Topological Quantum Chemistry

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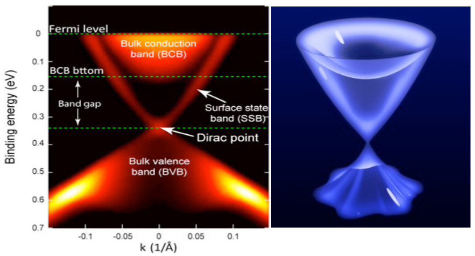
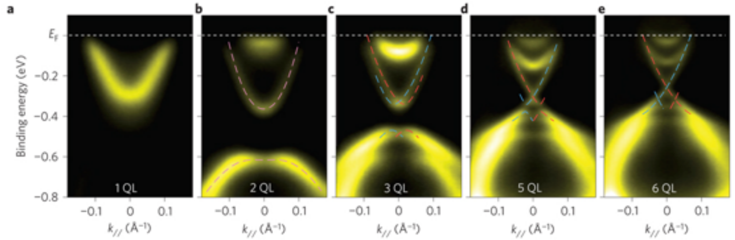
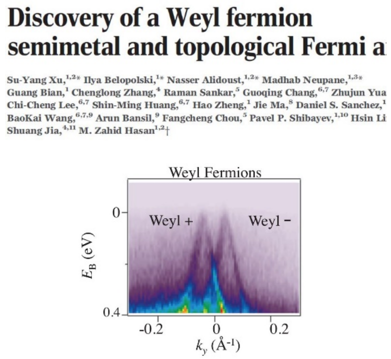
KITP

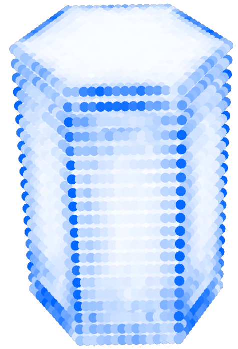
Topological Quantum Matter: Concepts and Realizations

Discovery of topological materials









Hsieh Nature (2008)
Zhang Nat Phys (2009)
Xia Nat Phys (2008)

3D TIs theory + exp protected by **TRS** : Bi_2Se_3

Chang Science (2013)

QAHE

Weng PRX (2015)
Xu Science (2015)

Weyl semimetals

New Fermions

Bradlyn (2016)

Nodal Lines

Bzdušek (2016)

2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018

Prediction HgTe 2D TI

Bernevig Science (2006)
König Science (2007)

Mirror Chern insulators

Hsieh Nat Comm (2012)
Tanaka Nat Phys (2012)

Type II Weyls

Soluyanov (2015)

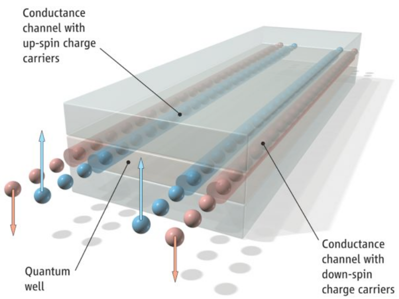
High Order TIs

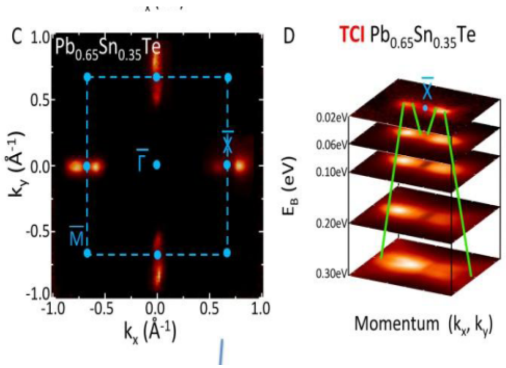
Schindler (2018)

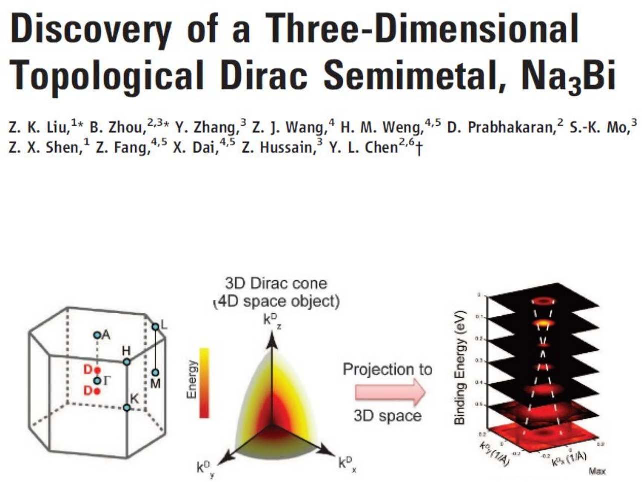
Dirac semimetals

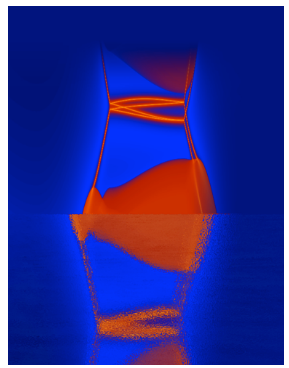
Non-symmorphic TIs

Alexandrinata (2016)









Kane & Mele, PRL (2015)

Recall: a space group is a set of symmetries that defines a crystal structure in 3D

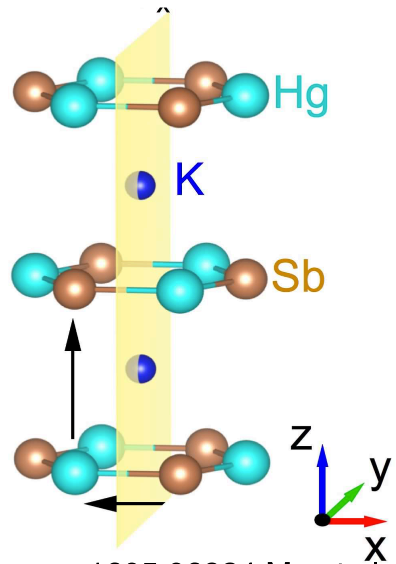


Image: 1605.06824 Ma et al

230 Space-Groups

Ingredients:

- unit lattice translations ($\mathbb{Z}^3$)
- point group operations (rotations, reflections)
- non-symmorphic (screw, glide)
- orbitals
- atoms in some lattice positions

How do we go from real space orbitals sitting on lattice sites to electronic bands (without a Hamiltonian)?

ELEMENTARY BAND REPRESENTATIONS

Zak PRB 26 (1982)

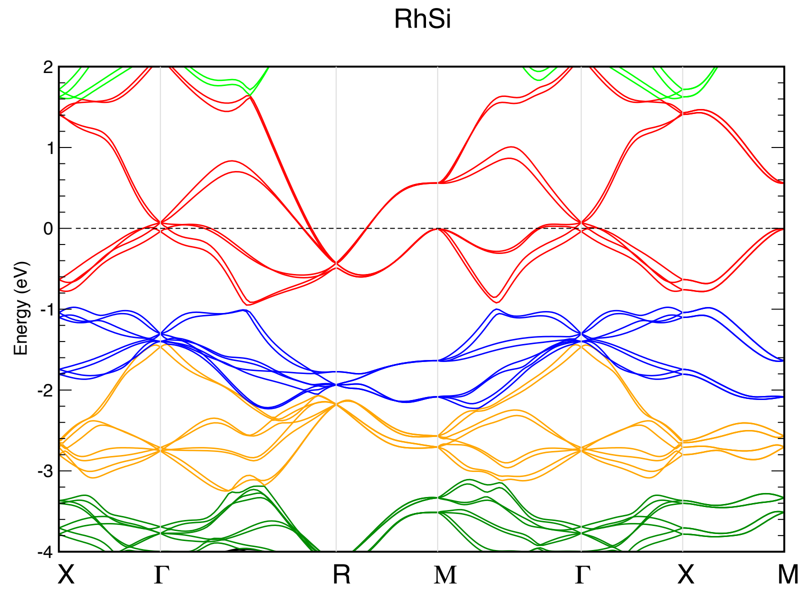
Band as Representations

Band Representation (BR): set of **bands linked to a localized orbital**
(respecting all the crystal symmetries and TRS)

↓

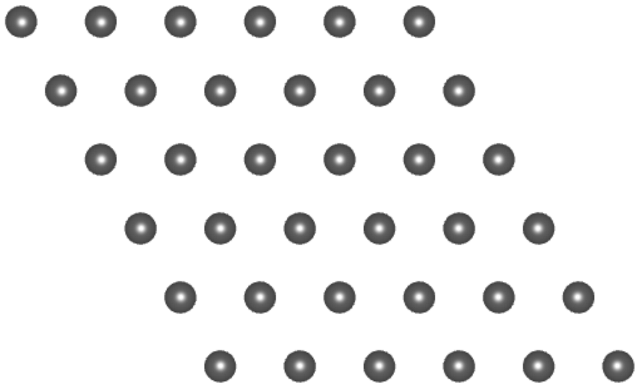
Elementary BR: smallest set of bands cannot be decomposed in elementary bands
Physical Elementary BR: when EBR also respects TR symmetry
Composite BR: A BR which is not elementary is a "composite"

(P)EBRs are connected along the BZ



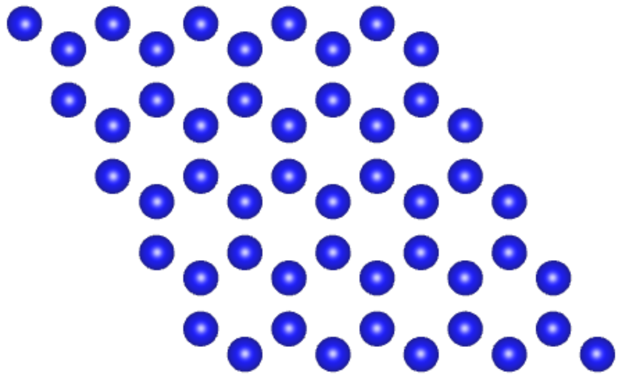
Zak PRB 26 (1982)

Induction of a (P)EBR



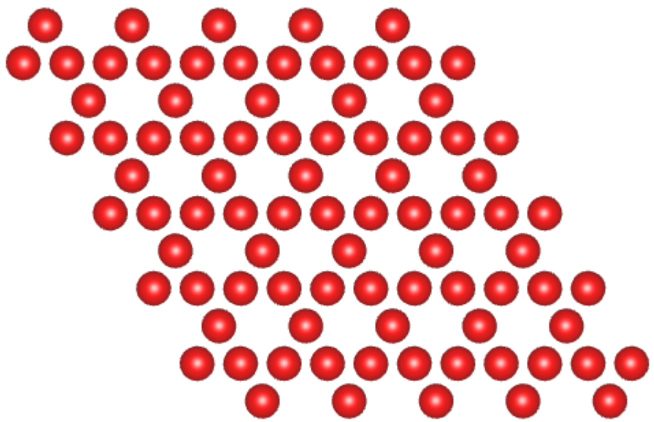
1 atom/unit cell
(triangular)

1a



2 atoms/unit cell
(honeycomb)

2b



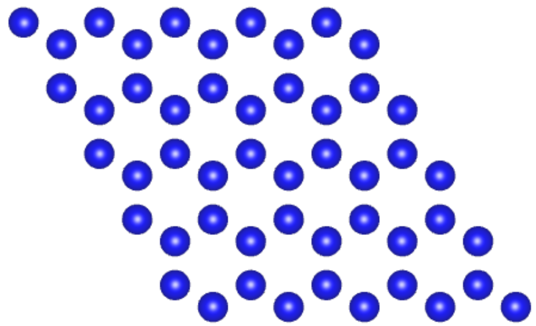
3 atoms/unit cell
(kagome)

3c

- Within the same SG many ways to arrange atoms
- Each arrangement determines different representations

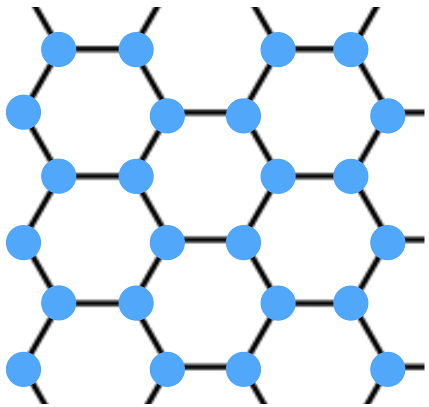
Induction of a (P)EBR

- Within the same lattice, different orbitals

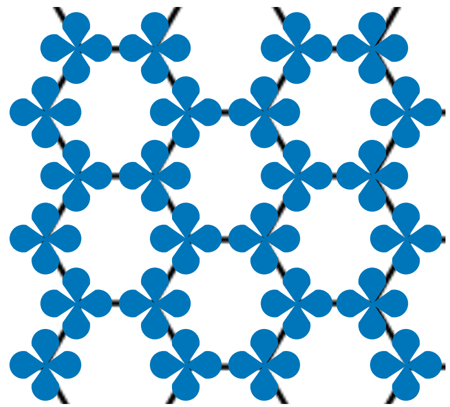


2 atoms/unit cell

s (or p_z) orbitals



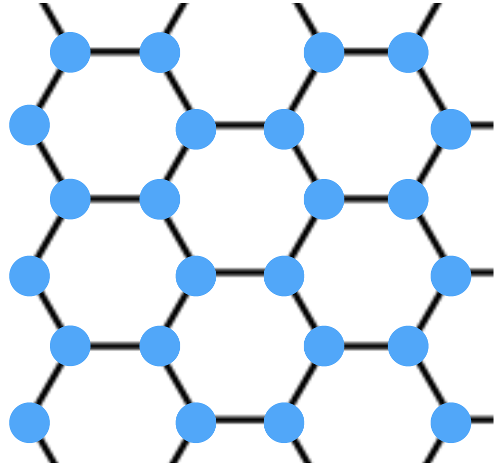
p_x and p_y orbitals



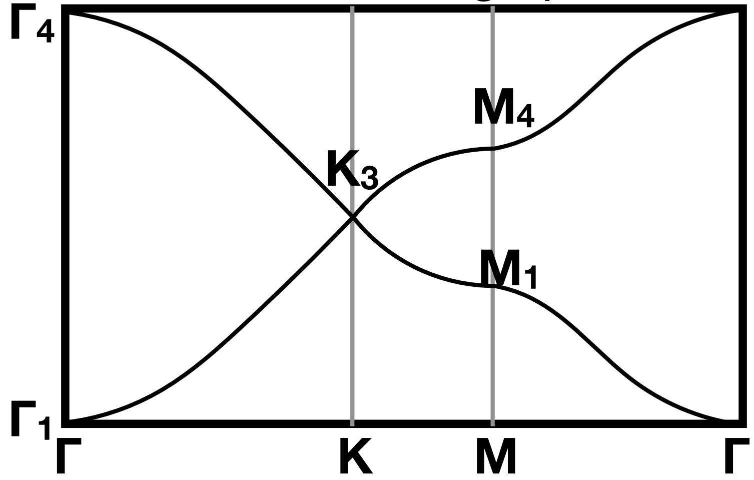
Induction of a (P)EBR

Site-symmetry group, G_q, leaves q invariant

s (or p_z) orbitals

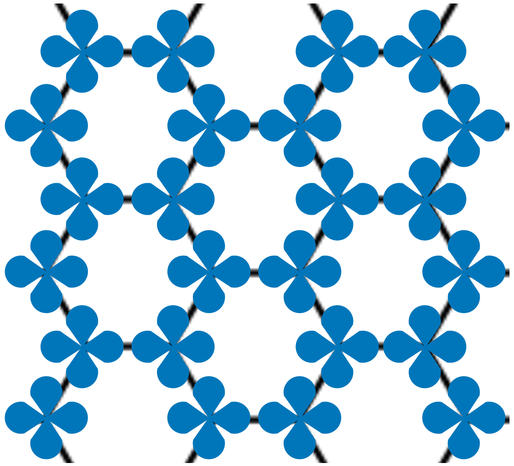


Band structure graphene

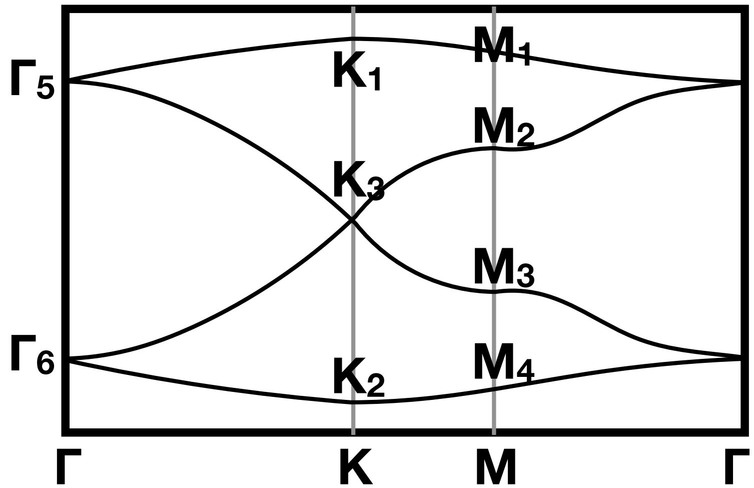


Real space vs momentum space

p_x and p_y orbitals



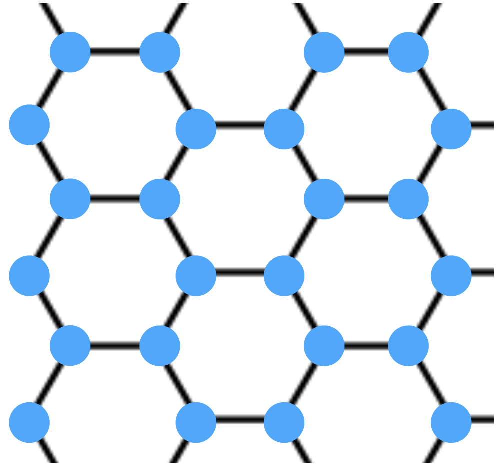
Band structure bismuthene



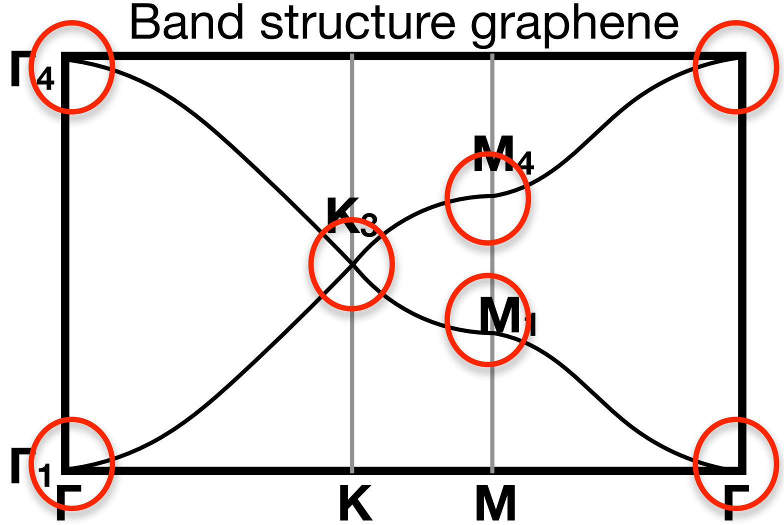
Induction of a (P)EBR

Each arrangement/orbital determines symmetry representations in the Brillouin zone

s (or p_z) orbitals

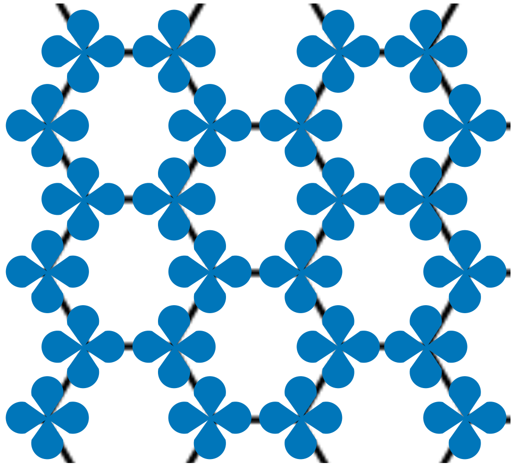


Band structure graphene

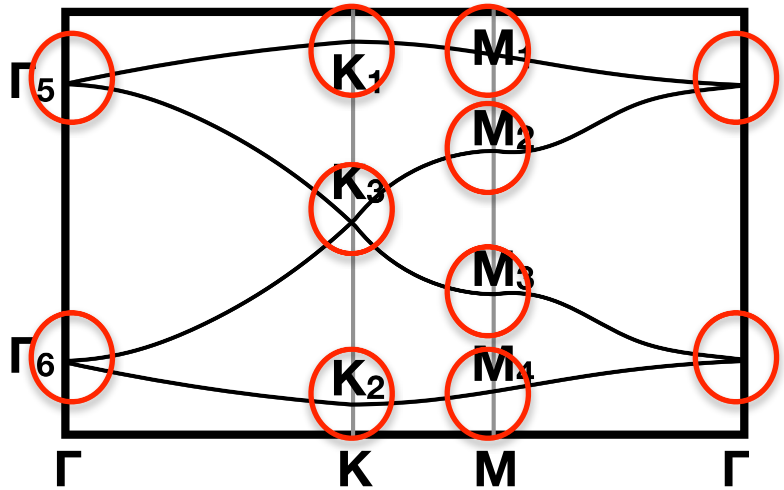


Real space vs momentum space

p_x and p_y orbitals



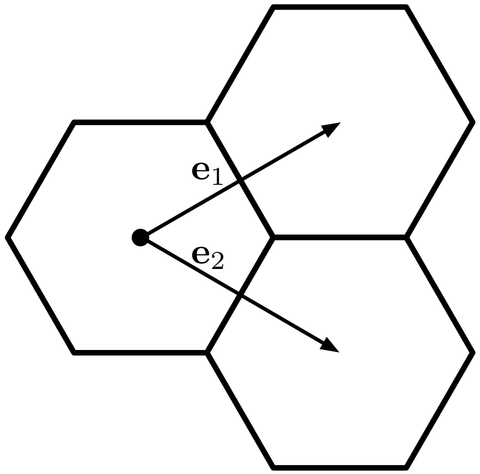
Band structure bismuthene



Induction of a (P)EBR: Example of the honeycomb lattice

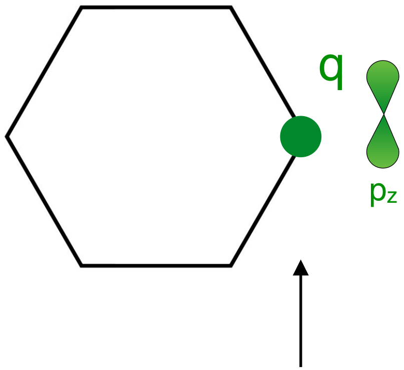
Lets consider the generators of 2D P6mm: $\{C_2, C_3, m_{1\bar{1}}\}$

Lattice vectors:



$$\begin{cases} \mathbf{e}_1 = \sqrt{3}/2\mathbf{x} + 1/2\mathbf{y} \\ \mathbf{e}_2 = \sqrt{3}/2\mathbf{x} - 1/2\mathbf{y} \end{cases}$$

Lattice site: Wyckoff 2b, spinfull p_z



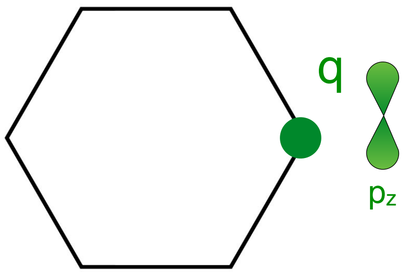
Site-symmetry group, G_q, leaves q invariant

Coset decomposition of a Space Group :

$$G = \bigcup_{\alpha=1}^{n} (g_\alpha)\ (G_q \ltimes \mathbf{Z}^3)\ ,\ g_\alpha \notin G_q$$

Induction of a (P)EBR: Example of the honeycomb lattice

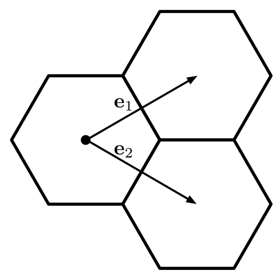
Consider one lattice site:



$$G = \bigcup_{\alpha} (g_{\alpha})\ (G_q \ltimes \mathbf{Z}^3)$$

(2) (1)

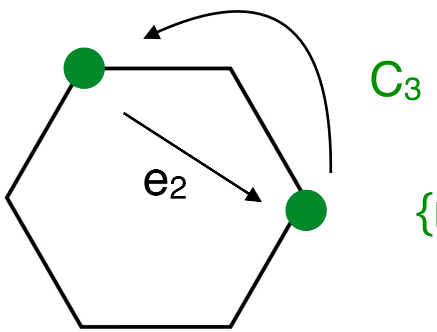
$\{C_2, C_3, m_{1\bar{1}}\}$



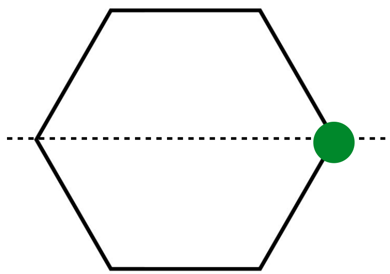
(1) Site-symmetry group, G_q, leaves q invariant $\{C_3|01\}, \{m_{1\bar{1}}|00\}$ $\approx C_{3v}$

→ Orbitals at q transform under a rep, ρ, of G_q

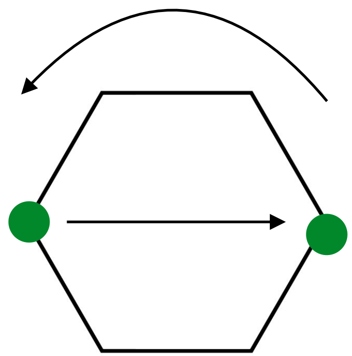
$\{C_3|01\}$



$\{m_{1\bar{1}}|00\}$

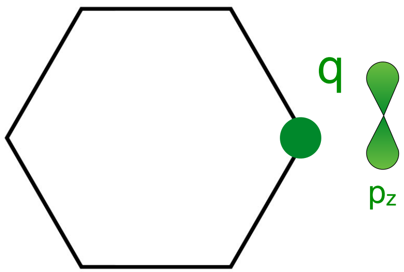


$\{C_2|?\}$



Induction of a (P)EBR: Example of the honeycomb lattice

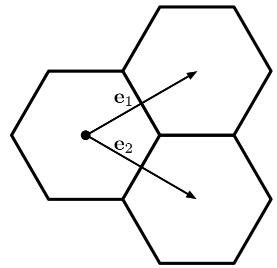
Consider one lattice site:



$$G = \bigcup_{\boldsymbol{\alpha}} (g_{\boldsymbol{\alpha}})\ (G_q \ltimes \mathbf{Z}^3)$$

(2) (1)

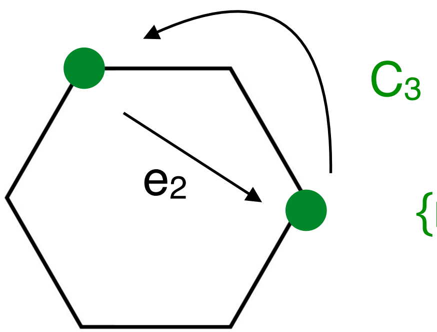
$\{C_2, C_3, m_{11}\}$



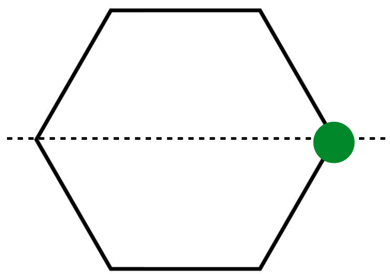
(1) Site-symmetry group, G_q, leaves q invariant $\{C_3|01\}, \{m_{1\bar{1}}|00\}$ $\approx C_{3v}$

⟶ Orbitals at q transform under a rep, ρ, of G_q

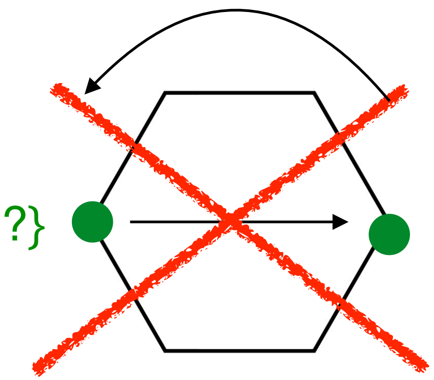
$\{C_3|01\}$



$\{m_{1\bar{1}}|00\}$

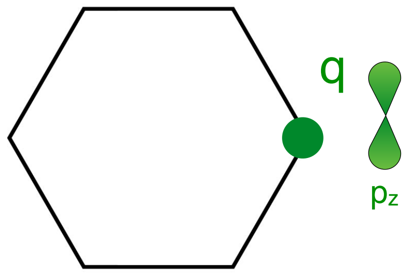


$\{C_2|?\}$



Induction of a (P)EBR: Example of the honeycomb lattice

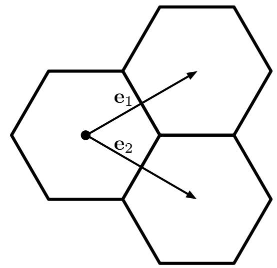
Consider one lattice site:



$$G = \bigcup_{\alpha} (g_\alpha)\ (G_q \ltimes \mathbb{Z}^3)$$

(2) (1)

$\{C_2, C_3, m_{11}\}$



(1) Site-symmetry group, G_q, leaves q invariant $\{C_3|01\}, \{m_{1\bar{1}}|00\}$ $\approx C_{3v}$

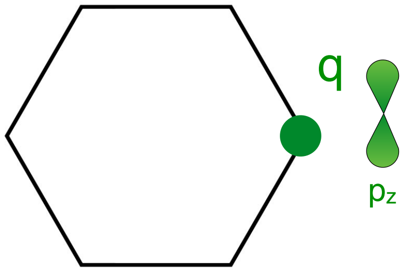
⟶ Orbitals at q transform under a rep, ρ, of G_q

Rep	E	C_3	M	$\bar{E}$
⟶ $\bar{\Gamma}_6$	2	1	0	-2

Character table for the double-valued representation of C_{3v}

Induction of a (P)EBR: Example of the honeycomb lattice

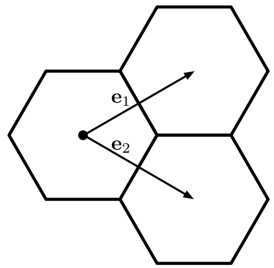
Consider one lattice site:



$$G = \bigcup_{\alpha} (g_{\alpha})\ (G_q \ltimes \mathbb{Z}^3)$$

(2) (1)

$\{C_2, C_3, m_{11}\}$

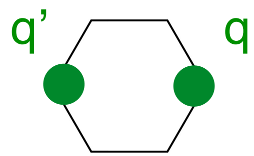


(1) Site-symmetry group, G_q, leaves q invariant $\{C_3|01\}, \{m_{1\bar{1}}|00\}$ $\approx C_{3v}$

⟶ Orbitals at q transform under a rep, ρ, of G_q

(2) Elements of space group $g \notin G_q$ (coset representatives) move sites in an orbit "Wyckoff position" $\{C_2|00\},\{E|00\}$

Wyckoff multiplicity: 2
orbit of q



Induction of a (P)EBR: Example of the honeycomb lattice

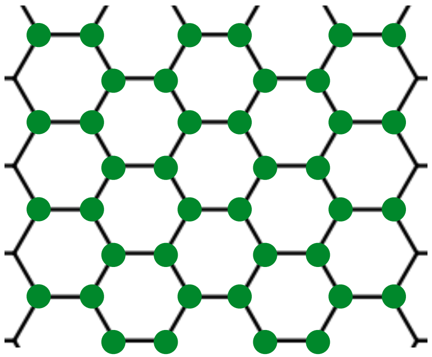
$\bar{\Gamma}_6$ induced in C_{6v}

electron bands sitting at pz orbitals in
Wyckoff 2b in wall paper group 17

$\rho_G = \rho \uparrow G$

Coset representative g: $\{C_2|00\},\{E|00\}$

h ∈ G, generators of
honeycomb lattice: C_2, C_3, σ



$$\rho_{i\alpha,j\beta}(h) = \rho_{ij}(g_{\alpha\beta})$$

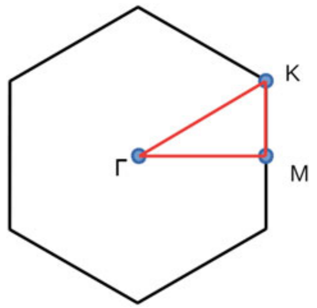
$$g_{\alpha\beta} = g_\alpha^{-1}\{E|t_{\alpha\beta}\}hg_\beta$$

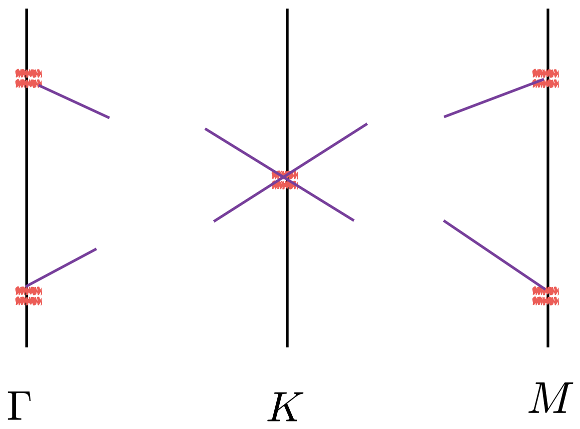
$$\rho_G^k(h) = e^{-(k \cdot t_{\alpha\beta})}\rho_{ij}(g_{\alpha\beta})$$

dimension of this band representations = connectivity in the Brillouin zone

Subduction in momentum space

$$(\rho \uparrow G) \downarrow G_k$$





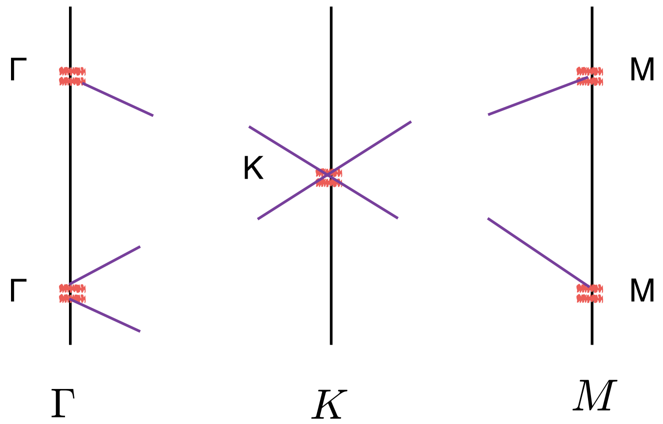
$$\rho_G^{\Gamma} = \bar{\Gamma}_7 \oplus \bar{\Gamma}_8$$

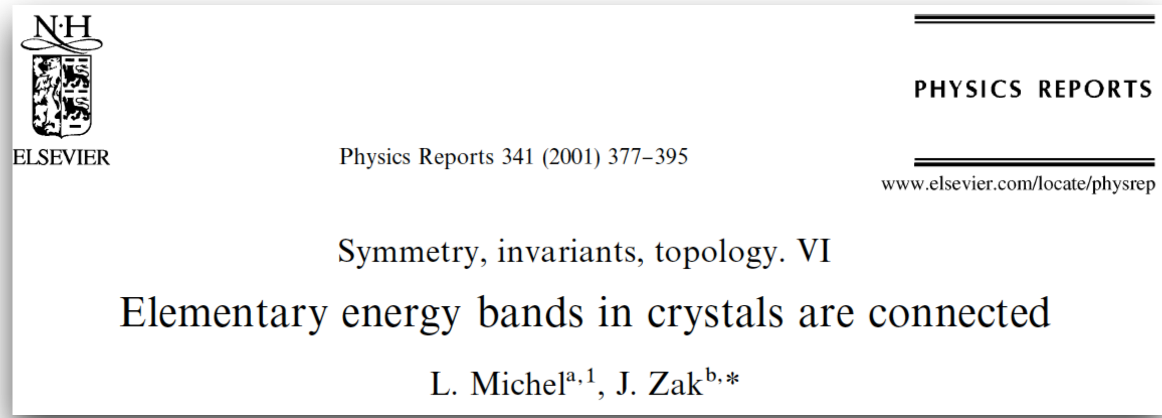
Table 1.5 Table of characters of the group C_{6v}

C_{6v}	E	$C_3^{\pm}$	$C_2, \bar{C}_2$	$C_6^{\pm}$	m_{11}	$m_{1\bar{1}}$	$\bar{E}$	$\bar{C}_3^{\pm}$	$\bar{C}_6^{\pm}$
ρ_G^{Γ}	4	2	0	0	0	0	−4	−2	0
$\bar{\Gamma}_7$	2	1	0	$-\sqrt{3}$	0	0	−2	−1	$\sqrt{3}$
$\bar{\Gamma}_8$	2	1	0	$\sqrt{3}$	0	0	−2	−1	$-\sqrt{3}$
$\bar{\Gamma}_9$	2	−2	0	0	0	0	−2	2	0

ATOMIC LIMIT

- Restricting to the little group at k to find irreps at each k point (subduction) -> **all bands connected**
- **-** EBR is defined by a **maximal Wyckoff position and the irreps in real space**





N·H
ELSEVIER
Physics Reports 341 (2001) 377–395
PHYSICS REPORTS
www.elsevier.com/locate/physrep

Symmetry, invariants, topology. VI

Elementary energy bands in crystals are connected

L. Michel[a,1], J. Zak[b,*]

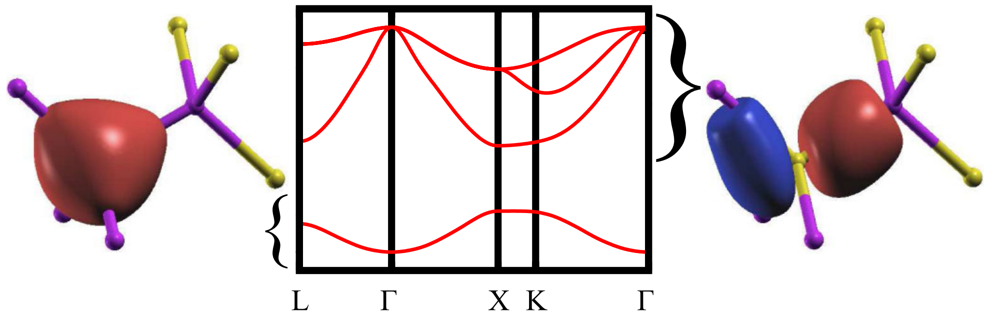
- **Topology?**

By construction, a **band representation has an atomic limit**,
and all atomic limits yield a band representation

↕

Recall: **Topological bands** **CANNOT Have Maximally Localized** Wannier Function

ATOMIC LIMIT



1) Bands in ρ_G are **connected** (this phase can always realized) in the Brillouin zone

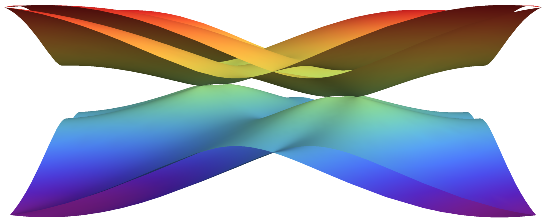
2) Bands in ρ_G are **not connected**: at least one **topological band**

(Disconnected (P)EBR = set of disconnected bands that connected form an (P)EBR)

GRAPHENE

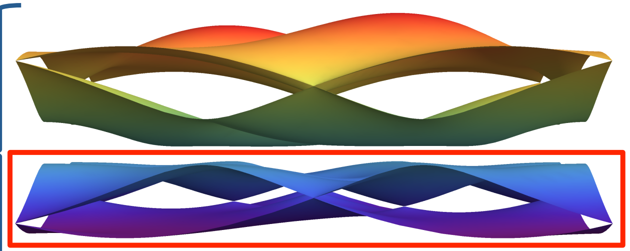
What makes the disconnected bands topological?

All four bands come from a single set of localized orbitals (p_z, spin up/down)



Symmetry enforced semi-metal

Local description:
Wannier functions ≈
atomic orbitals



Topological insulator

Cannot be described by localized Wannier functions while preserving symmetries (Soluyanov and Vanderbilt 2011)

Disconnected bands are topological because they lack localized Wannier functions that obey TR

Kane, Mele Phys. Rev. Lett (2005)

TQC Statement

All sets of bands induced from symmetric, localized orbitals, are topologically trivial by design.

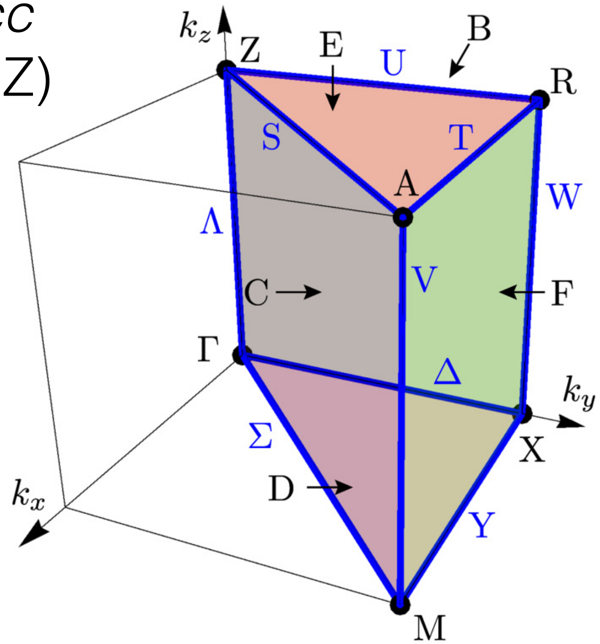
Nature 547, 298--305 (2017)

Maximal k-vectors and paths

For all the 230 SG:
maximal k-vectors + minimal set non-redundant **connections**

k vector in a manifold is maximal if its little co-group it's not a subgroup of another manifold of vectors **k'** (in general coincides with high-symmetry k-vector)

P4/ncc
(first BZ)



k-vec	mult.	Coordinates	Little	Maximal co-group	TR
Γ	1	(0,0,0)	$4/mmm(D_{4h})$	yes	yes
Z	1	(0,0,1/2)	$4/mmm(D_{4h})$	yes	yes
M	1	(1/2,1/2,0)	$4/mmm(D_{4h})$	yes	yes
A	1	(1/2,1/2,1/2)	$4/mmm(D_{4h})$	yes	yes
R	2	(0,1/2,1/2)	$mmm(D_{2h})$	yes	yes
X	2	(0,1/2,0)	$mmm(D_{2h})$	yes	yes
Λ	2	$(0,0,w), 0 < w < 1/2$	$4mm(C_{4v})$	no	no
V	2	$(1/2,1/2,w), 0 < w < 1/2$	$4mm(C_{4v})$	no	no
W	4	$(0,1/2,w), 0 < w < 1/2$	$mm2(C_{2v})$	no	no
Σ	4	$(u,u,0), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
S	4	$(u,u,1/2), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
Δ	4	$(0,v,0), 0 < v < 1/2$	$mm2(C_{2v})$	no	no
U	4	$(0,v,1/2), 0 < v < 1/2$	$mm2(C_{2v})$	no	no
Y	4	$(u,1/2,0), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
T	4	$(u,1/2,1/2), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
D	8	$(u,v,0), 0 < u < v < 1/2$	$m(C_s)$	no	no
E	8	$(u,v,1/2), 0 < u < v < 1/2$	$m(C_s)$	no	no
C	8	$(u,u,w), 0 < u < w < 1/2$	$m(C_s)$	no	no
B	8	$(0,v,w), 0 < v < w < 1/2$	$m(C_s)$	no	no
F	8	$(u,1/2,w), 0 < u < w < 1/2$	$m(C_s)$	no	no
GP	16	$(u,v,w), 0 < u < v < w < 1/2$	1(1)	no	no

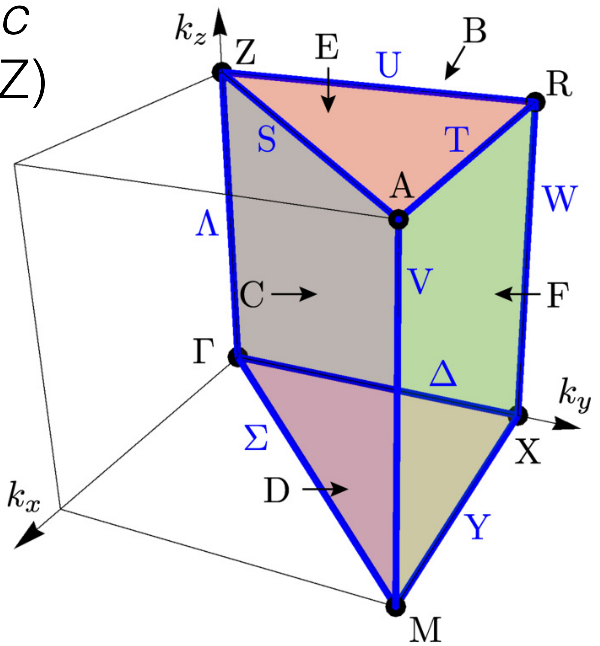
Physical Review E 96 (2), 023310

Maximal k-vectors and paths

For all the 230 SG:
maximal k-vectors + minimal set non-redundant **connections**

k vector in a manifold is maximal if its little co-group it's not a subgroup of another manifold of vectors **k'** (in general coincides with high-symmetry k-vector)

P4/ncc
(first BZ)



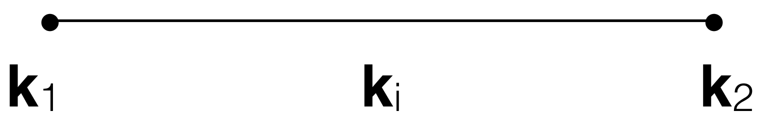
k-vec	mult.	Coordinates	Little	Maximal co-group	TR
Γ	1	(0,0,0)	$4/mmm(D_{4h})$	yes	yes
Z	1	(0,0,1/2)	$4/mmm(D_{4h})$	yes	yes
M	1	(1/2,1/2,0)	$4/mmm(D_{4h})$	yes	yes
A	1	(1/2,1/2,1/2)	$4/mmm(D_{4h})$	yes	yes
R	2	(0,1/2,1/2)	$mmm(D_{2h})$	yes	yes
X	2	(0,1/2,0)	$mmm(D_{2h})$	yes	yes
Λ	2	$(0,0,w), 0 < w < 1/2$	$4mm(C_{4v})$	no	no
V	2	$(1/2,1/2,w), 0 < w < 1/2$	$4mm(C_{4v})$	no	no
W	4	$(0,1/2,w), 0 < w < 1/2$	$mm2(C_{2v})$	no	no
Σ	4	$(u,u,0), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
S	4	$(u,u,1/2), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
Δ	4	$(0,v,0), 0 < v < 1/2$	$mm2(C_{2v})$	no	no
U	4	$(0,v,1/2), 0 < v < 1/2$	$mm2(C_{2v})$	no	no
Y	4	$(u,1/2,0), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
T	4	$(u,1/2,1/2), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
D	8	$(u,v,0), 0 < u < v < 1/2$	$m(C_s)$	no	no
E	8	$(u,v,1/2), 0 < u < v < 1/2$	$m(C_s)$	no	no
C	8	$(u,u,w), 0 < u < w < 1/2$	$m(C_s)$	no	no
B	8	$(0,v,w), 0 < v < w < 1/2$	$m(C_s)$	no	no
F	8	$(u,1/2,w), 0 < u < w < 1/2$	$m(C_s)$	no	no
GP	16	$(u,v,w), 0 < u < v < w < 1/2$	$1(1)$	no	no

Maximal k-vectors and paths

All possible connection between maximal and non-maximal **k**-vectors

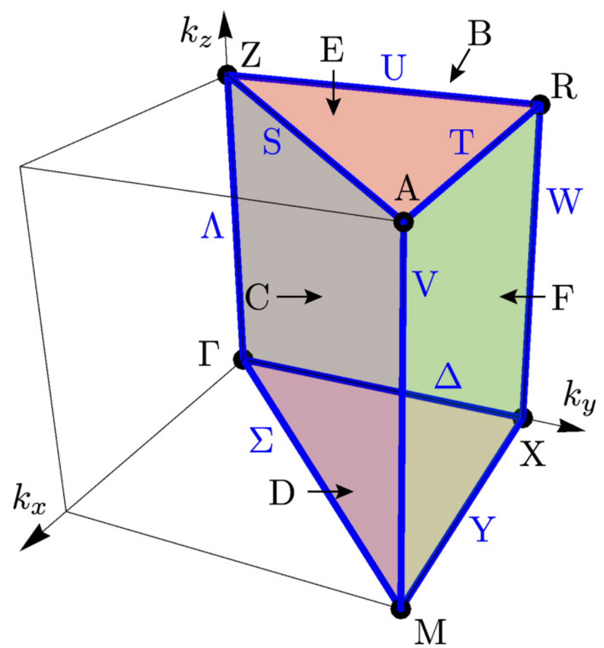
→ 2 manifolds are connected if:

$\mathbf{k}_i(\mathbf{u}_1)=\mathbf{k}_1$
$\mathbf{k}_i(\mathbf{u}_2)=\mathbf{k}_2$



for each max. **k** in ***k** and $\mathbf{k}_i$ non-maximal

P4/ncc
(first BZ)



Maximal **k**-vec	Connected **k**-vecs	Specific coordinates	Connections with the star
Γ: (0,0,0)	Λ: $(0,0,w)$	$w=0$	2
	Δ: $(0,v,0)$	$v=0$	4
	Σ: $(u,u,0)$	$u=0$	4
	B: $(0,v,w)$	$v=w=0$	8
	C: (u,u,w)	$u=w=0$	8
	D: $(u,v,0)$	$u=v=0$	8

Γ:3 lines and 3 planes

Compatibility relations

All possible connection between maximal and non-maximal **k**-vectors

→ 2 manifolds are connected if:

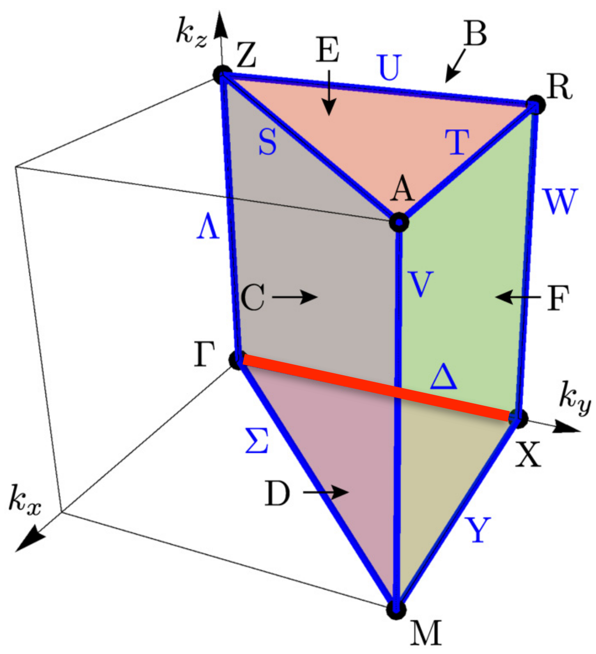
$\mathbf{k}_i\,(\mathbf{u}_1)=\mathbf{k}_1$

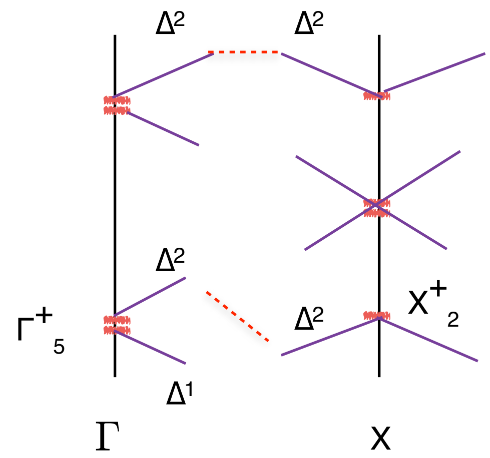
$\mathbf{k}_i\,(\mathbf{u}_2)=\mathbf{k}_2$

$\mathbf{k}_1$ $\mathbf{k}_i$ $\mathbf{k}_2$

for each max. **k** in ***k** and $\mathbf{k}_i$ non-maximal

P4/ncc
(first BZ)



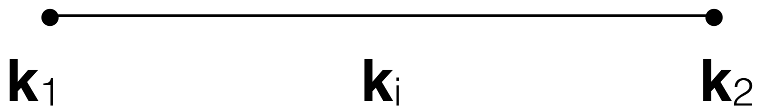


Compatibility relations

All possible connection between maximal and non-maximal **k**-vectors

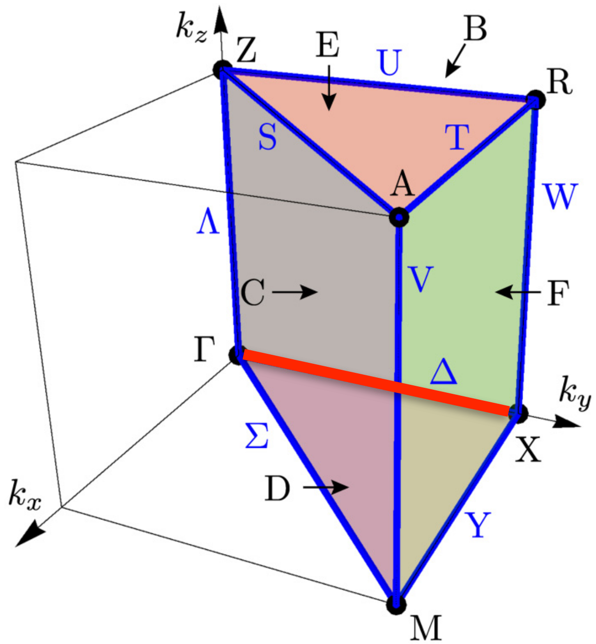
⟶ 2 manifolds are connected if:

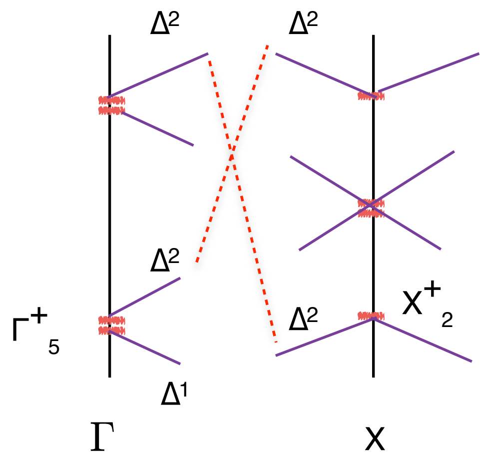
$$\mathbf{k}_i\,(\mathbf{u}_1)=\mathbf{k}_1$$
$$\mathbf{k}_i\,(\mathbf{u}_2)=\mathbf{k}_2$$



for each max. **k** in ***k** and $\mathbf{k}_i$ non-maximal

P4/ncc
(first BZ)





Compatibility relations

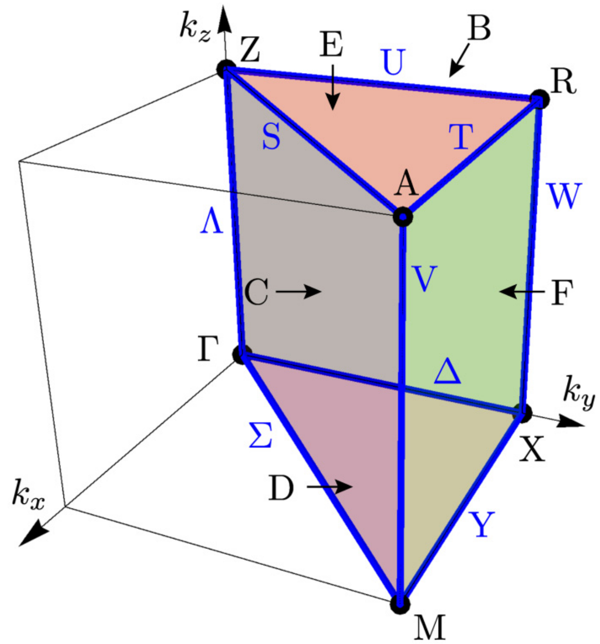
Reducing the number of paths

(i) Paths are subspace of other paths
k^1_M and k^2_M connect through k_p and k_l, k_p is redundant

(ii) **Paths related by symmetry operations**
A single line or plane of the *k gives all independent restrictions

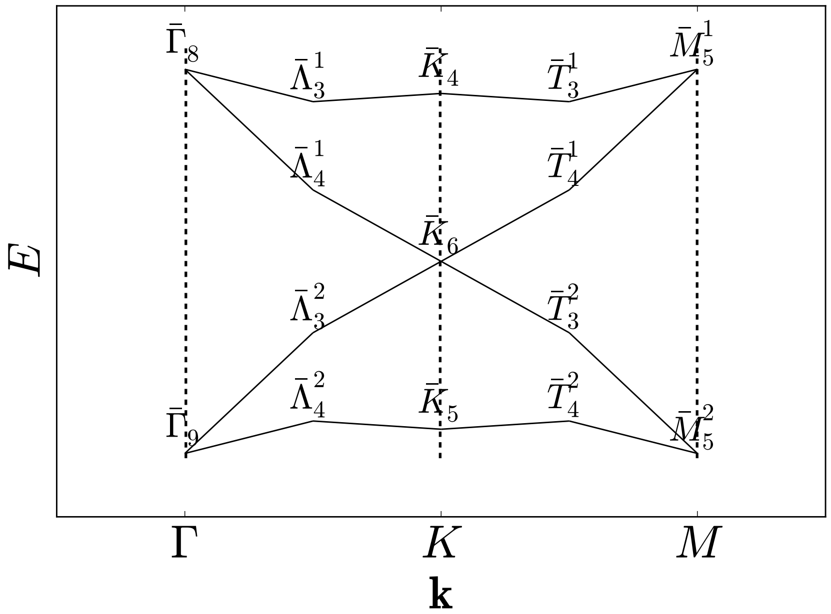
(iii) **Paths that are combinations of other paths**

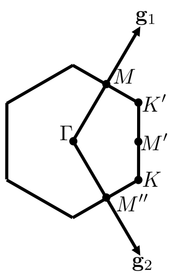
* additional restrictions in non-symmorphic groups (monodromy)

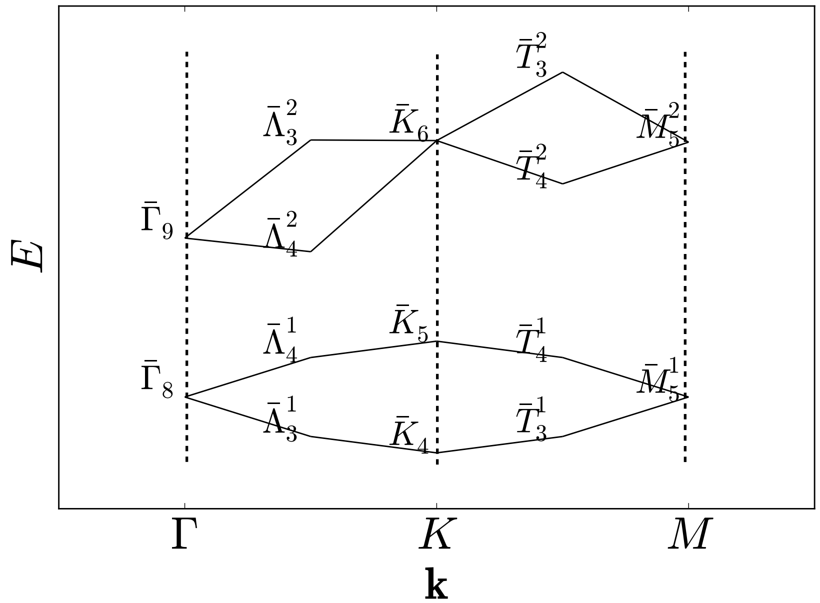


Compatibility relations

2 possible connectivities for $\bar{E}_1 \uparrow G(4)$







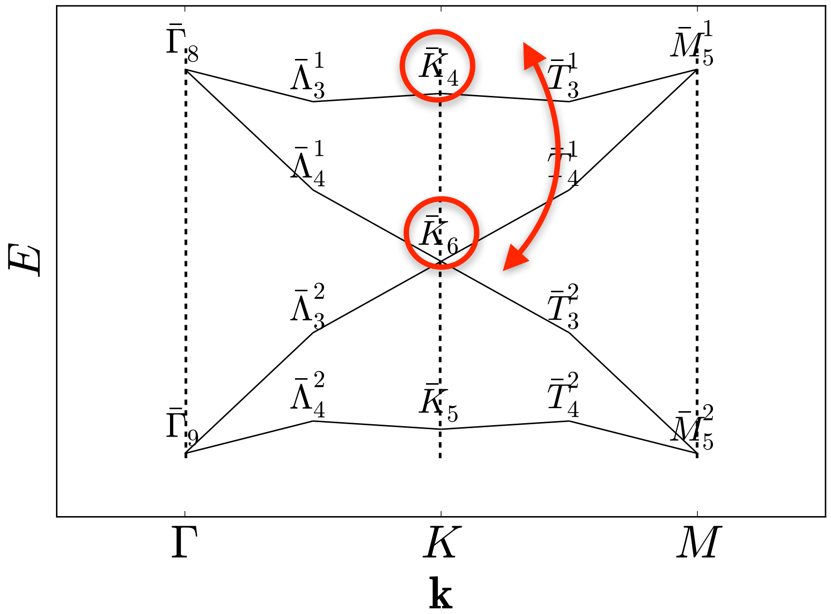
- Single connected component
→ Fully connected

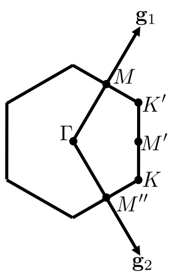
- Splitting of EBR
→ Topological bands

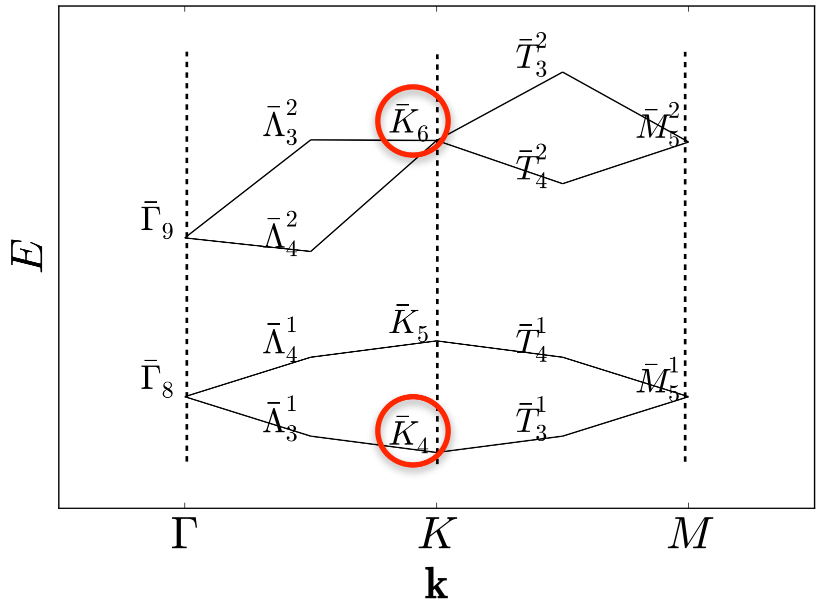
Vanderbilt, Soluyanov PRB 83, 035108 (2011)

Compatibility relations

2 possible connectivities for $\bar{E}_1 \uparrow G(4)$



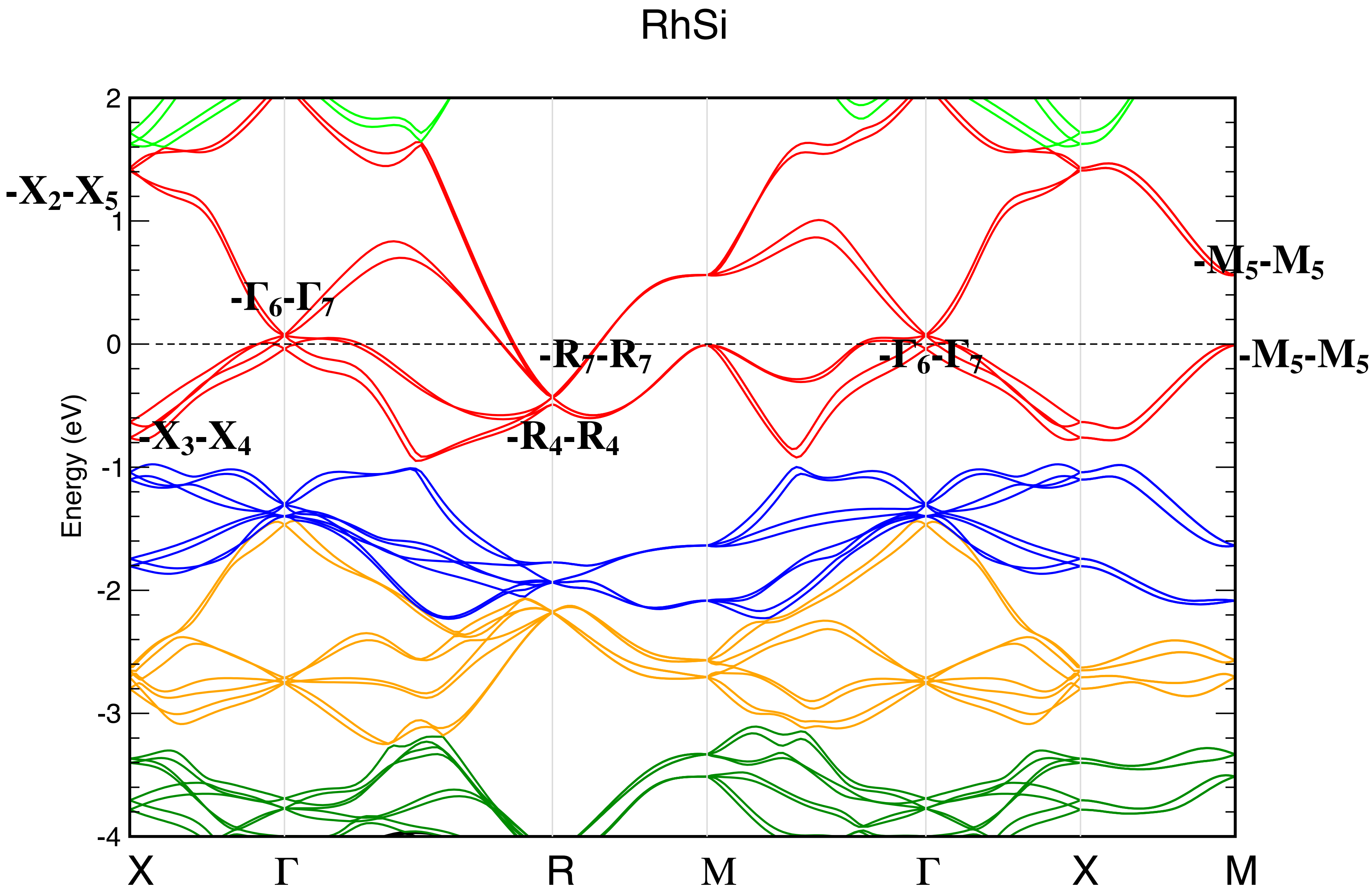




- Single connected component
→ Fully connected

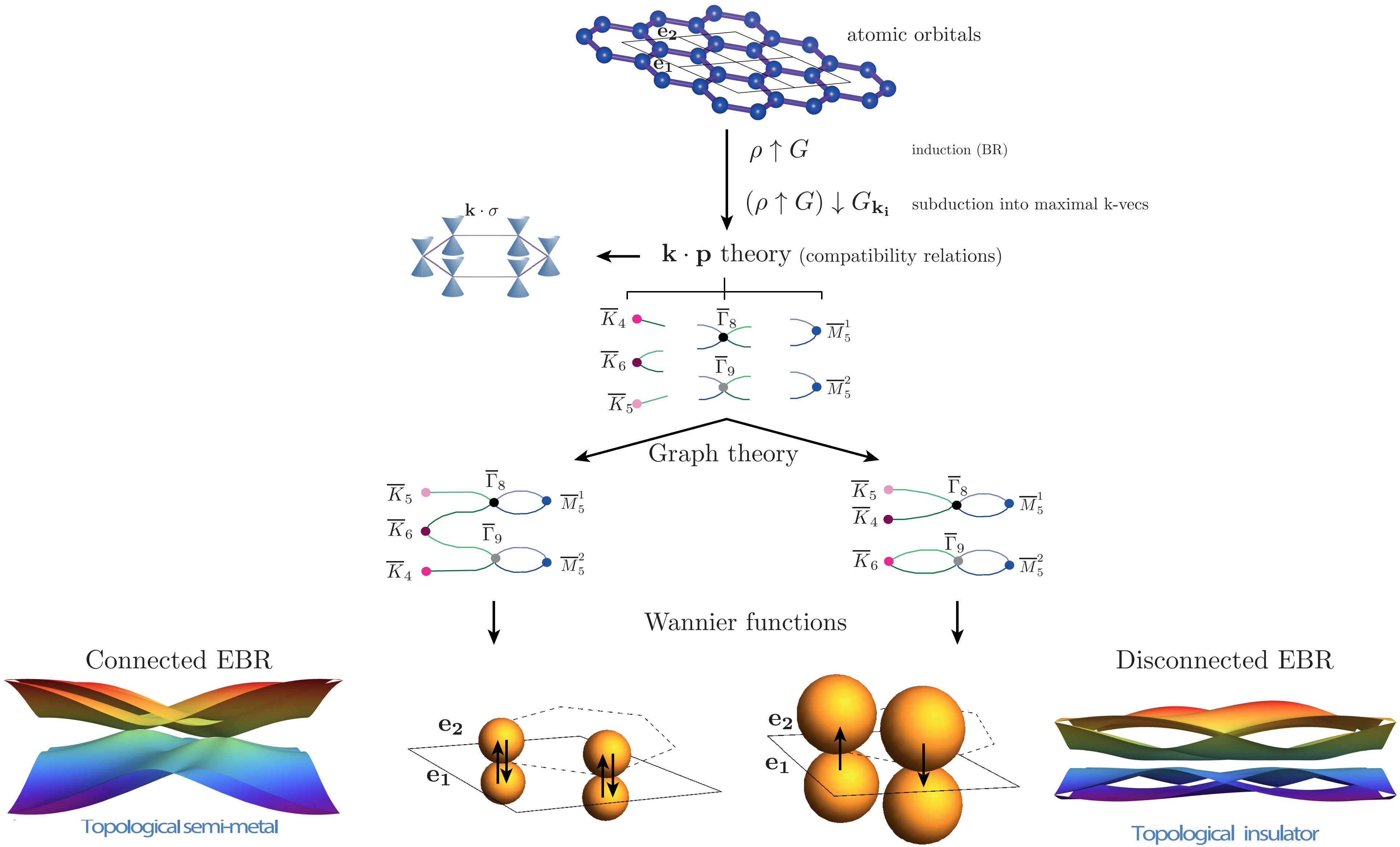
- Splitting of EBR
→ Topological bands

Vanderbilt, Soluyanov PRB 83, 035108 (2011)



RhSi
Energy (eV)
2
1
0
-1
-2
-3
-4
X
Γ
R
M
Γ
X
M
-X2-X5
-Γ6-Γ7
-R7-R7
-X3-X4
-R4-R4
-M5-M5
-Γ6-Γ7
-M5-M5

TOPOLOGICAL QUANTUM CHEMISTRY



Nature 547, 298--305 (2017)

Classification of crystalline atomic limits

10398 real-space **atomic limits** of materials

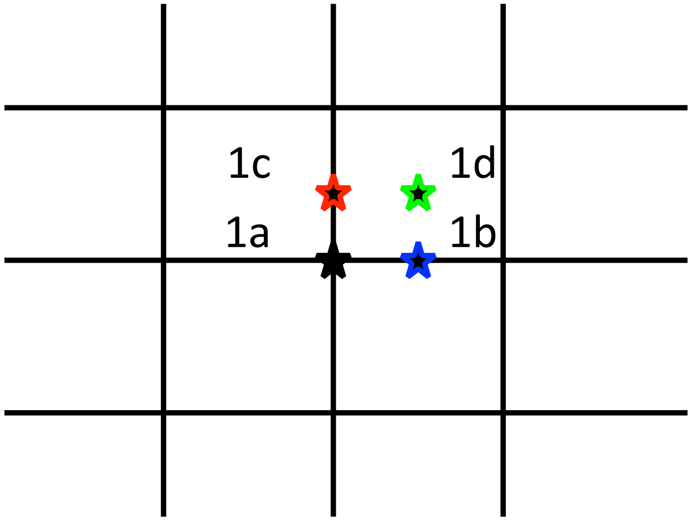
SG	MWP	WM	PG	Irrep	Dim	KR	Bands	Re	E	PE	SG	MWP	WM	PG	Irrep	Dim	KR	Bands	Re	E	PE
1	1a	1	1	Γ_1	1	1	1	1	e	e	131	2d	2	8	Γ_2^-	1	1	2	1	e	e
1	1a	1	1	$\bar{\Gamma}_2$	1	2	2	2	e	e	131	2d	2	8	Γ_4^+	1	1	2	1	e	e
2	1a	1	2	Γ_1^+	1	1	1	1	e	e	131	2d	2	8	Γ_4^-	1	1	2	1	e	e
2	1a	1	2	Γ_1^-	1	1	1	1	e	e	131	2d	2	8	Γ_3^+	1	1	2	1	e	e
2	1a	1	2	$\bar{\Gamma}_3$	1	2	2	2	e	e	131	2d	2	8	Γ_3^-	1	1	2	1	e	e
2	1a	1	2	$\bar{\Gamma}_2$	1	2	2	2	e	e	131	2d	2	8	$\bar{\Gamma}_5$	2	1	4	1	e	e
2	1b	1	2	Γ_1^+	1	1	1	1	e	e	131	2d	2	8	$\bar{\Gamma}_6$	2	1	4	1	e	e
2	1b	1	2	Γ_1^-	1	1	1	1	e	e	131	2e	2	14	Γ_1	1	1	2	1	e	e
2	1b	1	2	$\bar{\Gamma}_3$	1	2	2	2	e	e	131	2e	2	14	Γ_4	1	1	2	1	e	e

SG: Space Group
MWP: Maximal Wyckoff Position
WM: Wyckoff multiplicity in the primitive cell
PG: Point group number of the site-symmetry
Irrep: Name of the Irrep of the site-symmetry for each BR

KR: 1 for PEBR, 2 for EBR (f and s)
Bands: Total number of bands
Re: 1 for TRS at each k, 2 for connection with its conjugate
E: e for elementary, c for composite
PE: e for elementary, c for composite

Nature 547, 298--305 (2017)

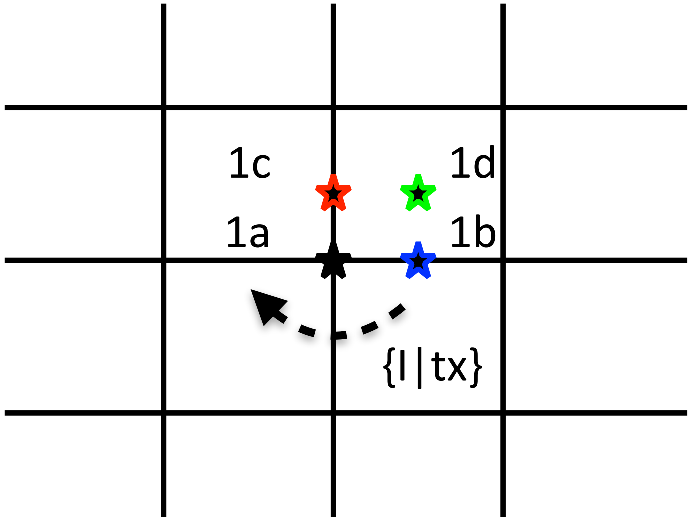
Spinless 2D material, $\mathcal{I}$, s and p orbitals



Zeroth Order: How To Use The Eigenvalues of EBRs to Find Topological Materials:

1. Find the Atomic Limit Real Space Orbitals

Spinless 2D material, I, s and p orbitals



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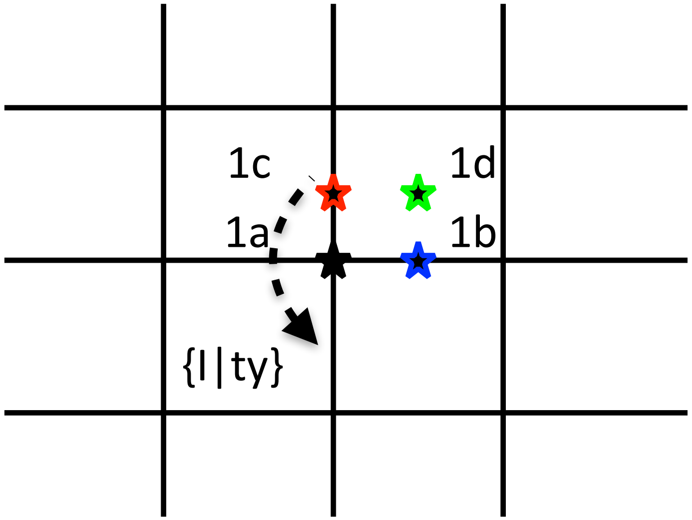
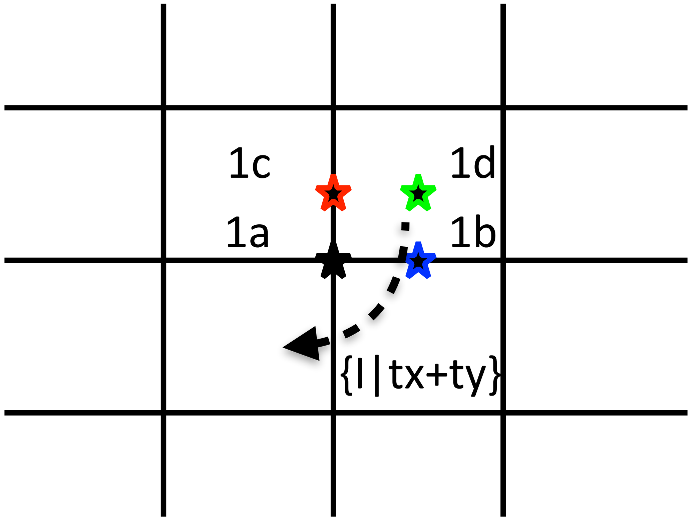


Zeroth Order: How To Use The Eigenvalues of EBRs to Find Topological Materials:

1. Find the Atomic Limit Real Space Orbitals

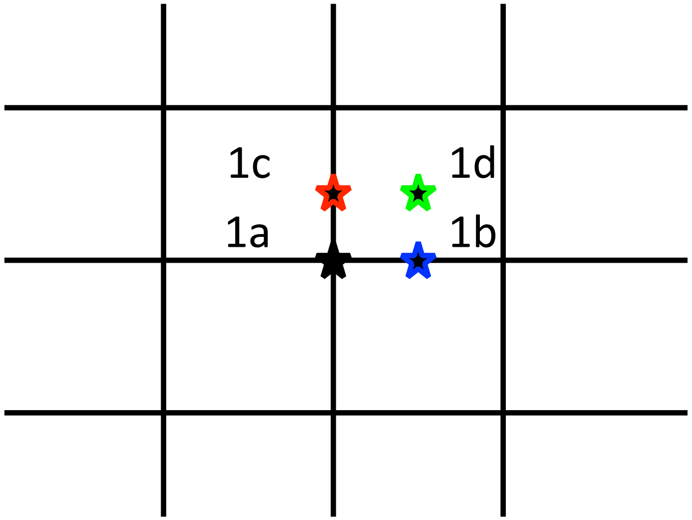
Spinless 2D material, I, s and p orbitals

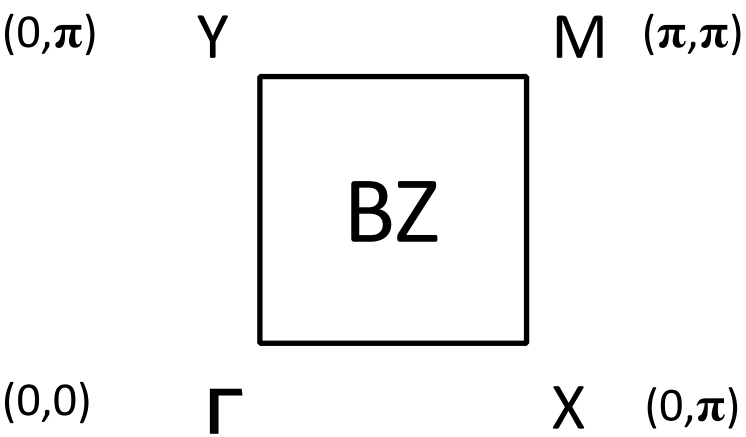


Zeroth Order: How To Use The Eigenvalues of EBRs to Find Topological Materials:

2.Obtain the Induced Representation in k(momentum) space

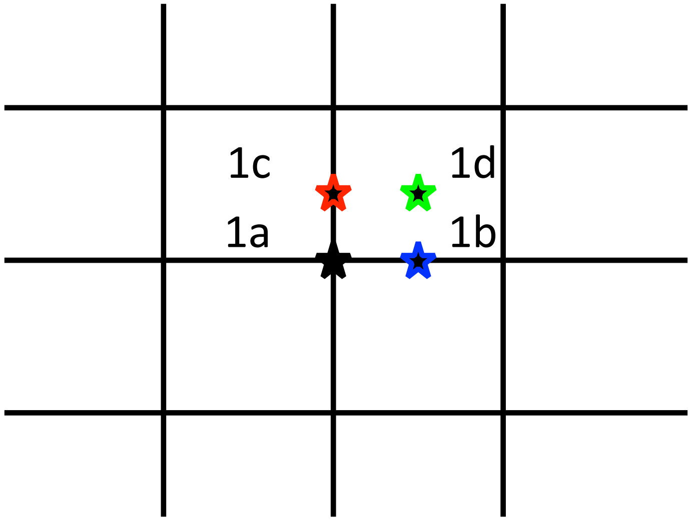
Spinless 2D material, I, **s** and **p** orbitals

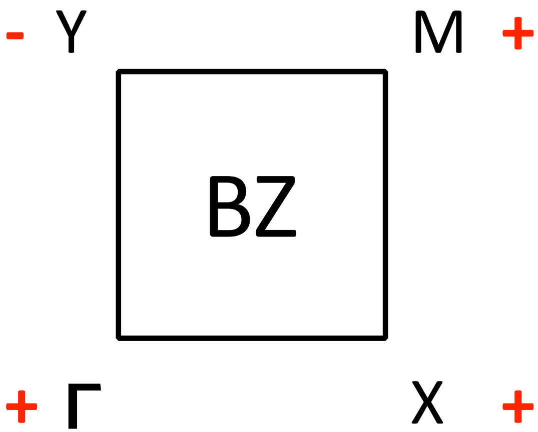




	Γ	X	Y	M
s 1a	+	+	+	+
p 1a	-	-	-	-
s 1b	+	-	+	-
p 1b	-	+	-	+
s 1c	+	+	-	-
p 1c	-	-	+	+
s 1d	+	-	+	-
p 1d	-	+	+	-

Spinless 2D material, $\mathcal{I}$, s and p orbitals

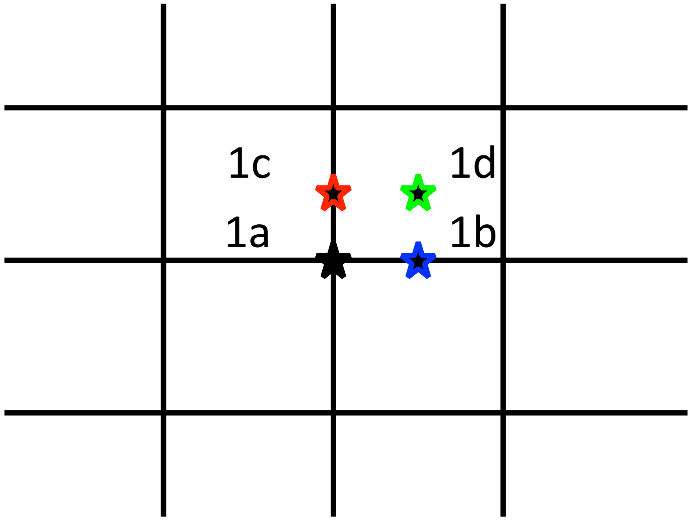


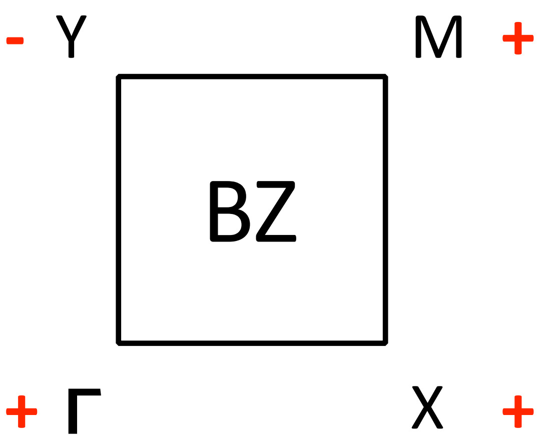


odd # in $\mathcal{I}$ eigenvalues

	Γ	X	Y	M
s 1a	+	+	+	+
p 1a	-	-	-	-
s 1b	+	-	+	-
p 1b	-	+	-	+
s 1c	+	+	-	-
p 1c	-	-	+	+
s 1d	+	-	+	-
p 1d	-	+	+	-

Spinless 2D material, $\mathcal{I}$, s and p orbitals



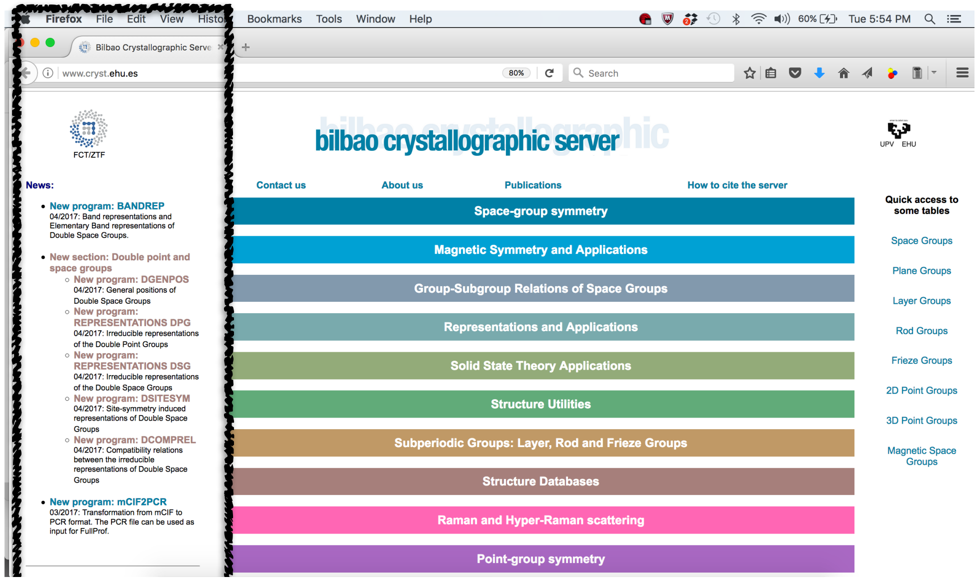


odd # in $\mathcal{I}$ eigenvalues

	Γ	X	Y	M
s 1a	+	+	+	+
p 1a	-	-	-	-
s 1b	+	-	+	-
p 1b	-	+	-	+
s 1c	+	+	-	-
p 1c	-	-	+	+
s 1d	+	-	+	-
p 1d	-	+	+	-

TOPOLOGICAL

http://www.cryst.ehu.es/cryst/bandrep



All 230 double groups

For each group, reps/wyckoff/k point reps

Compatibility relations in the Brillouin Zone

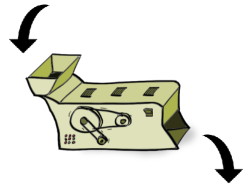
All 10398 Atomic limits

Disconnected EBR's/Graphs/Topological bands

Wyckoff pos.	1a(6mm)	1a(6mm)	1a(6mm)	1a(6mm)	1a(6mm)	1a(6mm)	2b(3m)
Band-Rep.	$A_1\uparrow G(1)$	$A_2\uparrow G(1)$	$B_1\uparrow G(1)$	$B_2\uparrow G(1)$	$E_1\uparrow G(2)$	$E_2\uparrow G(2)$	$A_1\uparrow G(2)$
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable
Γ:(0,0,0)	$\Gamma_1(1)$	$\Gamma_2(1)$	$\Gamma_4(1)$	$\Gamma_3(1)$	$\Gamma_6(2)$	$\Gamma_5(2)$	$\Gamma_1(1) \oplus \Gamma_4(1)$
A:(0,0,1/2)	$A_1(1)$	$A_2(1)$	$A_4(1)$	$A_3(1)$	$A_6(2)$	$A_5(2)$	$A_1(1) \oplus A_4(1)$
K:(1/3,1/3,0)	$K_1(1)$	$K_2(1)$	$K_2(1)$	$K_1(1)$	$K_3(2)$	$K_3(2)$	$K_3(2)$
H:(1/3,1/3,1/2)	$H_1(1)$	$H_2(1)$	$H_2(1)$	$H_1(1)$	$H_3(2)$	$H_3(2)$	$H_3(2)$
M:(1/2,0,0)	$M_1(1)$	$M_2(1)$	$M_4(1)$	$M_3(1)$	$M_3(1) \oplus M_4(1)$	$M_1(1) \oplus M_2(1)$	$M_1(1) \oplus M_4(1)$
L:(1/2,0,1/2)	$L_1(1)$	$L_2(1)$	$L_4(1)$	$L_3(1)$	$L_3(1) \oplus L_4(1)$	$L_1(1) \oplus L_2(1)$	$L_1(1) \oplus L_4(1)$

Atom arrangement

Orbital



High-symmetry points

Phys. Rev. E 96 023310 (2017)

Band Representations in the Bilbao Crystallographic Server

http://www.cryst.ehu.es/cryst/bandrep

Bilbao Crystallographic Server ➝ BANDREP | Help

Band representations of the Double Space Groups

Band Representations

This program calculates the band representations (BR) induced from the irreps of the site-symmetry group of a given Wyckoff position.
Alternatively, it gives the set of elementary BRs of a Double Space Group.
In both cases, it can be chosen to get the BRs with or without time-reversal symmetry.
The program also indicates if the elementary BRs are decomposable or indecomposable. If it is decomposable, the program gives all the possible ways to decompose it.

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A [choose it]

1. Get the elementary BRs without time-reversal symmetry [Elementary]
2. Get the elementary BRs with time-reversal symmetry [Elementary TR]
3. Get the BRs without time-reversal symmetry from a Wyckoff position [Wyckoff]
4. Get the BRs with time-reversal symmetry from a Wyckoff position [Wyckoff TR]

Bilbao Crystallographic Server
http://www.cryst.ehu.es

For comments, please mail to
administrador.bsc@ehu.eus

http://www.cryst.ehu.es/cryst/bandrep

Output

12b(2)	8a(3)	8a(3)	12b(2)
B↑G(6)	$^1\bar{E}^2\bar{E}$↑G(8)	$\bar{E}\bar{E}$↑G(8)	$^1\bar{E}^2\bar{E}$↑G(12)
Indecomposable	**Indecomposable**	Decomposable	Decomposable
$2\ \Gamma_4(3)$	$2\ \bar{\Gamma}_5(2) \oplus \bar{\Gamma}_6\bar{\Gamma}_7(4)$	$2\ \bar{\Gamma}_6\bar{\Gamma}_7(4)$	$2\ \bar{\Gamma}_5(2) \oplus 2\ \bar{\Gamma}_6\bar{\Gamma}_7(4)$
$H_1(1) \oplus H_2H_3(2) \oplus H_4(3)$	$2\ \bar{H}_5(2) \oplus \bar{H}_6\bar{H}_7(4)$	$2\ \bar{H}_6\bar{H}_7(4)$	$2\ \bar{H}_5(2) \oplus 2\ \bar{H}_6\bar{H}_7(4)$
$P_1(2) \oplus P_2(2) \oplus P_3(2)$	$\bar{P}_5(1) \oplus \bar{P}_6(1) \oplus 2\ \bar{P}_7(3)$	$2\ \bar{P}_4(1) \oplus 2\ \bar{P}_7(3)$	$\bar{P}_4(1) \oplus \bar{P}_5(1) \oplus \bar{P}_6(1) \oplus 3\ \bar{P}_7(3)$
$PA_1(2) \oplus PA_2(2) \oplus PA_3(2)$	$\overline{PA}_5(1) \oplus \overline{PA}_6(1) \oplus 2\ \overline{PA}_7(3)$	$2\ \overline{PA}_4(1) \oplus 2\ \overline{PA}_7(3)$	$\overline{PA}_4(1) \oplus \overline{PA}_5(1) \oplus \overline{PA}_6(1) \oplus 3\ \overline{PA}_7(3)$
$3\ N_1(1) \oplus 3\ N_2(1)$	$4\ \bar{N}_3\bar{N}_4(2)$	$4\ \bar{N}_3\bar{N}_4(2)$	$6\ \bar{N}_3\bar{N}_4(2)$

http://www.cryst.ehu.es/cryst/bandrep

Output

	branch 1	branch 2
1	$\overline{H}_5,\overline{\Gamma}_5,\overline{P}_5,\overline{P}_6,\overline{N}_4,\overline{N}_4$	$\overline{H}_6,\overline{H}_7,\overline{\Gamma}_6,\overline{\Gamma}_7,\overline{P}_4,\overline{P}_7,\overline{N}_3,\overline{N}_3,\overline{N}_4,\overline{N}_4$
2	$\overline{H}_6,\overline{\Gamma}_6,\overline{P}_4,\overline{P}_6,\overline{N}_4,\overline{N}_4$	$\overline{H}_7,\overline{H}_5,\overline{\Gamma}_5,\overline{\Gamma}_7,\overline{P}_5,\overline{P}_7,\overline{N}_3,\overline{N}_3,\overline{N}_4,\overline{N}_4$
3	$\overline{H}_7,\overline{\Gamma}_7,\overline{P}_4,\overline{P}_5,\overline{N}_4,\overline{N}_4$	$\overline{H}_5,\overline{H}_6,\overline{\Gamma}_5,\overline{\Gamma}_6,\overline{P}_6,\overline{P}_7,\overline{N}_3,\overline{N}_3,\overline{N}_4,\overline{N}_4$

http://www.cryst.ehu.es/cryst/bandrep

Output

Elementary band-representations without time-reversal symmetry of the Double Space Group $I2_13$ (No. 199)

The first row shows the Wyckoff position from which the band representation is induced.
In parentheses, the symbol of the point group isomorphic to the site-symmetry group.

The second row gives the symbol ρ↑G, where ρ is the irrep of the site-symmetry group.
In parentheses, the dimension of the representation.

The output shows the decomposition of the band representations into irreps of the little groups of the given k-vectors in the first column.
In parentheses, the dimensions of the representations.

Minimal set of paths and compatibility relations to analyse the connectivity

Show all types of k-vectors

http://www.cryst.ehu.es/cryst/bandrep

Output

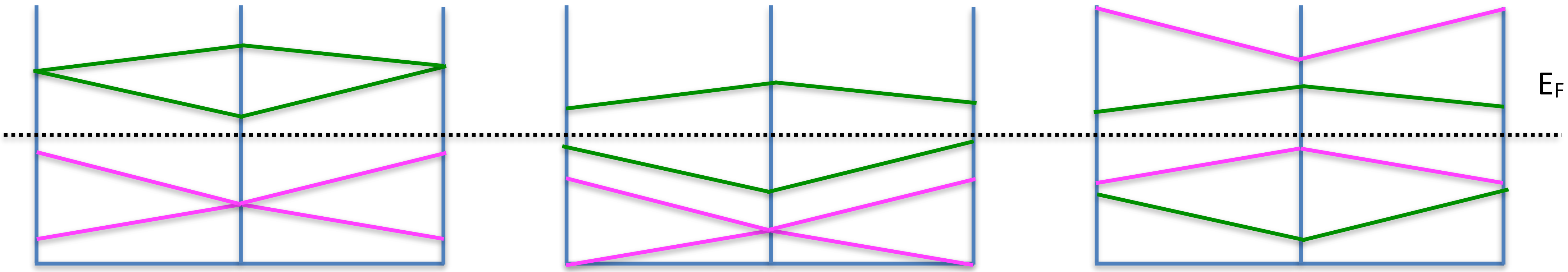
Maximal k-vec	Compatibility relations	Intermediate path	Compatibility relations	Maximal k-vec
Γ:(0,0,0)	$\Gamma_1(1)\to\Delta_1(1)$ $\Gamma_2(1)\to\Delta_1(1)$ $\Gamma_3(1)\to\Delta_1(1)$ $\Gamma_4(3)\to\Delta_1(1) \oplus 2\,\Delta_2(1)$ $\bar{\Gamma}_5(2)\to\bar{\Delta}_3(1) \oplus \bar{\Delta}_4(1)$ $\bar{\Gamma}_6(2)\to\bar{\Delta}_3(1) \oplus \bar{\Delta}_4(1)$ $\bar{\Gamma}_7(2)\to\bar{\Delta}_3(1) \oplus \bar{\Delta}_4(1)$	Δ:(0,v,0)	$H_1(1)\to\Delta_2(1)$ $H_2(1)\to\Delta_2(1)$ $H_3(1)\to\Delta_2(1)$ $H_4(3)\to 2\,\Delta_1(1) \oplus \Delta_2(1)$ $\bar{H}_5(2)\to\bar{\Delta}_3(1) \oplus \bar{\Delta}_4(1)$ $\bar{H}_6(2)\to\bar{\Delta}_3(1) \oplus \bar{\Delta}_4(1)$ $\bar{H}_7(2)\to\bar{\Delta}_3(1) \oplus \bar{\Delta}_4(1)$	H:(1,1,1)
Γ:(0,0,0)	$\Gamma_1(1)\to\Lambda_1(1)$ $\Gamma_2(1)\to\Lambda_2(1)$ $\Gamma_3(1)\to\Lambda_3(1)$ $\Gamma_4(3)\to\Lambda_1(1) \oplus \Lambda_2(1) \oplus \Lambda_3(1)$ $\bar{\Gamma}_5(2)\to\bar{\Lambda}_5(1) \oplus \bar{\Lambda}_6(1)$ $\bar{\Gamma}_6(2)\to\bar{\Lambda}_4(1) \oplus \bar{\Lambda}_6(1)$ $\bar{\Gamma}_7(2)\to\bar{\Lambda}_4(1) \oplus \bar{\Lambda}_5(1)$	Λ:(-u,u,-u)	$H_1(1)\to\Lambda_1(1)$ $H_2(1)\to\Lambda_2(1)$ $H_3(1)\to\Lambda_3(1)$ $H_4(3)\to\Lambda_1(1) \oplus \Lambda_2(1) \oplus \Lambda_3(1)$ $\bar{H}_5(2)\to\bar{\Lambda}_5(1) \oplus \bar{\Lambda}_6(1)$ $\bar{H}_6(2)\to\bar{\Lambda}_4(1) \oplus \bar{\Lambda}_6(1)$ $\bar{H}_7(2)\to\bar{\Lambda}_4(1) \oplus \bar{\Lambda}_5(1)$	H:(1,1,1)
Γ:(0,0,0)	$\Gamma_1(1)\to\Lambda_1(1)$ $\Gamma_2(1)\to\Lambda_2(1)$ $\Gamma_3(1)\to\Lambda_3(1)$ $\Gamma_4(3)\to\Lambda_1(1) \oplus \Lambda_2(1) \oplus \Lambda_3(1)$ $\bar{\Gamma}_5(2)\to\bar{\Lambda}_5(1) \oplus \bar{\Lambda}_6(1)$ $\bar{\Gamma}_6(2)\to\bar{\Lambda}_4(1) \oplus \bar{\Lambda}_6(1)$ $\bar{\Gamma}_7(2)\to\bar{\Lambda}_4(1) \oplus \bar{\Lambda}_5(1)$	Λ:(-u,u,-u)	$P_1(2)\to\Lambda_1(1) \oplus \Lambda_2(1)$ $P_2(2)\to\Lambda_2(1) \oplus \Lambda_3(1)$ $P_3(2)\to\Lambda_1(1) \oplus \Lambda_3(1)$ $\bar{P}_4(1)\to\bar{\Lambda}_4(1)$ $\bar{P}_5(1)\to\bar{\Lambda}_5(1)$ $\bar{P}_6(1)\to\bar{\Lambda}_6(1)$ $\bar{P}_7(3)\to\bar{\Lambda}_4(1) \oplus \bar{\Lambda}_5(1) \oplus \bar{\Lambda}_6(1)$	P:(1/2,1/2,1/2)

Materials search

Topological "insulating" classes { EBR1, EBR2

$\mathbf{b}=\sum_i n_i(\mathbf{k})=\sum_m a_m \mathrm{EBR}$

LCEBR	SEBR	NLC
Linear Combination EBR	Split EBR	Non Linear Combination



b=EBR1	**b**=EBR1+1/2*EBR2	**b**=?

* Fragile: EBR_F=EBR1-EBR2

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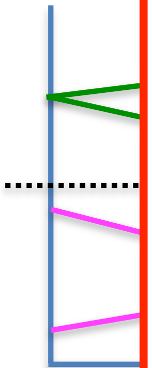
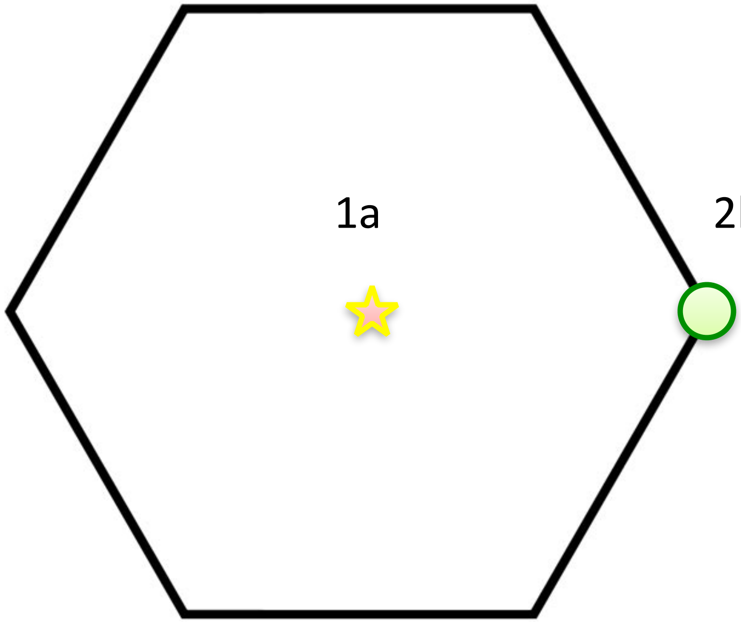
Materials search

Topological "insulating" classes { EBR1, EBR2

Line

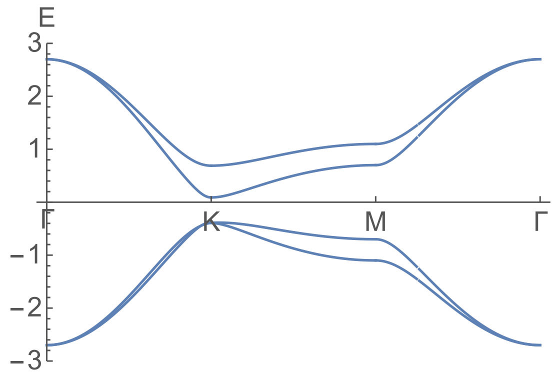


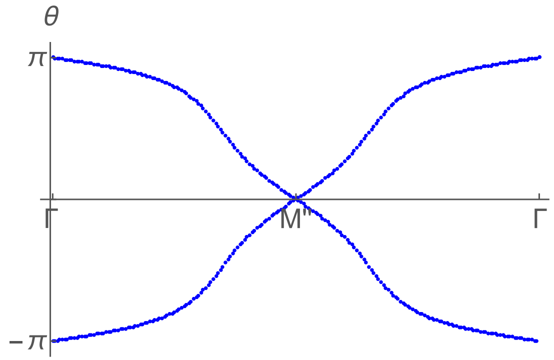


EBR1 = EBR2 + TOP_BANDS

EBR induced at 1a

EBR induced at 2b - EBR induced at 1a





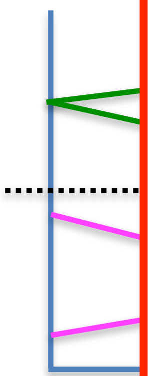
* Fragile: EBR_F=EBR1-EBR2

Phys. Rev. Lett. 120, 266401 (2018)

Materials search

Topological "insulating" classes { EBR1, EBR2

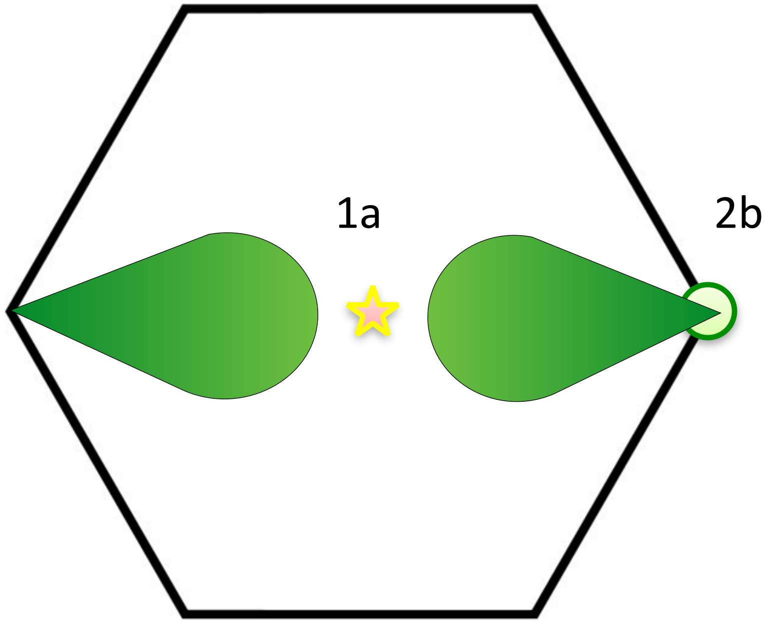
Line

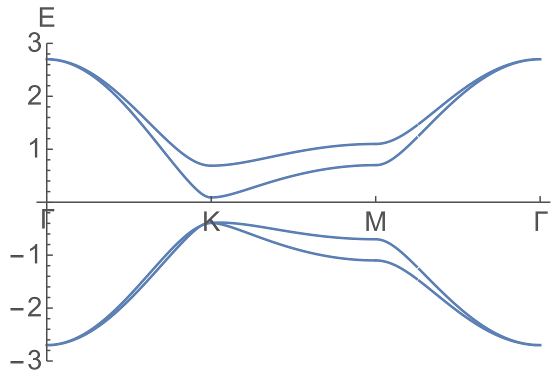


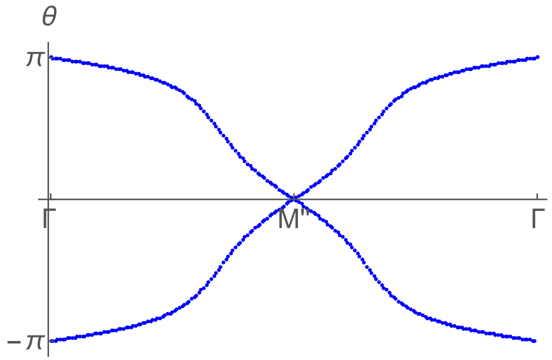
EBR1 = EBR2 + TOP_BANDS

EBR induced at 1a

EBR induced at 2b - EBR induced at 1a







* Fragile: EBR_F=EBR1-EBR2

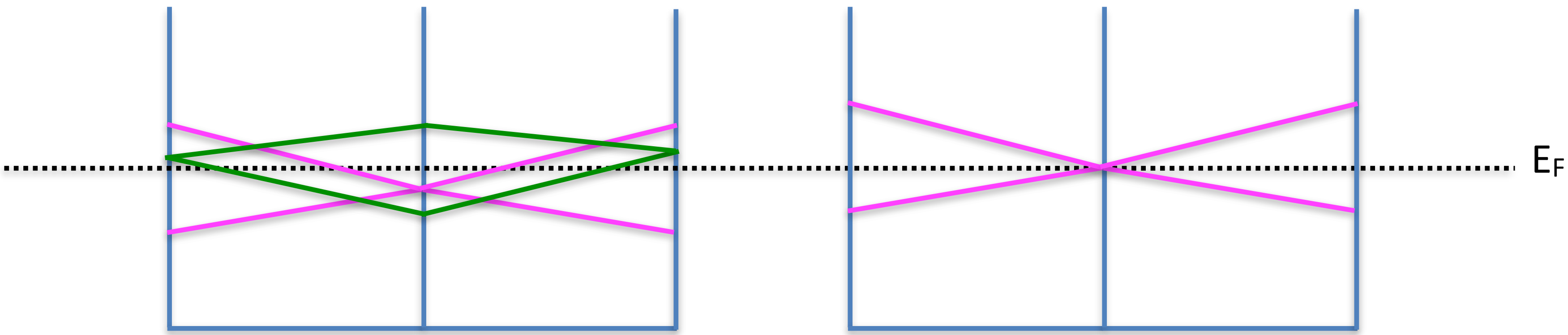
Phys. Rev. Lett. 120, 266401 (2018)

Materials search

Topological "metalic" classes { EBR1 / EBR2

ES
Enforced semimetals

ESFD
ES Fermi Degeneracy



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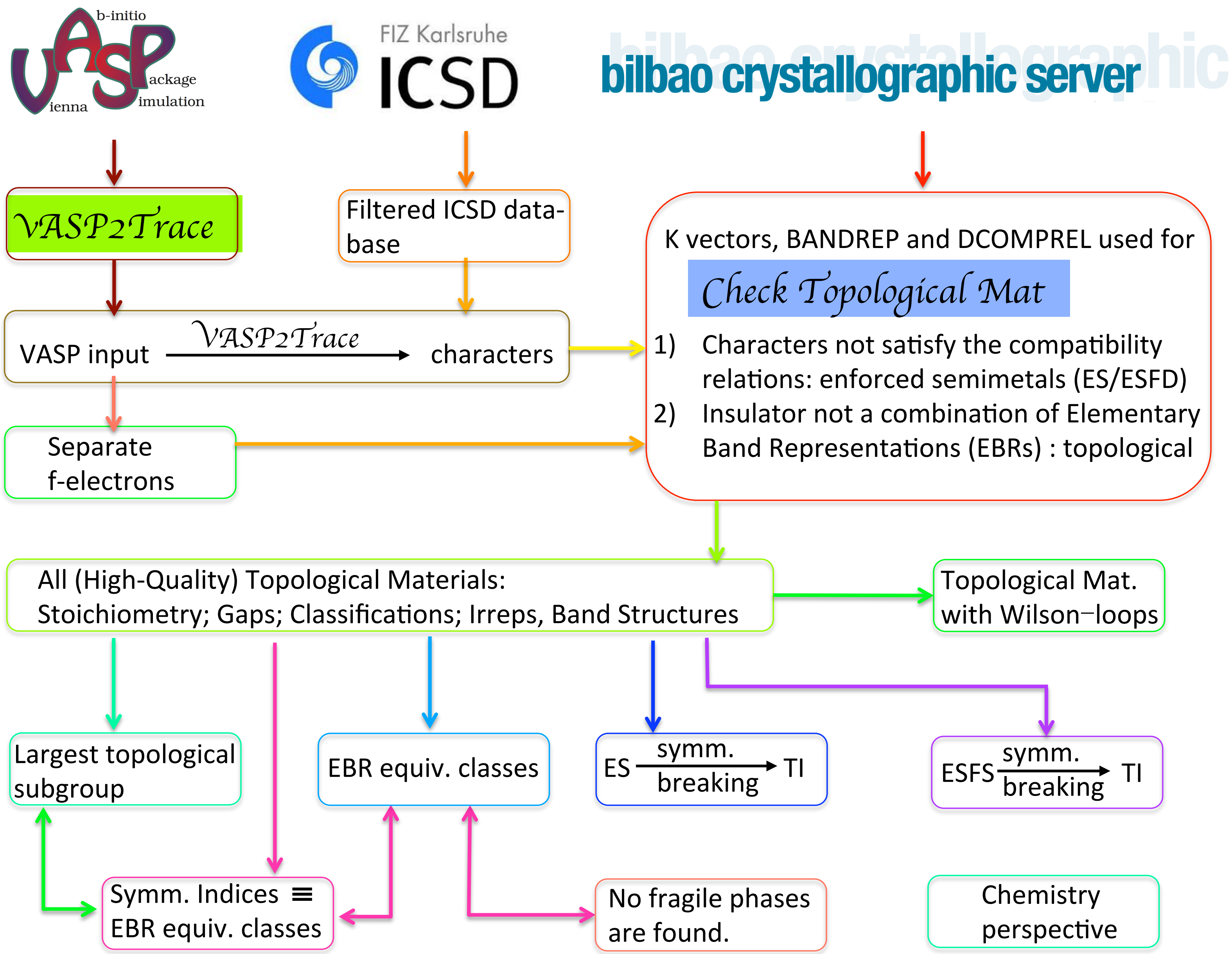

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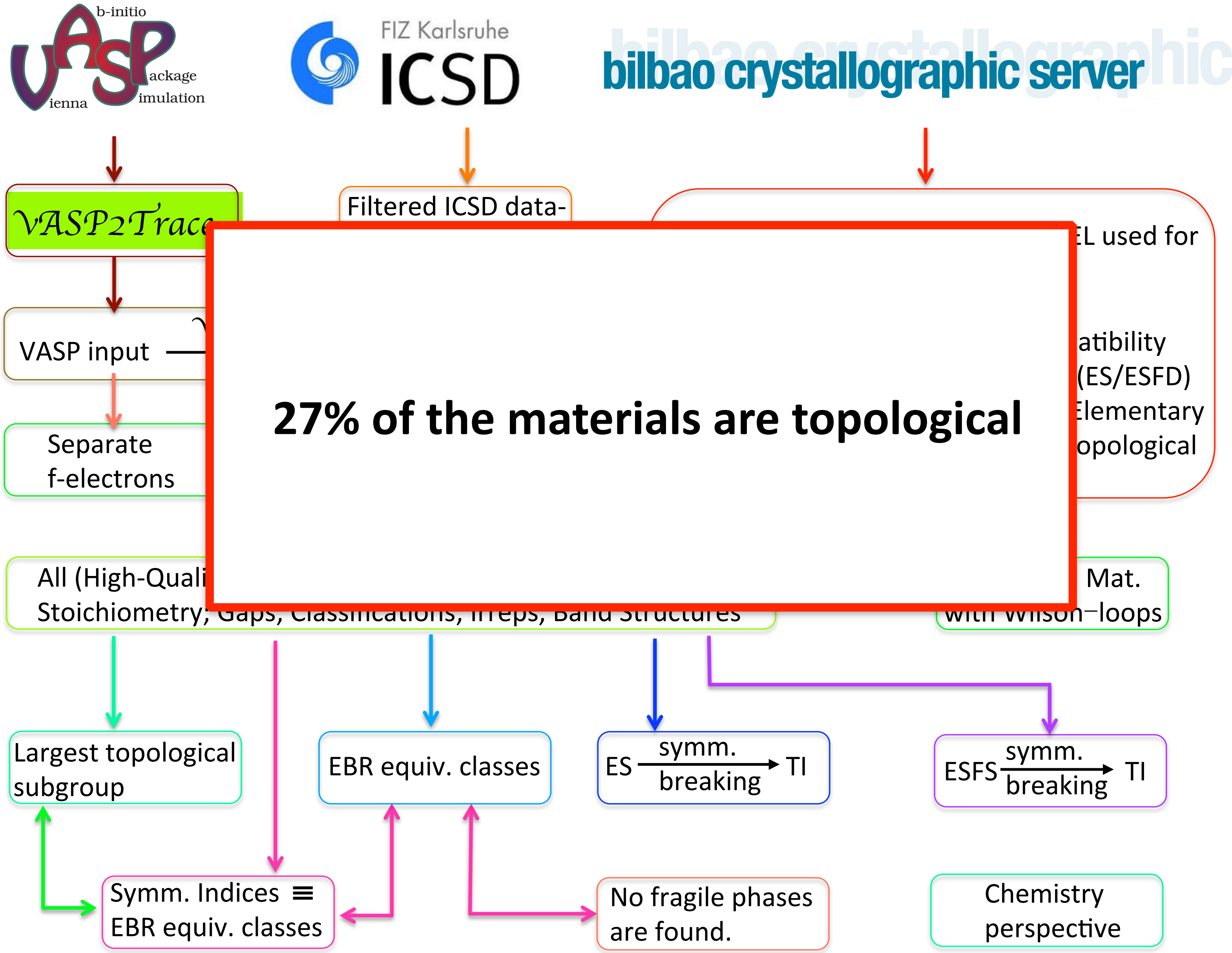

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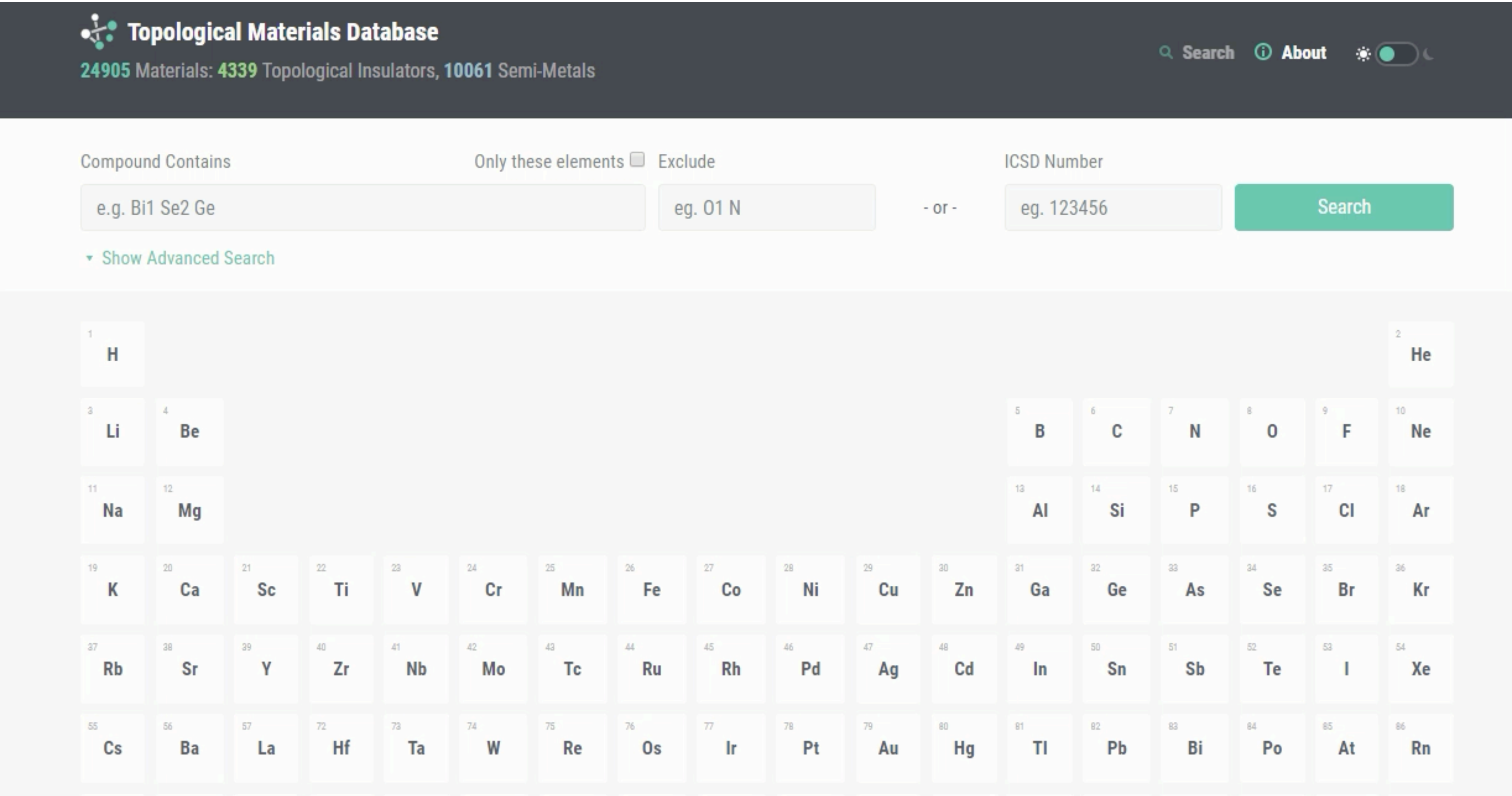
Topological Materials Database

https://www.topologicalquantumchemistry.org



Check Topology

www.cryst.ehu.es/cryst/checktopologicalmat

Check Topological Mat

Check Topological Mat.

Given a file that contain the eigenvalues at each maximal k-vec of a space group, the program gives the set of irreducible representations at each maximal k-vec (time-reversal is assumed). Then, using the compatibility relations and the set of Elementary Band Representations (EBRs), it checks whether the set of bands can be put as linear combinations of EBRs. This (self-explanatory) file shows the format of the file to be uploaded in the menu on the right:

File_Description

You can download examples of input files here:

Example_Ag1Ge1Li2 Example_Ag1O2Sc1
Example_B2Ca3Ni7 Example_Ba3Co10O17
Example_Ba3Ca1O9Ru2

You can generate the "trace.txt" file in your own computer using VASP and this program (fortran).

vasp2trace

Read the "README.pdf" file for help on the use of vasp2trace.
If you are using "Check Topological Mat." and/or "vasp2trace" programs in the preparation of an article, please cite this reference:

M.G. Vergniory, L. Elcoro, C. Felser, B.A. Bernevig, Z. Wang (2018) arXiv:1807.10271

Upload your traces.txt file

Browse... No file selected.

Show

1. A number of bands that is **not a sum of EBRs is topological**
2. A number of bands that does **not satisfy the compatibility relations** cannot be separated from other bands and describes a **semimetal**

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Check Topology

www.cryst.ehu.es/cryst/checktopologicalmat

Bilbao Crystallographic Server ➝ Check Topological Mat.

Result of the analysi

- The material is a topological insulator.
- List of topological indices:

  z2w,1=0

  z2w,2=0

  z2w,3=0

  z4=0

  z2=0

  z8=4

- The material belongs to the strong topological class: 1
- Clicking on See the irreps you can see the details about the number of bands and the ide
- The set of bands can be put as linear combination of Elementary Band Representations (I to get some possible linear combinations of EBRs and partial EBRs.
- Click on Subgroups to check the topological character of the structure in each of its (trans

```
Number of electrons=10
Number of maximal k-vectors=4
Symbols of the k-vectors, number of bands up to fermi level and set of irreps.
     -GM     -X        -L     -W
      10     10        10     10
 -GM6(2) -X6(2)    -L9(2) -W6(2)
 -GM6(2) -X6(2)    -L8(2) -W7(2)
 -GM8(2) -X8(2)    -L8(2) -W7(2)
-GM11(4) -X8(2) -L4-L5(2) -W6(2)
         -X9(2)    -L9(2) -W7(2)
```

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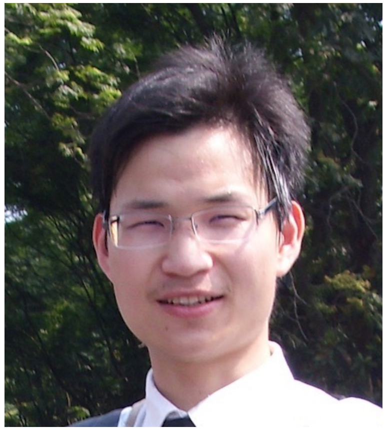

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