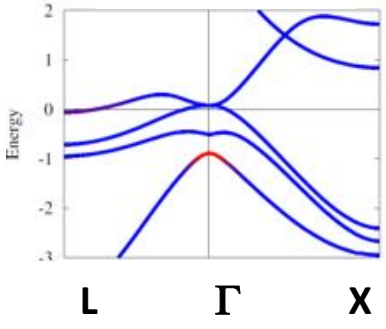
HgTe



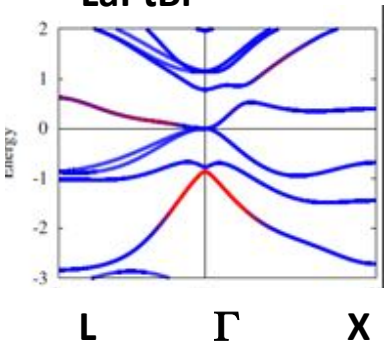
Graphite



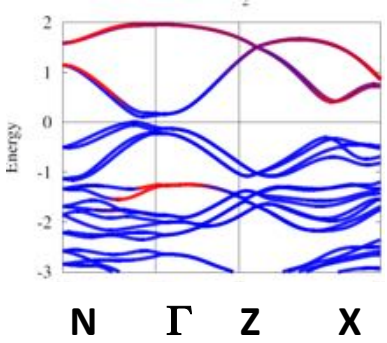
α Ag_2Te



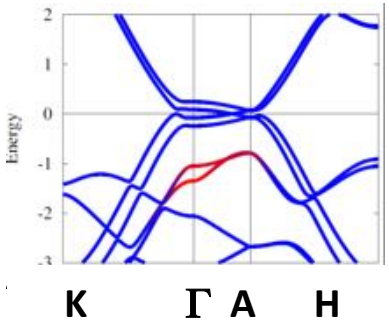
LaPtBi



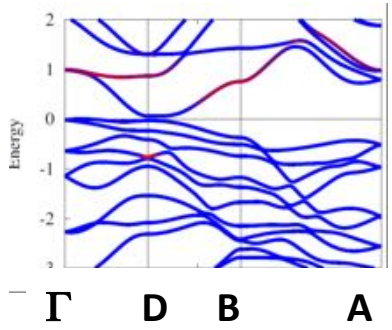
$AuTlTe_2$



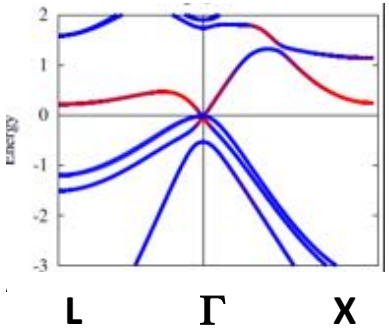
LiAuTe



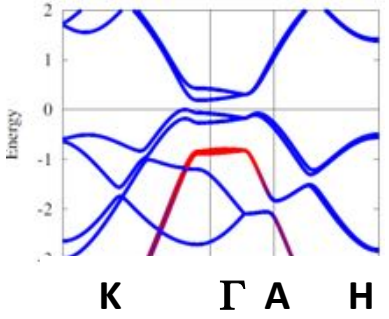
β Ag_2Te



Li_2AgSb

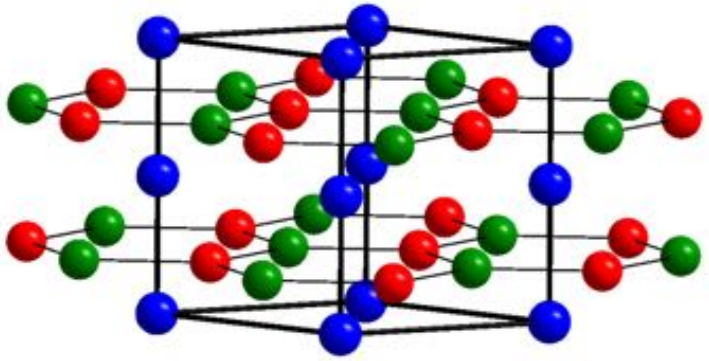


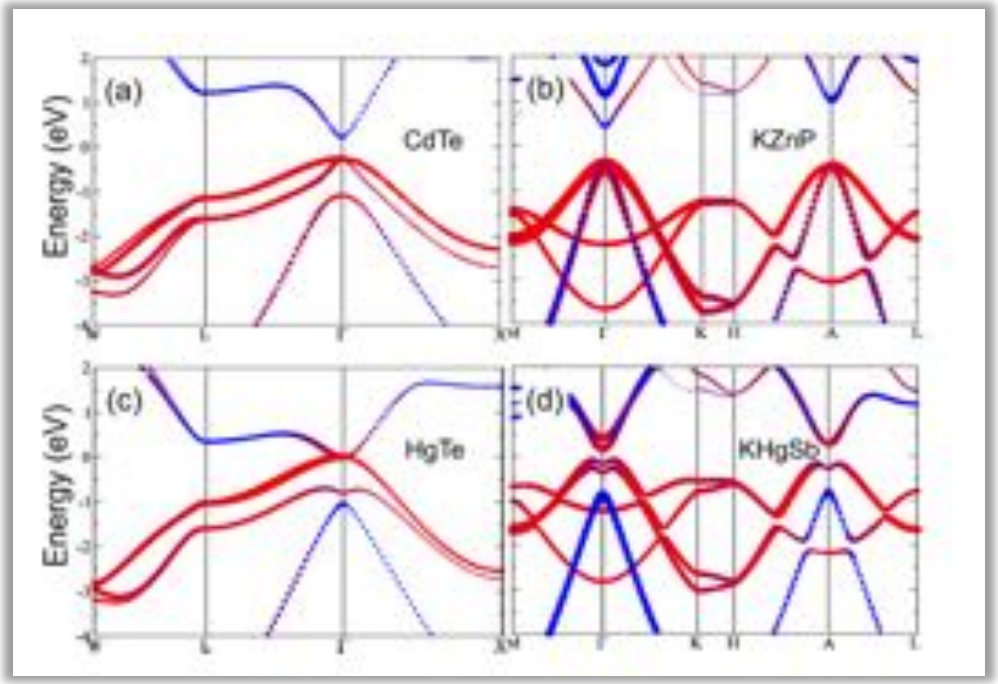
KHgSb



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

Honeycomb from sp^3 to sp^2

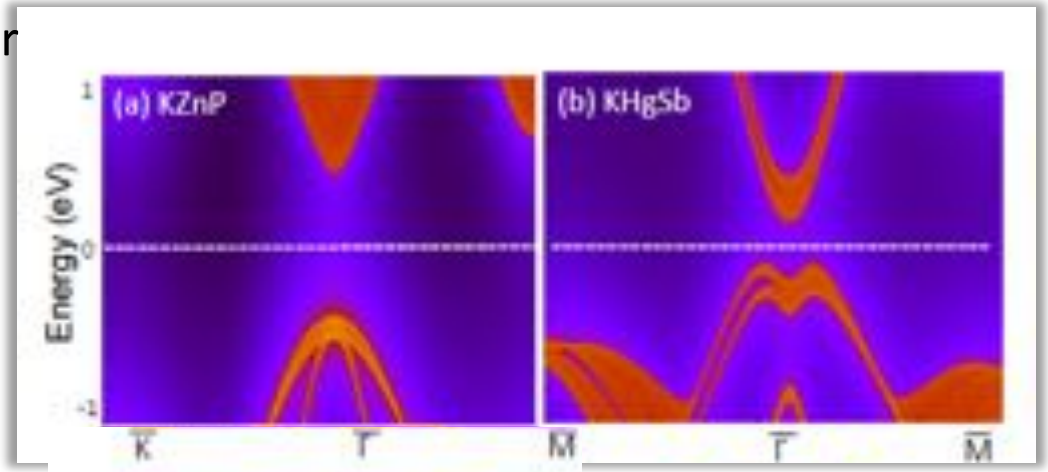




Band inversion is found in the heavier compounds

No surface state? Why ?

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

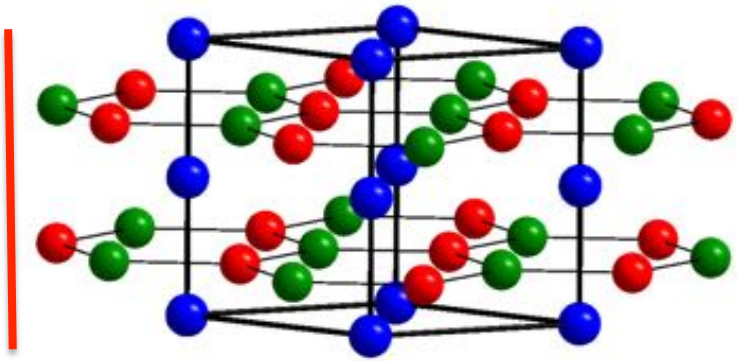


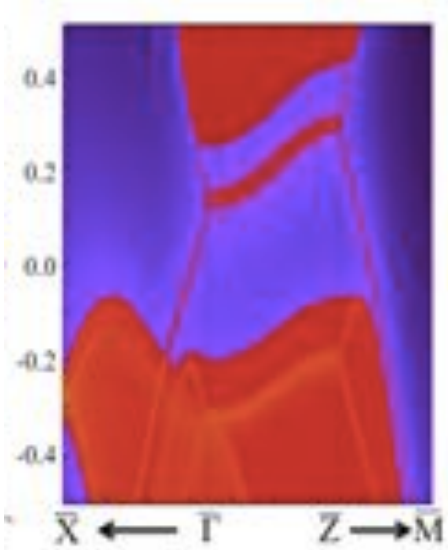
Zhang, Chadov, Müchler, Yan, Qi, Kübler, Zhang, Felser, Phys. Rev. Lett. 106 (2011) 156402 arXiv:1010.2195v1

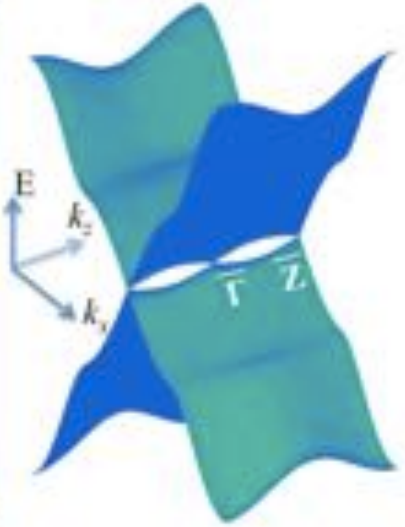
a)

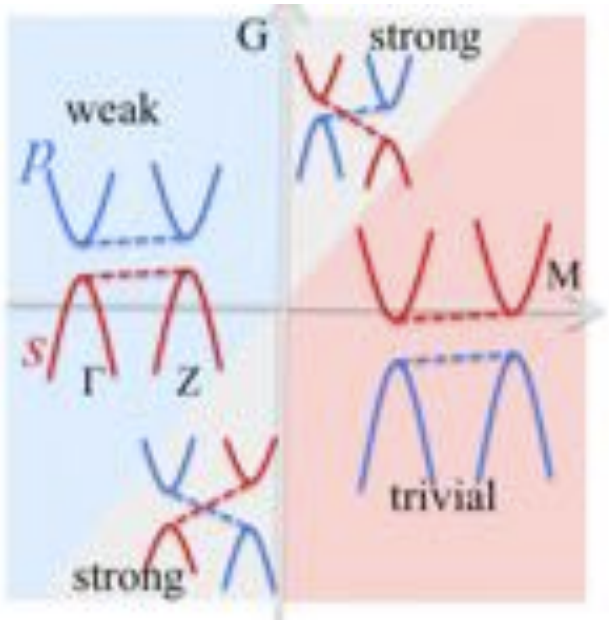
b)

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

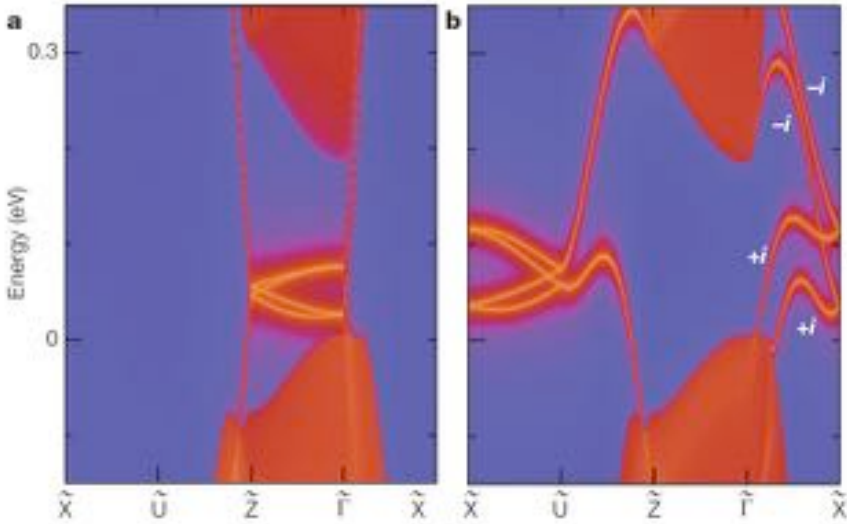
Yan, Müchler, Felser, Physical Review Lett. 109 (2012) 116406

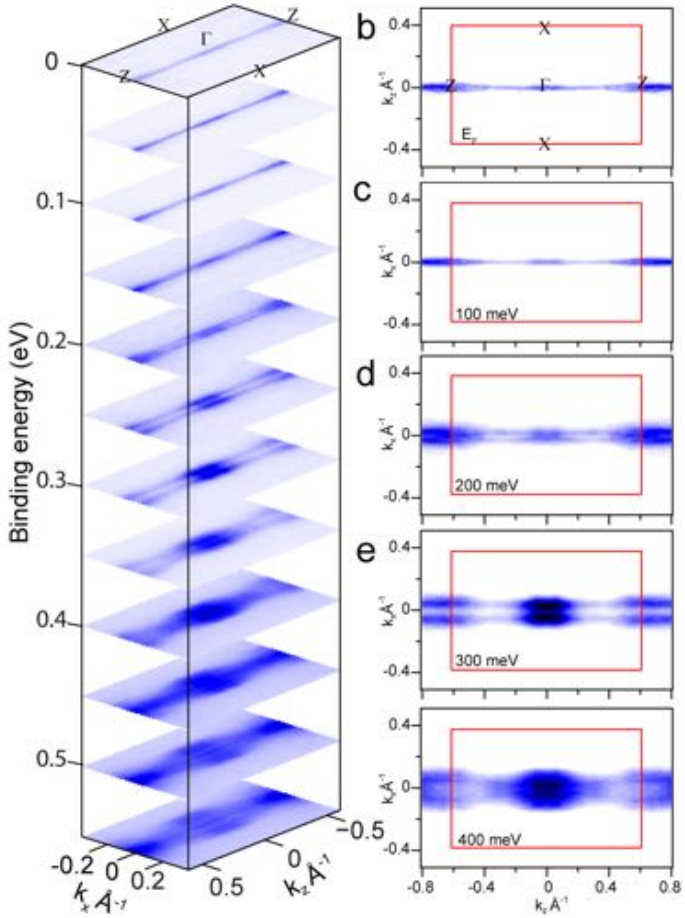
Hourglass

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

Dirac - Weyl Semimetals

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.

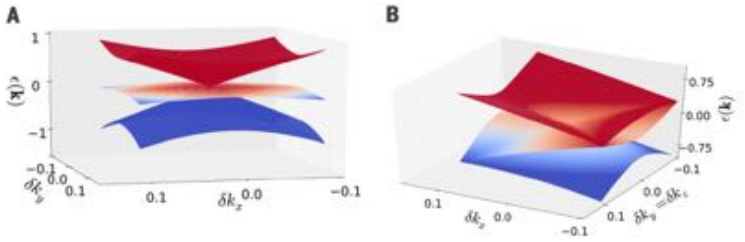
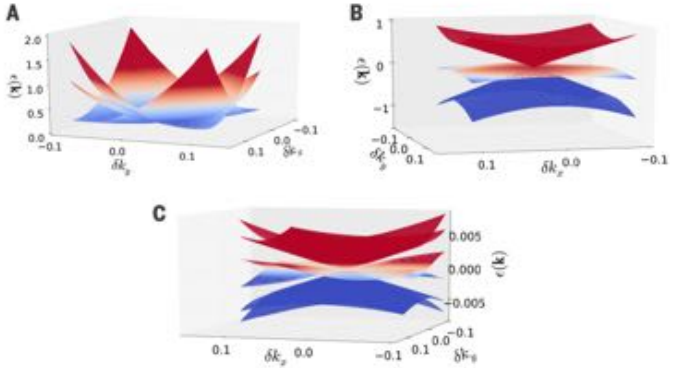
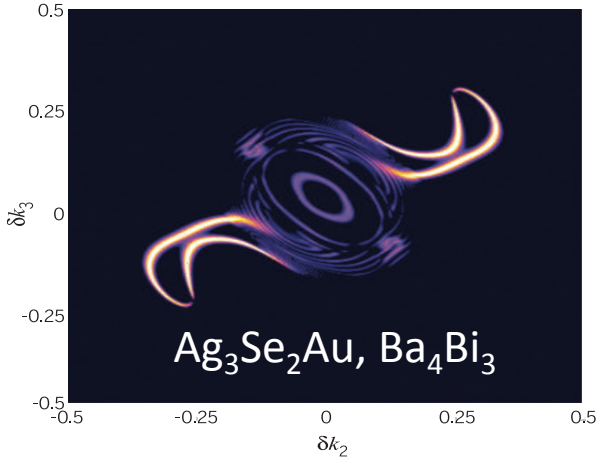


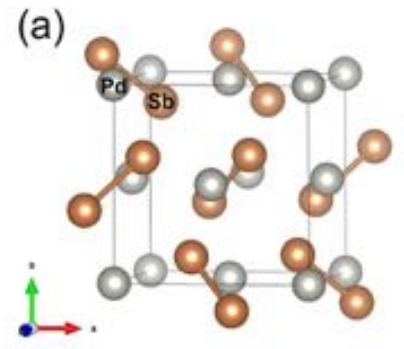
Fig. 1. Energy dispersion near a threefold degeneracy at the *P* point. (**A** and **B**) Shown are threefold degenerate points in (A) SGs 199 and 214 and (B) SG 220. In the latter case, pairs of bands remain degenerate in energy along the high-symmetry lines $|\delta k_x| = |\delta k_y| = |\delta k_z|$.

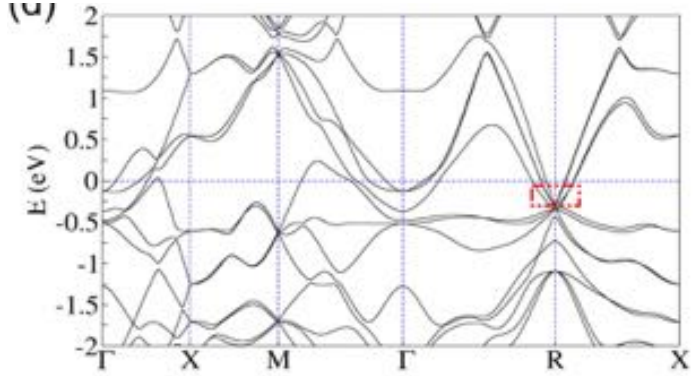


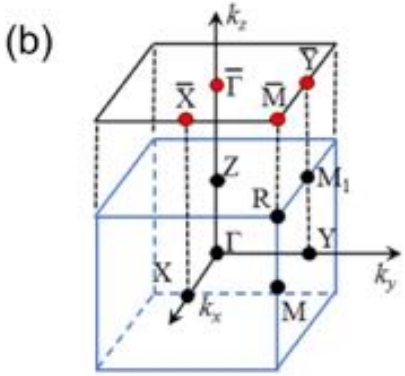


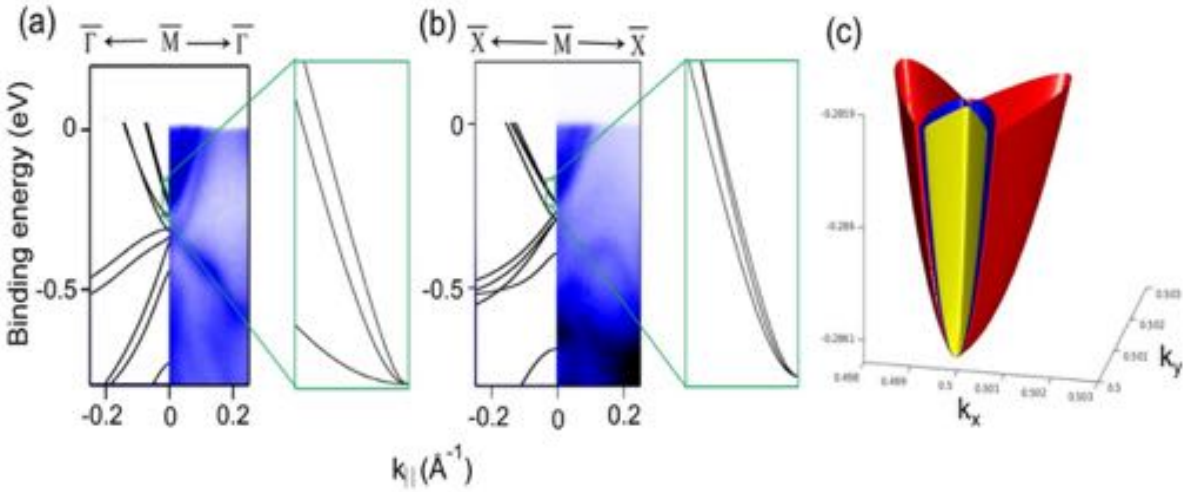
Science, 353, 6299, (2016)

Example: $PdSb_2$









6-fold fermions at the R point

Since SG 205 contains inversion symmetry, all bands are doubly degenerate

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

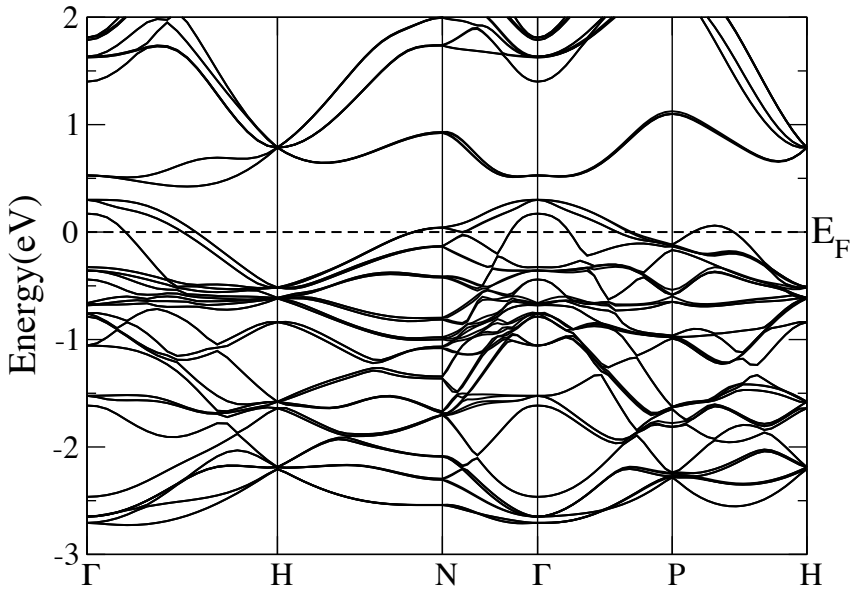
Andrei slide

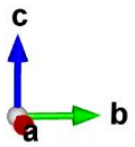
- Cubic crystal structure for high degenerations
- Non symmorphic is essential for stabilizing six- and eight-fold degenerate points.

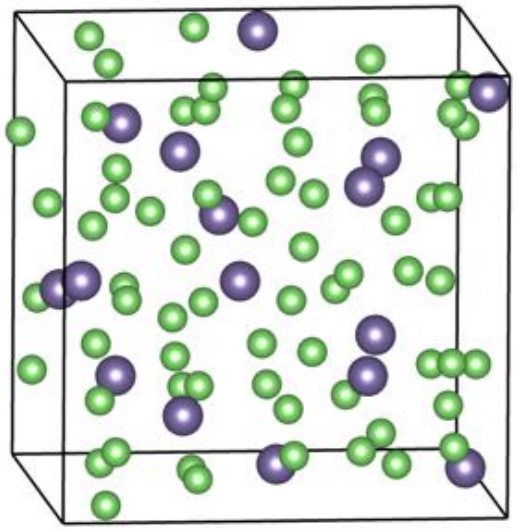
Novel Metals

Barry, Andrei slide

- SG I-43d (220) has elementary band representations with *16* branches -> 16fold connected metal if topologically trivial
- Filling -1/8 (lowest filling possible in a material is 1/24)
- Examples in the $A_{15}B_4$ material class (Here $Li_{15}Ge_4$)







Topology – interdisciplinary

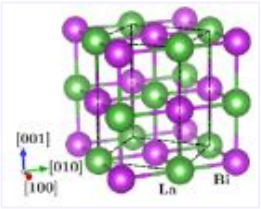
Chemistry

Real space - local

Crystals

LaBi

Crystal structure

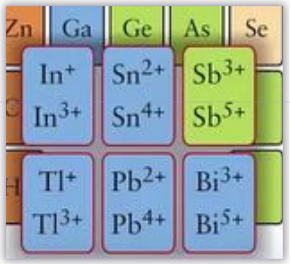


Position of the atoms

Orbitals

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

Inert pair effect

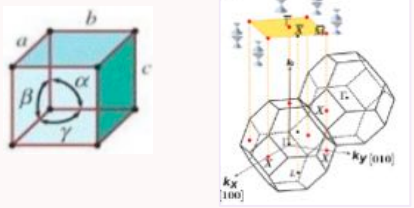


Physics

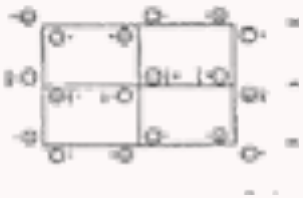
Recipro. space - delocalized

Brillouin zone

Symmetry

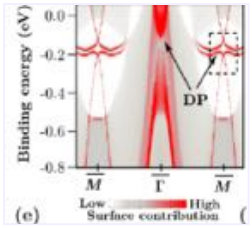


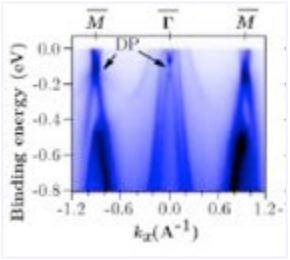
Local symmetry



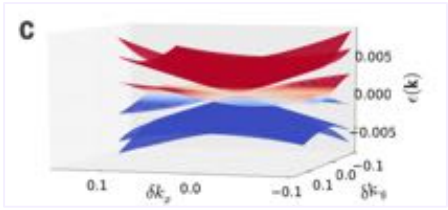
Relativistic effects

Electronic structure





Band connectivity



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)