Elementary Band Representations and Group Theory from the Perspective of Condensed Matter Physics

Aussois GDR School, May 2024

Benjamin J. Wieder

Outline

1. Basics of Group Theory and Point Groups

2. Crystals and Space Groups in Real and Momentum Space

3. Elementary Band Representations and Topological Quantum Chemistry

Part 1:
Basics of Group Theory and Point Groups

Sets

- *g* (or *h*) is an **operator** that acts on states and coordinates
  - Later: *g* will be a **symmetry group element**

- CMT rules: a **set** is a collection of **operators** (elements)
  - Implicit (sometimes unstated): Rules (**algebra** or relations) between elements

- **Ex:** {2,5,7,9} is a set of integers
  - *Implicit algebra* – **additivity:** $g_i g_j = g_{i+j}$
  - Algebra keeps *some* elements in set: $g_1 = 2,\ g_2 = 5 \rightarrow \boldsymbol{g_3 = 7 = 2 + 5}$ 
  - **But not every element:** $g_2 = 5,\ g_3 = 7 \rightarrow \boldsymbol{g_4 = 9 \neq 5 + 7}$ 
    - This set is **open** (not **closed**)

Groups

- A **group** G is a set (+ element algebra) with four constraints:

1. Closure: every product element is also in set:

- If $g_1 \in G,\ g_2 \in G$, then $g_1 g_2 \in G$

2. Associativity:

- Take 3 elements $g_{1,2,3}$ and define $g_i g_j = g_{ij}$
- Demand $g_1 g_{23} = g_{12} g_3$

3. Unique Identity Element in Set:

- There exists an element $E \in G$ for which $E g_i = g_i E = g_i$ for all *i*

4. Unique Inverse Elements in Set:

- For each $g \in G$, there also exists one $h \in G$ for which $hg = gh = E$

Group or Set?

- Even additive integers $2\mathbb{Z}$?
  - **Yes, a group**
- Odd additive integers?
  - **No, just a set**
  - ***Open, no identity***

Note: uniqueness of identity & identical left/right inverses not strictly required, see *Bradley & Cracknell, The Mathematical Theory of Symmetry in Solids, Chap. 1*

Finite Groups

- Given a set or group H, the **order** $|H|$ of H is the number of elements in H

- A **finite group** G has a finite order $|G|$
  - An **infinite group** does not

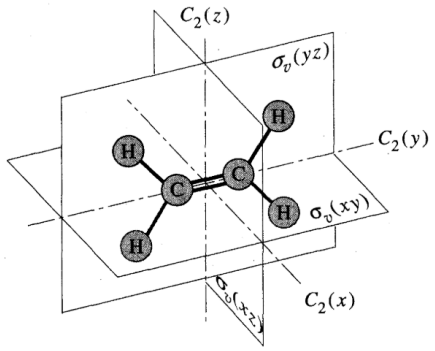
- Finer distinction of ∞:
  - A **continuous group** has infinite elements with infinitesimally spacing
    - *Example:* SO(3) rotations
  - A **discrete infinite group** has countably infinite discretely spaced elements
    - *Example:* additive integers $\mathbb{Z}$

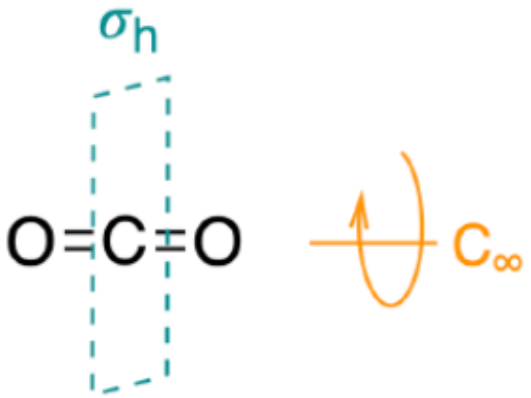
Point Groups (finally something concrete)

- **Point groups** leave points in space invariant, contain symmetries of:
  - *Molecules*
  - *Points (sites) in infinite crystals*

- Molecular point groups can be *discrete* or *continuous*
  - σ_i is mirror in chemistry

Discrete point group of ethene (C_2H_4)
McQuarrie and Simon, Chapter 12



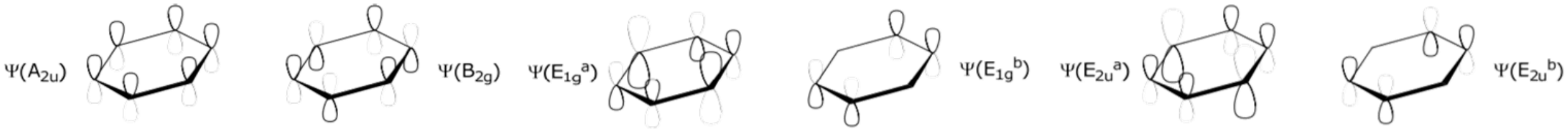


Continuous point group of CO_2
Haas, Fundamentals of Inorg. Chem., LibreTexts

- Site-symmetry groups in 2D and 3D crystals are *always finite groups*
  - Isomorphic to the 2D and 3D **crystallographic point groups**
  - Isomorphic = same group elements and algebra under redefinition

Representations of Finite Groups

- The representations (reps) ρ of groups are abstract mathematical objects
  - **<u>All molecular energy eigenstates "transform in" point group reps</u>**



molecular WFs and reps of benzene (C_6H_6), *<u>Nocera, Fundamentals of Inorg. Chem. II, LibreTexts</u>*

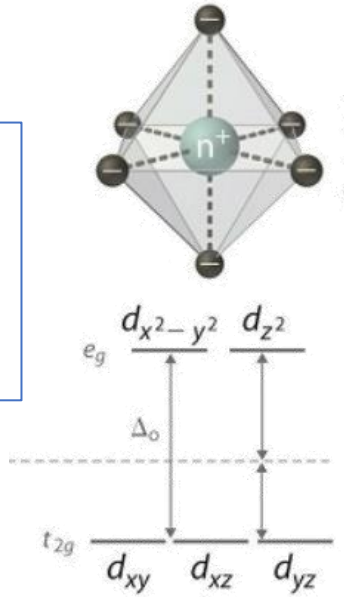
- Unitarity distinctions:
  - *G* contains <u>only unitary elements:</u> **ρ is a representation**
  - *G* contains <u>unitary & antiunitary elements:</u> **ρ is a corepresentation (corep)**
    - Nonmagnetic systems have time-reversal symmetry *T*, all group reps are coreps
      - Note: all nonmagnetic groups with symmetries like C_2 and *T* also have product C_2T
- Today, focus on groups with only unitary elements
  - "Type-I magnetic symmetry groups"

See *Bradley & Cracknell & L. Elcoro*, **BJW*** et al., Nat. Comm.* (2021)

Characters and Irreducible Representations

- Matrices and characters define reps
  - $\Delta_\rho(g)$ is the **matrix representative of g in ρ**
  - $\chi_\rho(g) = \mathrm{Tr}\left[\Delta_\rho(g)\right]$ is the **character of g in ρ**
    - Unitary symmetry g eigenvalue sum
    - **Crucial for detecting topology** (later)

Irreps are basis for "crystal field theory" **(here octahedral group O_h)**
Supp. Modules and Websites (Inorg. Chem.), LibreTexts



- ρ is an **irreducible rep (irrep)** of a group G if (and only if) the only matrix M for which $\Delta_\rho(g) M \Delta_\rho^{-1}(g) = M$ for all $g \in G$ is the identity matrix $M \propto \mathbb{I}$

- **Physical consequence:** given a molecular Hamiltonian *H*, there is a 1:1 correspondence between **robust spectral degeneracies and irreps**
  - Warmup for band degeneracies (later)

Character Tables

- **Character tables** define group irreps through symmetry eigenvalues
  - In groups with unitary and antiunitary elements, only unitary elements have characters
    - Because antiunitary elements g_A have $\Delta_\rho(g_A) = UK$, and $\mathrm{Tr}[K]$ is not defined
  - **Rows and columns are orthogonal**

Irreducible representations of the Point Group 222 (No. 6)

Table of characters

(1)	(2)	(3)	C_1	C_2	C_3	C_4
GM_1	A	GM_1	1	1	1	1
GM_3	B_1	GM_2	1	1	-1	-1
GM_4	B_3	GM_3	1	-1	-1	1
GM_2	B_2	GM_4	1	-1	1	-1

C_1: 1
C_2: 2_{001}
C_3: 2_{010}
C_4: 2_{100}

Symmetry element g

Irrep ρ label

Character $\chi_\rho(g)$

Example unitary group from Bilbao Crystallographic Server
https://www.cryst.ehu.es/cgi-bin/cryst/programs/representations_point.pl?tipogrupo=spg

All magnetic and nonmagnetic point group tables now available:
https://www.cryst.ehu.es/html/cryst/mpointrepres.html

L. Elcoro*, **BJW*** *et al.*, *Nat. Comm.* (2021)

Single and Double Groups

- Same point group has two forms: single and double
  - **Single group**: twofold rotations $C_{2,xyz}$ commute, $\chi_\rho\left(\mathrm{C}_{2\mathrm{i}}^2\right) = \chi_\rho(E)$
    - For phonons, magnons, electrons with no spin-orbit coupling (per spin), "spinless fermions"
  - **Double group:** new element $\bar{E}$, $C_{2x}C_{2y} = \bar{E}C_{2y}C_{2x}$, $\chi_{\bar{\rho}}\left(C_{2i}^2\right) = \chi_{\bar{\rho}}(\bar{E})$
    - **Double-valued reps of double group:** $\chi_{\bar{\rho}}(\bar{E}) = -\chi_{\bar{\rho}}(E)$, implies anticommutation
    - For electrons, "spinful fermions"

Irreducible representations of the Double Point Group 222 (No. 6)

Identity element E

Table of characters

Lists of symmetry operations in the conjugacy classes

(1)	(2)	(3)	C_1	C_2	C_3	C_4	C_5
GM_1	A	GM_1	1	1	1	1	1
GM_3	B_1	GM_2	1	1	-1	-1	1
GM_4	B_3	GM_3	1	-1	-1	1	1
GM_2	B_2	GM_4	1	-1	1	-1	1
GM_5	$\bar{E}$	$\overline{GM_5}$	2	0	0	0	-2

C_1: 1

C_2: 2_{001}, $^d2_{001}$

C_3: 2_{010}, $^d2_{010}$

C_4: 2_{100}, $^d2_{100}$

C_5: $^d1$

Single-valued irreps ρ

Double-valued irrep $\bar{\rho}$

$\bar{E}$ element

Example double group from Bilbao Crystallographic Server

https://www.cryst.ehu.es/cgi-bin/cryst/programs/representations_point.pl?tipogrupo=dbg

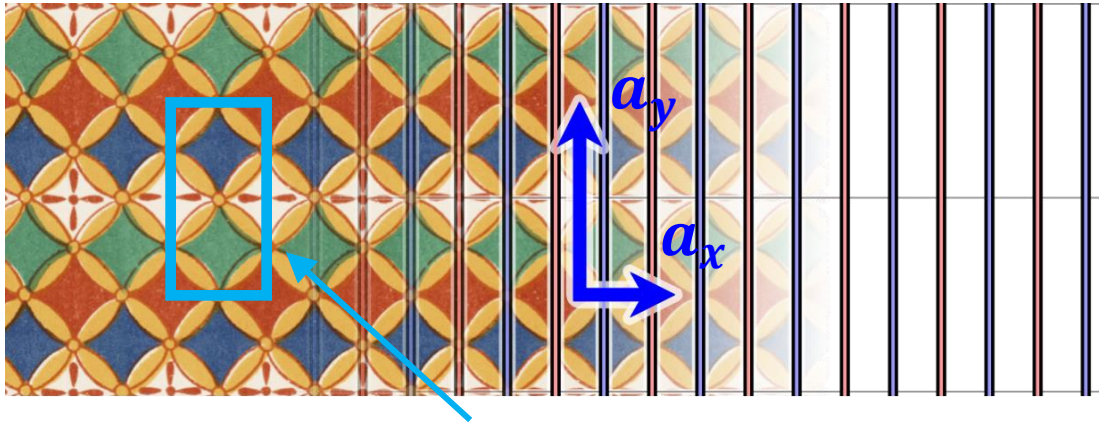
Part 2:
Crystals and Space Groups in Real and Momentum Space

Crystals and Translation Symmetry

- **Crystals** are objects with discrete translation symmetry
  - **Lattice vectors** a_i – shortest linearly independent translations

This pattern is a crystal

von Gagern, https://en.wikipedia.org/wiki/Wallpaper_group



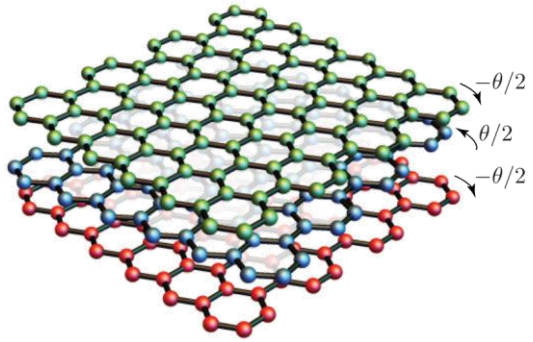
- Crystals have repeated periodic motifs termed **unit cells**

- Crystals are infinite and pristine – **free of defects and boundaries**
  - **Results derived from crystal models say *nothing* about boundaries and defects response without using other methods**
    - ***e.g.* topology, continuum field theory, long-wavelength semiconductor physics, chemistry, etc.**

Crystal Symmetry Groups

- Crystals have **infinite symmetry groups (SGs)**
  - Crystal symmetries have the form $g = \{R|\boldsymbol{v}\}$
  - R is point group element, $\boldsymbol{v}$ is a translation
  - Primitive (generating) lattice translations are $t_{\boldsymbol{a_i}} = \{E|\boldsymbol{a_i}\}$

Mirror-symmetric twisted trilayer graphene model has layer group symmetry
Khalaf et al., PRB (2019)



- SG defined by **dimensionality** of $\boldsymbol{R}$, number of independent $\boldsymbol{a_i}$
  - If dim $\boldsymbol{R}$ > number of $\boldsymbol{a_i}$, group is **subperiodic**

See further reading in:
Conway et al., The Symmetries of Things

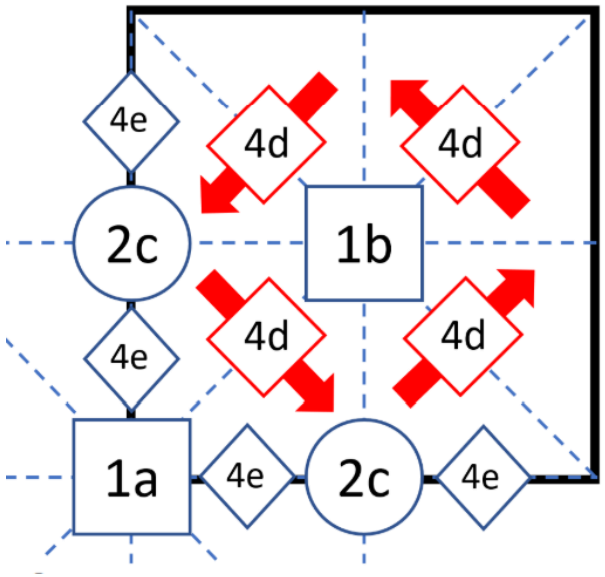
dim R	num a_i	Group Name	Subperiodic?	Physical System
1	1	Line		Toy model?
2	1	Frieze	✓	Flat polymer on substrate
2	2	Wallpaper		Few-layer on substrate, TI surface
3	2	Layer	✓	Floating few-layer (*e.g.* Moiré model)
3	3	Space		Bulk crystalline solid

Wyckoff Positions

- **Site-symmetry groups** $G_{\boldsymbol{q}_\alpha}$ define finer unit cell structure of crystal w/ SG G
  - For a site with coordinates $\boldsymbol{q}_\alpha$, $g\boldsymbol{q}_\alpha = \boldsymbol{q}_\alpha$ (**in same unit cell**) for each g $\in G_{\boldsymbol{q}_\alpha}$
  - $G_{\boldsymbol{q}_\alpha} \subset G$, but $G_{\boldsymbol{q}_\alpha}$ **isomorphic to point group, *has same irreps***

- **Wyckoff orbit**: set $\{\boldsymbol{q}_\alpha\}$ *in same unit cell* permuted by $g \in G, g \notin G_{\boldsymbol{q}_\alpha}$
  - **Multiplicity** of orbit defined by size of set $\{\boldsymbol{q}_\alpha\}$

Unit Cell of Wallpaper group *p4m*
BJW *et al., Nat. Comm.* (2020)



Some Wyckoff positions

$\boldsymbol{q}_{1a} = (0,0)$

$\boldsymbol{q}_{1b} = (1/2,1/2)$

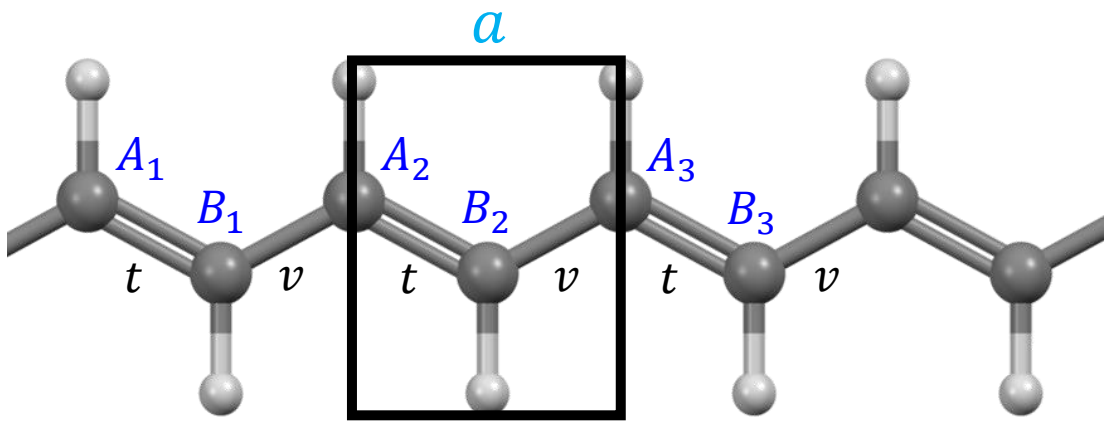
$\boldsymbol{q}_{4d} = \{(\pm x, \pm x)\}$

- **Wyckoff position**: set of Wyckoff orbits with same multiplicity related by smooth coordinate deformation (*e.g.* 4d and 4e above for all x)

Crystal Momentum Space

- Typical Hamiltonians for crystals (*e.g.* real-material electrons) are **off-diagonal** in unit-cell indices
  - **Note:** unit cell origin and shape are choices

$$H_x = \begin{array}{c} \begin{matrix} A_1 & B_1 & A_2 & B_2 \end{matrix} \\ \begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & 0 & t & 0 & 0 & \cdots \\ \cdots & t & 0 & v & 0 & \cdots \\ \cdots & 0 & v & 0 & t & \cdots \\ \cdots & 0 & 0 & t & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \end{array} \begin{matrix} \\ A_1 \\ B_1 \\ A_2 \\ B_2 \end{matrix}$$

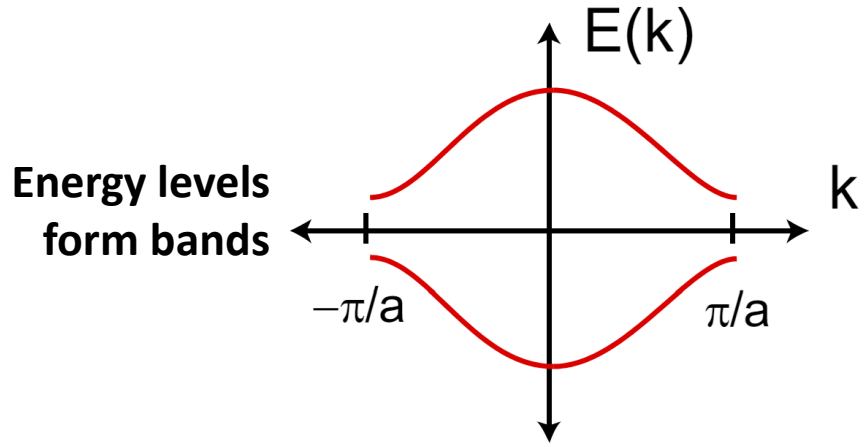


Nearest-neighbor hopping model of trans polyacetylene
https://en.wikipedia.org/wiki/Polyacetylene

- Block-diagonalize by Fourier transforming

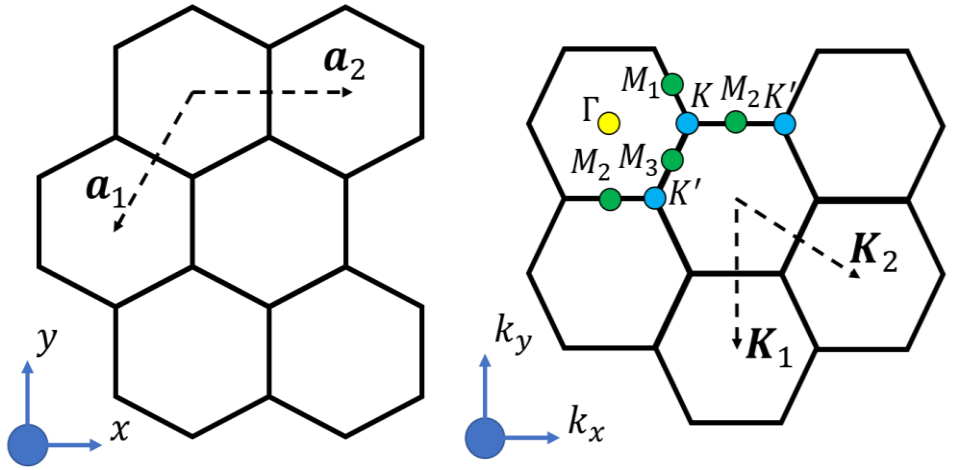
$$|A/B_\alpha> = \sum_k e^{ix_{\alpha,A/B}} |A/B_k>$$

$$H_x = \sum_k H_k = \sum_k \begin{array}{c} \begin{matrix} A_k & B_k \end{matrix} \\ \begin{bmatrix} 0 & te^{-ika/2} + ve^{ika/2} \\ te^{ika/2} + ve^{-ika/2} & 0 \end{bmatrix} \end{array} \begin{matrix} A_k \\ B_k \end{matrix}$$



Symmetry in $\boldsymbol{k}$ Space

- Unit cells in **x** are physically distinct, but only "1st unit cell in **k**" (BZ) is physical
  - **k** is just a Fourier parameter
  - **k** unit cells are *Brillouin zones* (BZs)
  - **Reciprocal lattice vectors** $\boldsymbol{K}_i$ relate BZs
    - Orthogonality $\boldsymbol{a}_i \cdot \boldsymbol{K}_j = 2\pi\delta_{ij}$



x-space unit cells and **k**-space BZs in graphene
***BJW** et al., Nat. Comm. (2020)*

- **k** points can be related by symmetry
  - Termed "momentum stars" (**k**-space analog of Wyckoff orbit)
  - Stars & **multiplicities** in graphene: 1: Γ, 2: K & K', 3: $M_{1,2,3}$

- Like sites in crystals, **k** points have symmetry
  - Given crystal SG G, **little group** $G_{\boldsymbol{k}} \subseteq G$ contains all symmetries g *including translations* that return $\boldsymbol{k}$ to itself *up to a BZ*: $g\boldsymbol{k} \bmod \boldsymbol{K}_{1,2,3} = \boldsymbol{k}$
  - $G_{\boldsymbol{k}}$ is isomorphic to an SG, ***not a point group*** (unlike site-symmetry group $G_{\boldsymbol{q}_\alpha}$)

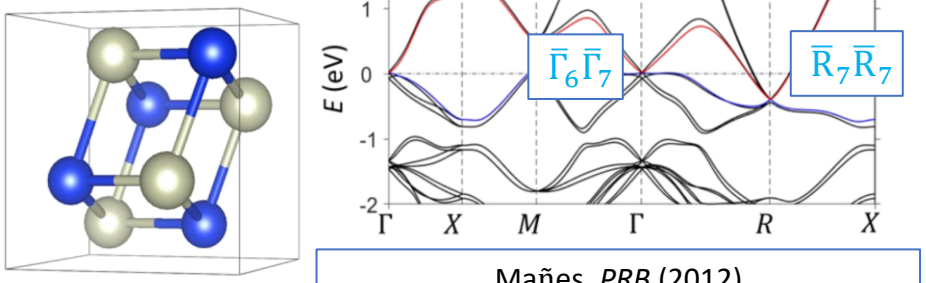
Irreducible Small Representations

- $G_{\boldsymbol{k}}$ is an *infinite group* (contains translation group G_T), implies infinite irreps
  - Could try constructing abstract "projective" point group from $G_{\boldsymbol{k}}$ see *Bradley & Cracknell, Chapter 5*

- For us: define finite number of **small irreps** $\sigma_{\boldsymbol{k}}$ of $G_{\boldsymbol{k}}$ by coset decomposition:
  - $G_{\boldsymbol{k}} = G_T \cup g_1 G_T \cup g_2 G_T \cup \cdots$, where each g_i is unique & $g_i \neq G_T$
  - For pure translation $t = \{E|\boldsymbol{t}\} \in G_T$, choose $\Delta_{\sigma_{\boldsymbol{k}}}(t) = e^{-i\boldsymbol{k}\cdot\boldsymbol{t}}\mathbb{I}$
  - Finite $\{\sigma_{\boldsymbol{k}}\}$ from unique matrix reps of coset symmetries using $\Delta_{\sigma_{\boldsymbol{k}}}(tg_i) = \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\boldsymbol{t}}\Delta_{\sigma_{\boldsymbol{k}}}(g_i)$

- **Most band degeneracies enumerable from $\boldsymbol{\sigma_k}$**
  - Led to discovery of many topological semimetals

RhSi structure and bands



Mañes, *PRB* (2012)
BJW *et al., PRL* (2016)
Bradlyn, …, Vergniory, *et al., Science* (2016)
Chang*, Xu*, **BJW***, *et al., PRL* (2017)

- **Tool for all SG small (co)reps**
  - https://www.cryst.ehu.es/cgi-bin/cryst/programs/corepresentations.pl

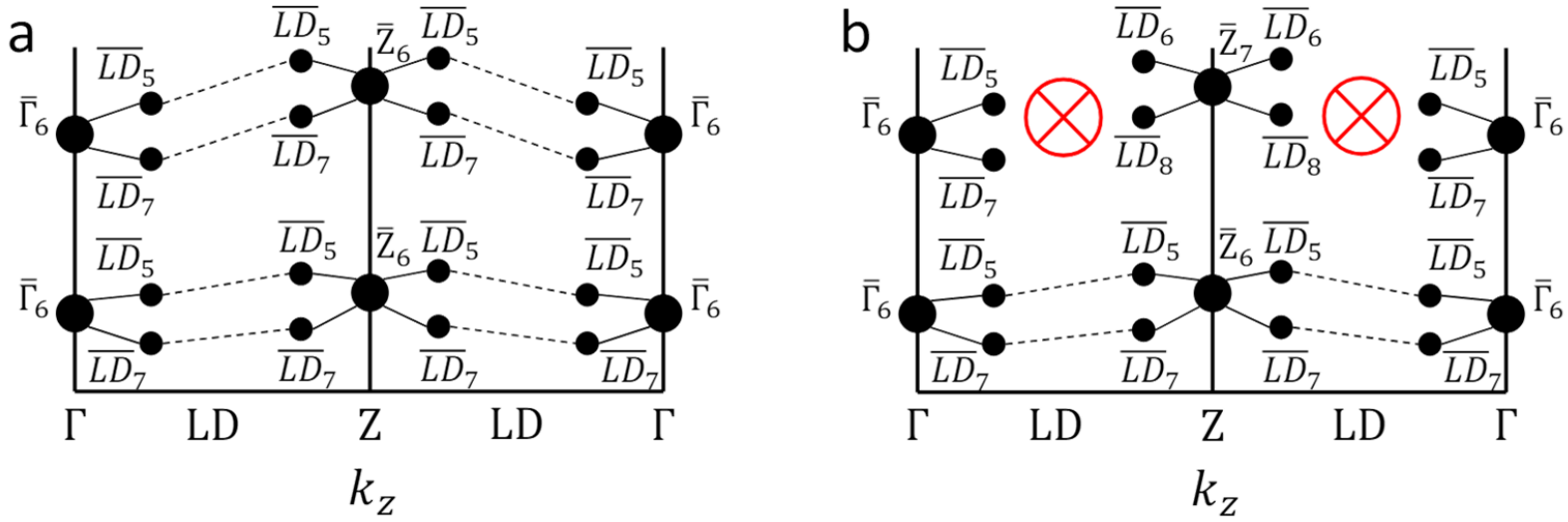
Xu, Elcoro, Song, **BJW**, Vergniory *et al., Nature* (2020)
Elcoro*, **BJW*** *et al., Nat. Comm.* (2021)

Compatibility Relations

- Given $\boldsymbol{k}_1$ & $\boldsymbol{k}_2$ in <u>connected</u> momentum stars, $G_{\boldsymbol{k}_2} \subset G_{\boldsymbol{k}_1}$
  - Small irreps are dependent by subduction: $\sigma_{i,\boldsymbol{k}_1} \downarrow G_{\boldsymbol{k}_2} = \bigoplus_j n_{i,j}^{\boldsymbol{k}_1,\boldsymbol{k}_2} \sigma_{j,\boldsymbol{k}_2}$
  - $n_{i,j}^{\boldsymbol{k}_1,\boldsymbol{k}_2}$ define the small irrep **<u>compatibility relations</u>**

- Compatibility relations can diagnose **<u>enforced semimetal (ES) states</u>**
  - "Occupied" high-symmetry-point small irreps termed **<u>symmetry data vector</u>**

a (b) Symmetry data vector (not) satisfying the compatibility relations
Elcoro, **BJW*** et al., Nat. Comm. (2021)*



Bilbao Tools for Real and Momentum Space

- The **bilbao crystallographic server** (BCS) is the leading open-access tool for symmetry group properties
  - (Relatively) unified notation with

- **<u>Partial lists of Bilbao tools for point groups and 3D SGs</u>**
  - Symmetries and irreducible coreps of all **<u>32 nonmagnetic and 90 magnetic point groups</u>**: https://www.cryst.ehu.es/html/cryst/mpointrepres.html
  - Generating symmetries of all **<u>230 nonmagnetic and 1,421 magnetic space groups (SGs):</u>** https://www.cryst.ehu.es/cgi-bin/cryst/programs/magget_gen.pl
  - Wyckoff positions and site-symmetry groups of all SGs: https://www.cryst.ehu.es/cgi-bin/cryst/programs/magget_wp.pl
  - Momentum stars of all SGs: https://www.cryst.ehu.es/cgi-bin/cryst/programs/magget_wp.pl

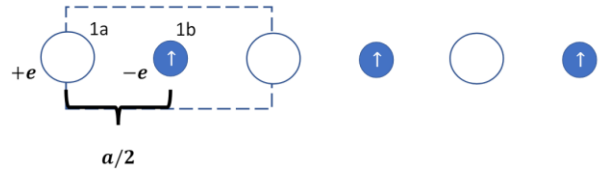
Xu, Elcoro, Song, **BJW**, Vergniory *et al., Nature* (2020)
Elcoro*, **BJW*** *et al.*, *Nat. Comm.* (2021)

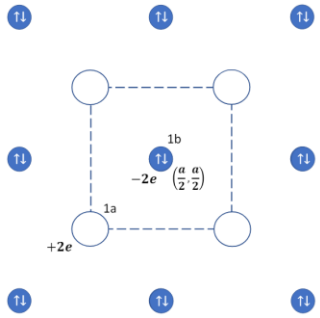
Part 3:
Elementary Band Representations and Topological Quantum Chemistry

Atomic Limits and Wannier Orbitals

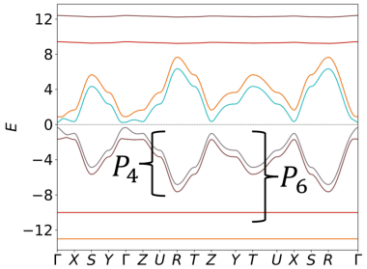
- An **atomic limit** is an insulator with (nearly) decoupled, exponentially localized orbitals in **x**-space in each unit cell
  - Define **atomic limit** to have **trivial stable topology**

Atomic limits in 1D and 2D
BJW *et al., Nat. Comm.* (2020)





- Separate question: given band(s) in **k**-space, can I inverse-Fourier-transform bands into an atomic limit of **Wannier** functions that:
  - Have exponential (and not power-law) tails?
  - Respect the system SG?



Wannierization can be attempted for any isolated bands

- If no, band(s) carry **nontrivial stable topology** (in a complicated, SG-dependent way)
  - **Stable** – remains topological if atomic limit bands added to projector

- **Caution:** many properties of Wannier functions are gauge-dependent!
  - Stable topology is gauge-invariant

see Marzari *et al., RMP* (2012), Soluyanov and Vanderbilt, *PRB* (2012)

Elementary Band Representations from Atomic Limits

- Consider an atomic limit w/ orbitals at high-symmetry **maximal Wyckoff positions**
  - Not connected to a higher-symmetry Wyckoff position
  - Corresponds to a sum of small irreps $\sigma_{i,\boldsymbol{k}}$ in $\boldsymbol{k}$ space
  - Symmetry eigenvalues, but also more Berry phases

BJW *et al.*, *Nat. Comm.* (2020)
Cano *et al.*, *PRB* (20202

- Formally, given SG G and site-symmetry group $G_{\boldsymbol{q}}$, orbitals generate a **k**-space **band representation** $\rho_{\boldsymbol{q}}^{G}$ via induction:

$$\rho_{\boldsymbol{q}} \uparrow G = \rho_{\boldsymbol{q}}^{G} = \bigoplus_{\boldsymbol{k}} \sigma_{\boldsymbol{k},\boldsymbol{q}}^{G} = \bigoplus_{\boldsymbol{k}} \bigoplus_{i} a_{i}^{\boldsymbol{k},\boldsymbol{q}} \sigma_{i,\boldsymbol{k}}$$

- Distinct maximal Wyckoff positions sometimes produce **equivalent band reps,** termed *exceptional cases*
  - Deducible through "sliding" procedure termed **Wannier center homotopy**

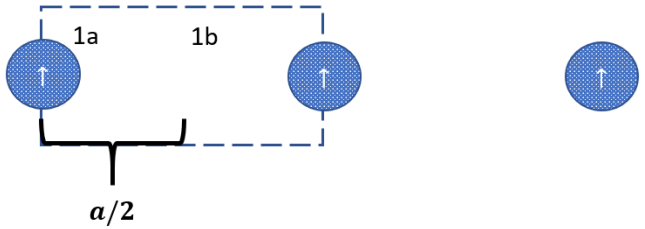
- The inequivalent band reps are termed **elementary (EBRs)**

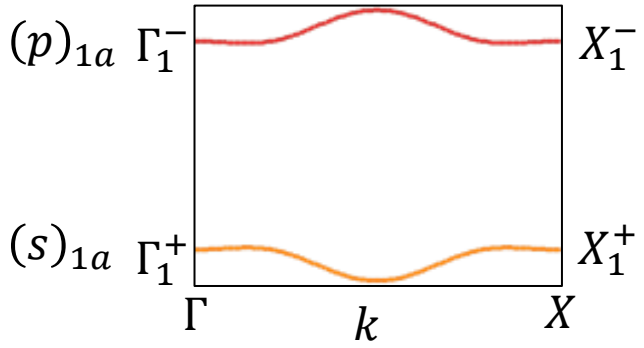
J. Zak, *PRB* (1981)

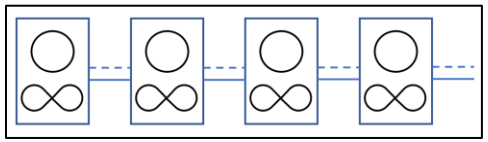
OAL Example 1: Rod Group $p\bar{1}$

- Consider a 1D chain with inversion symmetry & spinless *s* and *p* orbitals at 1a
  - Characters are inversion eigenvalues

Atomic Limit



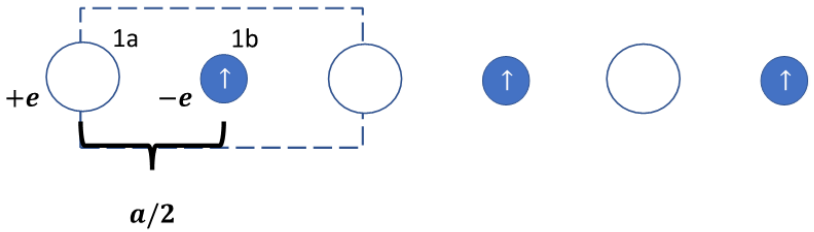


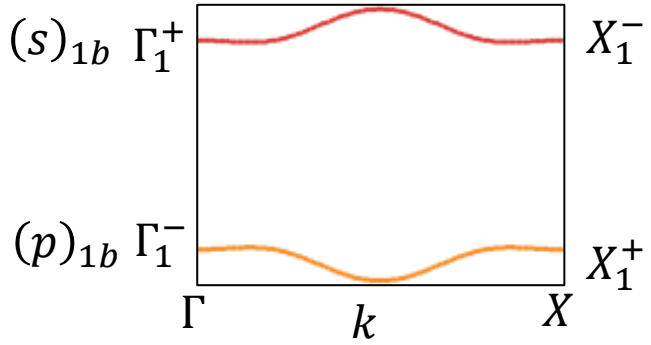


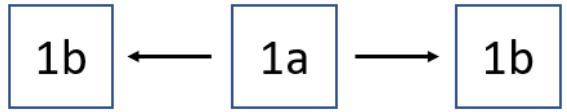
Orbital	Site-Symmetry Irrep	Wyckoff Position	Induced Small Irrep at Γ	Induced Small Irrep at X
s	A_g	1a	Γ_1^+	X_1^+
p	A_u	1a	Γ_1^-	X_1^-
s	A_g	1b	Γ_1^+	X_1^-
p	A_u	1b	Γ_1^-	X_1^+

- Invert bands at $k = 0$ to slide Wannier orbitals
  - **Important:** single degeneracy at intermediate 2c position $\pm x$
  - **Important: OALs are not stable topological, dangerous to predict in real materials due to Wannier gauge issues**

Obstructed Atomic Limit (OAL)



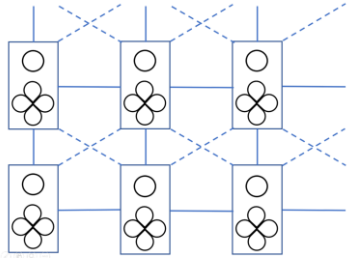




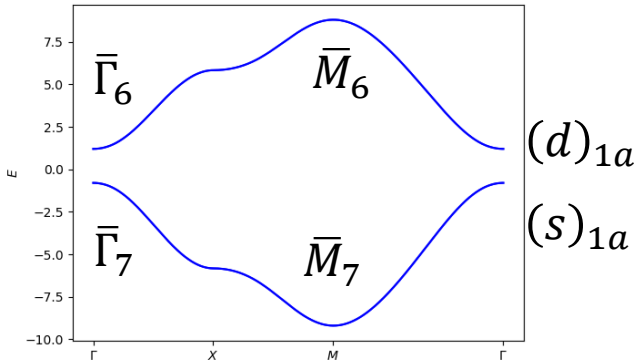
Bradlyn, …, Vergniory, *et al.*, *Nature* (2017)

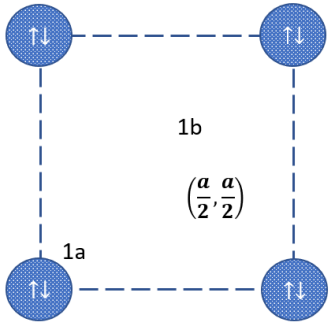
OAL Example 2: Double Wallpaper Group $p4m$

- Consider a 2D square lattice with mirror & C_{4z} & spinful pairs of *s* and *d* orbitals at 1a
  - Characters are (sums of) spinful C_{4z} eigenvalues



Atomic Limit

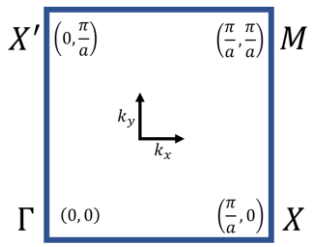


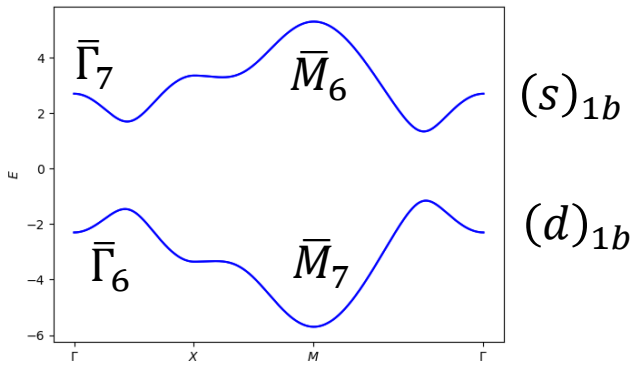


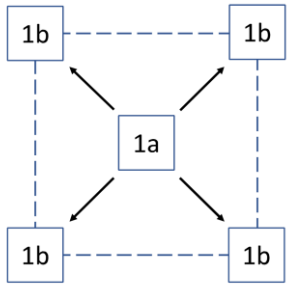
Orbital	Site-Symmetry Irrep	Wyckoff Position	Induced Small Irrep at Γ	Induced Small Irrep at *M*
s	$\bar{E}_1$	1a	$\bar{\Gamma}_7$	$\bar{M}_7$
d	$\bar{E}_2$	1a	$\bar{\Gamma}_6$	$\bar{M}_6$
s	$\bar{E}_1$	1b	$\bar{\Gamma}_7$	$\bar{M}_6$
d	$\bar{E}_2$	1b	$\bar{\Gamma}_6$	$\bar{M}_7$

- Invert bands at $\boldsymbol{k = 0}$ to slide Wannier orbitals
  - **Important:** single degeneracy at intermediate 4d position $(\pm x, \pm x)$

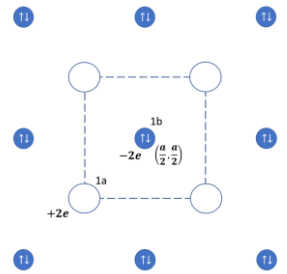
Obstructed Atomic Limit







Checkboard Charge Order



BJW *et al.*, *Nat. Comm.* (2020)

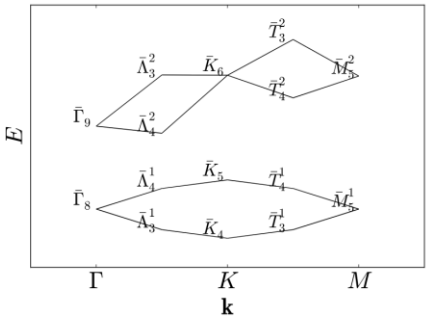
Topological Quantum Chemistry (TQC)

- **<u>Complete theory of band topology</u>** in Classes A, AI, AII with crystal symmetries
  - Both magnetic and nonmagnetic SGs

Bradlyn, …, Vergniory, *et al., Nature* (2017)
Elcoro*, **BJW***, *et al., Nat. Comm.* (2021)

- Basic idea of TQC – **<u>topology by brute force</u>**
  - Enumerate all possible EBRs for every SG
  - Pick out a band in a model or material
  - **If band is not equivalent to integer linear combo of EBRs, it is stable topological**

- Clarifies **<u>two routes towards stable topology</u>** in real materials
  - Band inversion
  - Fractionally fill a split EBR (not all EBRs are connected)



A disconnected (split) EBR
Frequently (but not always) stable topological
For "fragile" case, see H. C. Po, et al., PRL (2018)

Symmetry-Based Indicators

- If a set of bands *P* do not "transform" (eigenvalues and Berry phases) in an integer linear combination of EBRs, *P* is stable topological

- For **<u>just eigenvalues</u>**, *some SGs* support generalized Fu-Kane $\mathbb{Z}_N$ formulas for topology termed **<u>Symmetry-Based Indicators (SIs)</u>**
  - Obtainable algorithmically via EBRs (Smith normal decomposition)
  - Nontrivial SI indicates either:
    - <u>*P* is stable topological</u>
    - <u>*P* is semimetal satisfying compatibility relations</u>

Fu and Kane, *PRB* (2007)
Fang, Gilbert, Bernevig, *PRB* (2012)
Kruthoff *et al., PRX* (2017)
Po *et al., Nat. Comm.* (2017)
Song *et al., Nat. Comm.* (2018)

Typical SI Computer Output

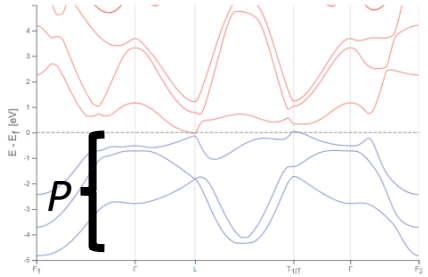
k point	Irreducible representations
Γ	$2E_{\frac{1}{2}g}+E_{\frac{1}{2}u}+F_{\frac{3}{2}u}$
L	$E_{\frac{3}{2}g}+2E_{\frac{1}{2}g}+2E_{\frac{1}{2}u}$
W	$2E_{\frac{3}{2}}+3E_{\frac{1}{2}}$
X	$2E_{\frac{1}{2}g}+2E_{\frac{1}{2}u}+E_{\frac{3}{2}u}$

↓

$z_8 = 4$

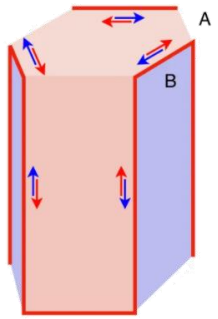
- **<u>Cons:</u>**
  - Have to figure out the right linear combo of computer output for **<u>physical basis of SI formula</u>**
  - **<u>Only a partial classification</u>** – some invariants like Chern number are $\mathbb{Z}$-valued
    - Complete *P* diagnosis requires other tools like Wilson loops and layer constructions

$Z_{2w,1} = 0, Z_{2w,2} = 0, Z_{2w,3} = 0, Z_4 = 2$



- **<u>Pros:</u>**
  - Reveal new topological states (*e.g.* bismuth)
  - Numerically efficient *ab initio*

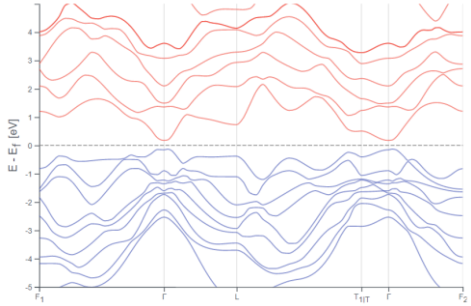
$Z_4 = 2$ "higher-order TI" in bismuth, still mysterious…
see Schindler et al., Nat. Phys. (2018),
*Schindler, …, **BJW,** Nat. Comm. (2022), Lin, …, **BJW**, Nat. Comm. (2024)*



High-Throughput Topological Materials Discovery

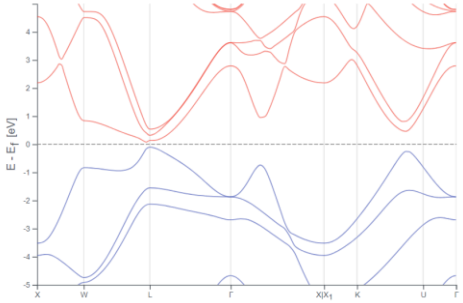
- SIs applied to high-throughput first principles (DFT) calculations reveal ***O*(10,000) topological insulators, semimetals, flat bands, magnons, and phonons**
  - Leading teams: Bernevig (Princeton), Vishwanath (Harvard), Fang (IOP China)
  - Confirm known examples and recontextualize others

Bi_2Se_3



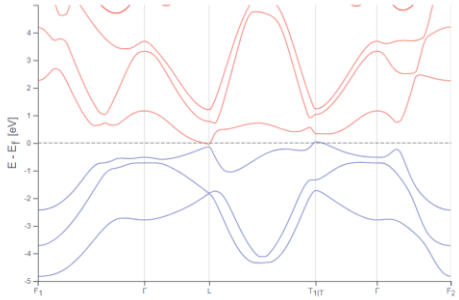
$Z_{2w,1} = 0, Z_{2w,2} = 0, Z_{2w,3} = 0, Z_4 = 3$

SnTe



$Z_{2w,1} = 0, Z_{2w,2} = 0, Z_{2w,3} = 0, Z_4 = 0, Z_2 = 0, Z_8 = 4$

Rhombohedral Bismuth



$Z_{2w,1} = 0, Z_{2w,2} = 0, Z_{2w,3} = 0, Z_4 = 2$

Our results are freely available here:

Topological Materials Database

www.topologicalquantumchemistry.com

Partial list of DFT papers

Vergniory, …, Regnault, *Nature* (2019)
Tang, *et al., Nature* (2019)
Zhang *et al., Nature* (2019)
Xu, …, **BJW**, Vergniory, …, *Nature* (2020)
Vergniory,* **BJW***, …., Regnault, *Science* (2022)
BJW, …, Vergniory, Regnault, …, *Nat. Rev. Mater.* (2022)
Regnault *et al., Nature* (2022)
Karaki *et al., Sci. Adv.* (2023)
Xu, Vergniory, *et al., Science* (2024)

Elementary Band Representations and Group Theory from the Perspective of Condensed Matter Physics

Aussois GDR School, May 2024

Benjamin J. Wieder

Fin. Merci!