MAX PLANCK INSTITUTE
FOR CHEMICAL PHYSICS OF SOLIDS

Topological Quantum Chemistry

Hands-on-session

Aussois GDR School, May 2024

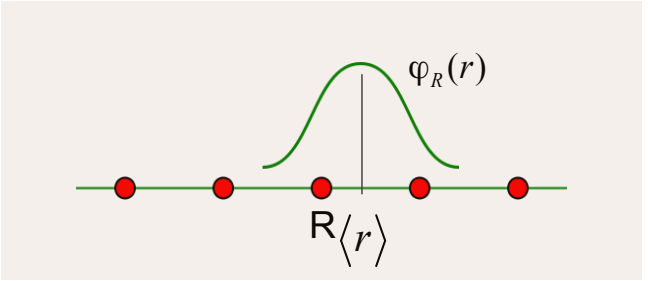
Maia G. Vergniory & Mikel Iraola

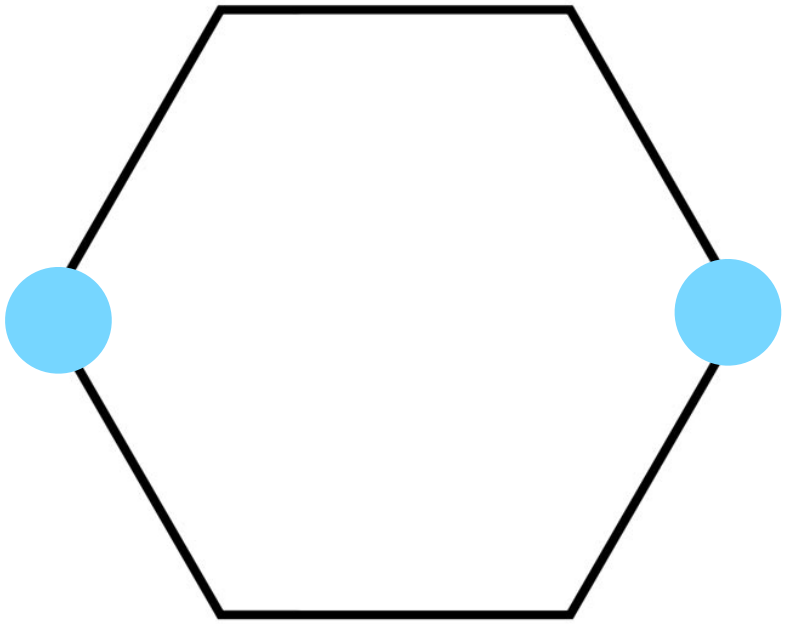
Wannier functions

Bloch states $\psi_k(r) = e^{ikr} u_k(r)$ are defined for periodic boundary conditions

Define localized **Wannier States** :

$$|\varphi(R)\rangle = \oint_{BZ} \frac{dk}{2\pi} e^{-ikR} |\psi_k\rangle = \oint_{BZ} \frac{dk}{2\pi} e^{-ik(R-r)} |u_k\rangle$$





Vanderbilt and Soluyanov PRB (2011)

Wannier functions

D. Vanderbilt "Berry phases in electronic structure theory "

Definition of a Wannier function :

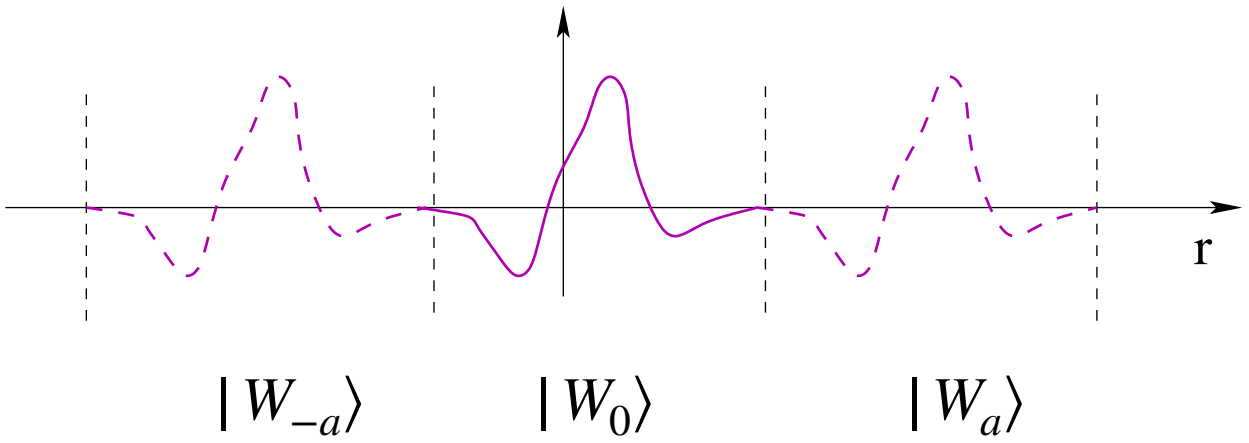
$$|W_R\rangle = \frac{a}{2\pi}\int_0^{2\pi/a} d\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}} |\psi_\mathbf{k}\rangle$$

$$|\psi_\mathbf{k}\rangle = \sum_\mathbf{R} e^{i\mathbf{k}\cdot\mathbf{r}} |W_R\rangle$$

If $|\psi_\mathbf{k}\rangle(x)$ is a smooth function of k,
then $|W_R\rangle(x)$ is a localized function centred near R

Properties of a Wannier function :

1. WFs with different R are periodic images of one another



Properties of a Wannier function :

2. WFs form an orthonormal set

$$\langle W_{R'} | W_R \rangle = \delta_{RR'}$$

3. WFs span the **same subspace** of the Hilbert space as is spanned by the **Bloch wave functions** from which they are constructed

Properties of a Wannier function :

→

Let it be P_n the projector operator onto band n

$$\hat{P}_n = \frac{a}{2\pi}\int_{BZ} |\psi_{nk}\rangle\langle\psi_{nk}| = \sum_R |W_R\rangle\langle W_R|$$

From this also follows that the total charge density ρ_n in a band n is

$$\rho_n = -e\langle r|\hat{P}_n|r\rangle = -e\frac{V_{cell}}{(2\pi)^3}\int_{BZ} |\psi_{nk}(r)|^2 d^3k = -e\sum_R |W_{nR}(r)|^2$$

Properties of a Wannier function :

4. Matrix elements between of operators between Wannier functions

$$\langle W_{n0} | H | W_{nR} \rangle = E_{nR}$$

$$\langle W_{n0} | \mathbf{r} | W_{nR} \rangle = \mathbf{A}_{nR}$$

Fourier transform coefficients of the Berry connection $A_n(k)$

5. The centers of Wannier are related to the Berry phase.

$$\bar{\mathbf{r}} = \langle W_{n0} | \mathbf{r} | W_{n0} \rangle$$

Properties of a Wannier function :

$$\bar{\mathbf{r}} = \frac{V_{cell}}{(2\pi)^3}\int_{BZ} A_n(\mathbf{k})d^3\mathbf{k} = \frac{V_{cell}}{(2\pi)^3}\int_{BZ} \langle u_{n\mathbf{k}} | i\nabla u_{n\mathbf{k}}\rangle d^3\mathbf{k}$$

In 1D

$$\bar{\mathbf{x}} = \frac{a}{2\pi}\int_0^{2\pi/a} \langle u_{nk} | i\partial_k u_{nk}\rangle dk = a\cdot\frac{\gamma}{2\pi}$$

Berry phase evolving from 0 to 2π, would just correspond to a Wannier center evolving from x=0 to x=1

Hybrid Wannier functions

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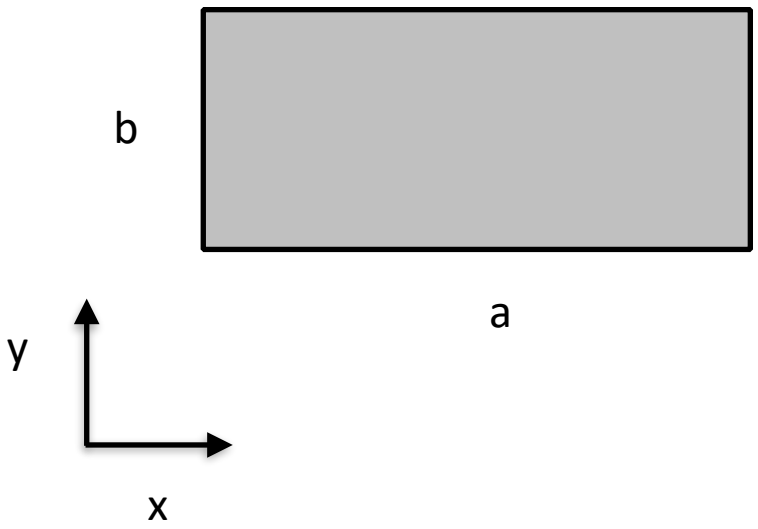
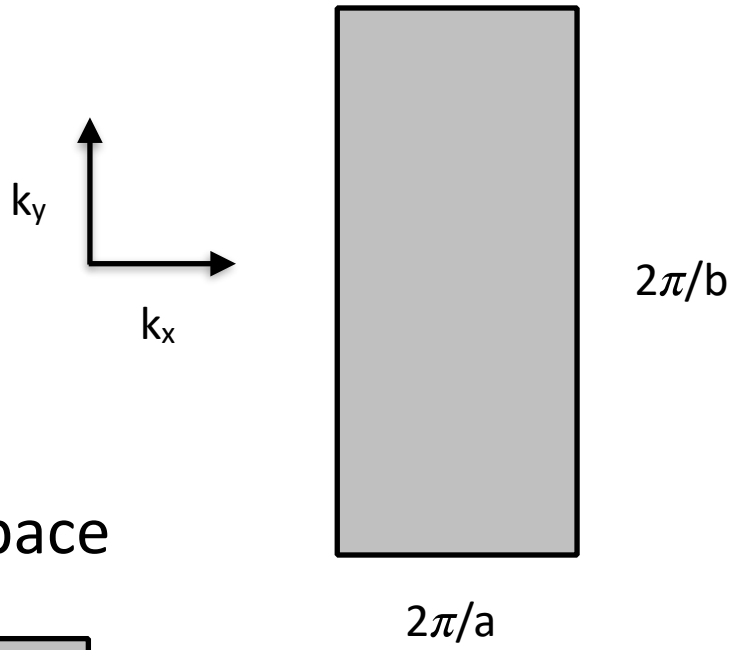
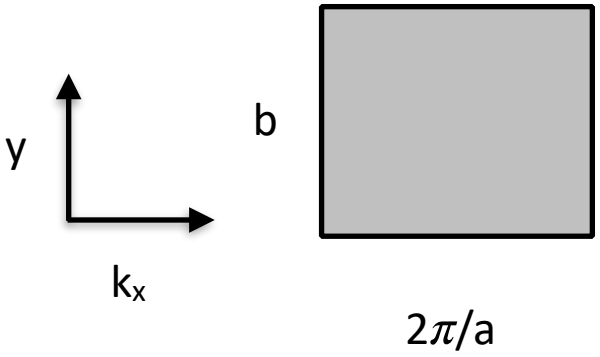
Real-space unit cell



Reciprocal-space unit cell



Hybrid space



Hybrid Wannier functions

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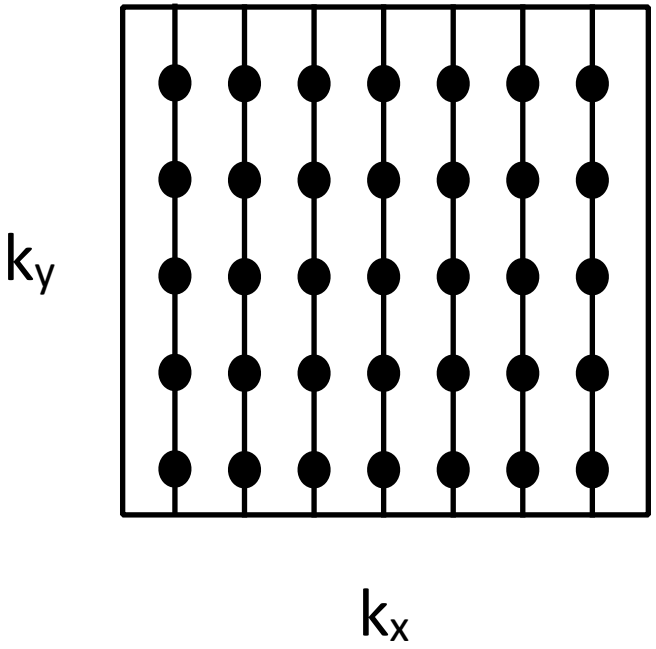
At each k_x find 1D WF along y, and their centers



$$\bar{\mathbf{y}}(k_x) = \langle W_{nk_x} | y | W_{nk_x} \rangle dk$$

$$\gamma(k_x)^{(y)} = \int_0^{2\pi/b} i\langle u | \partial_{k_y} u \rangle dk y_y$$

$$\downarrow$$

$$\bar{\mathbf{y}}(k_x) = b\frac{\gamma(k_x)}{2\pi}$$

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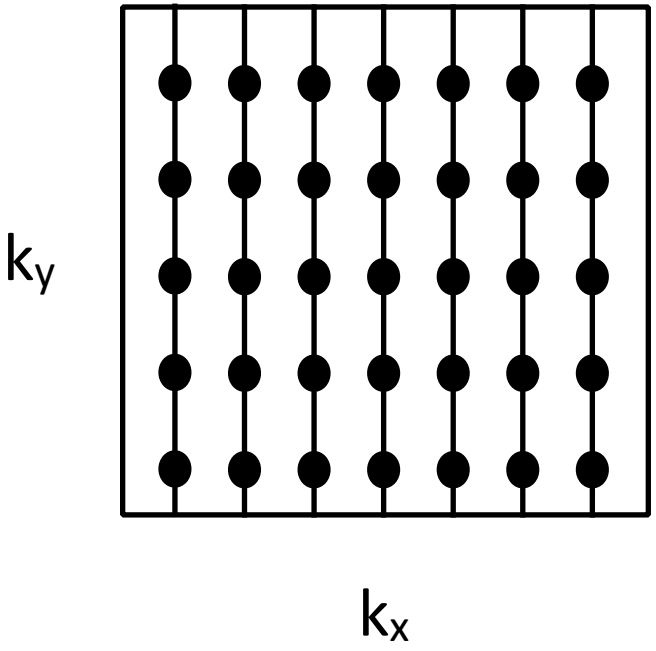

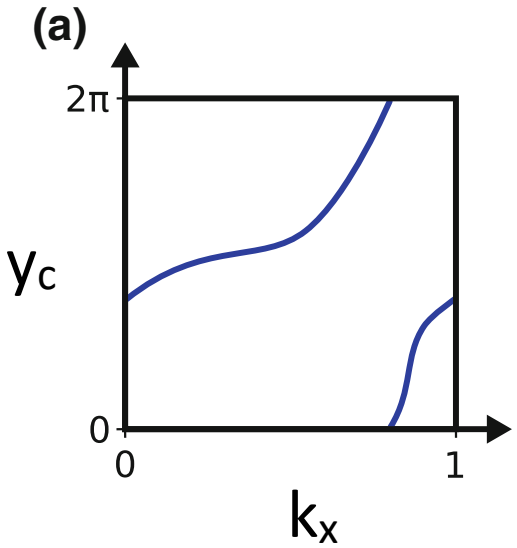

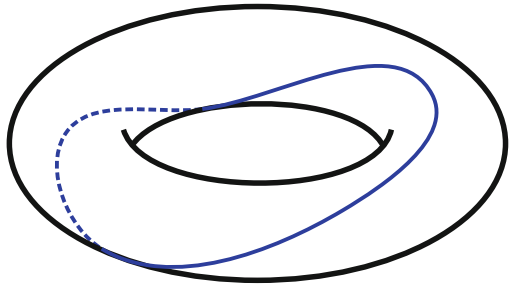

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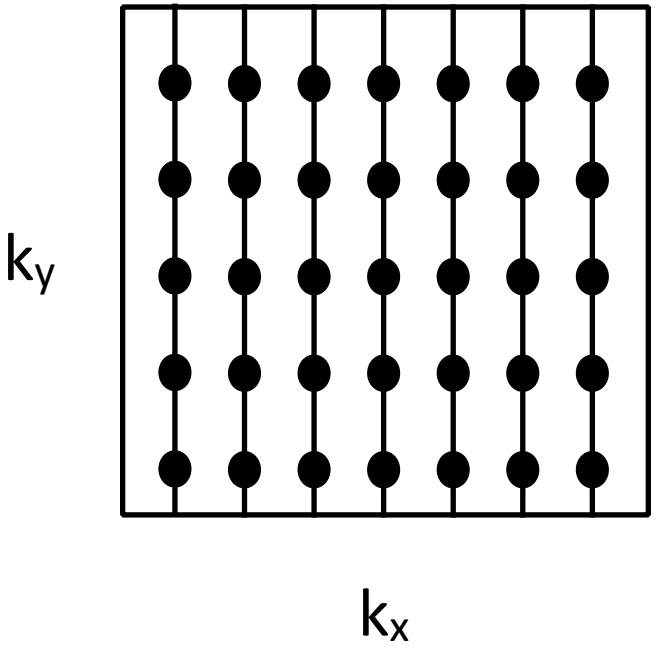

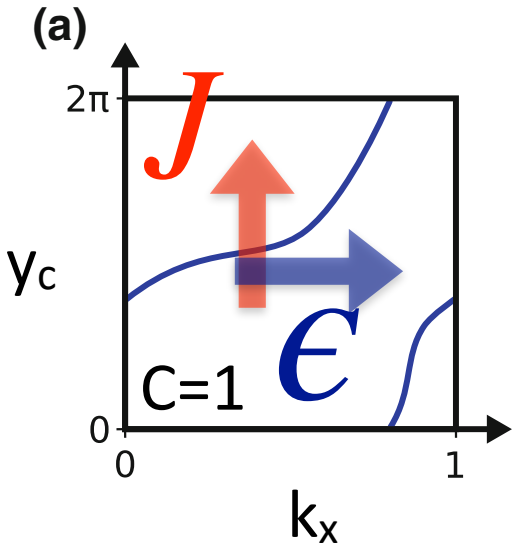

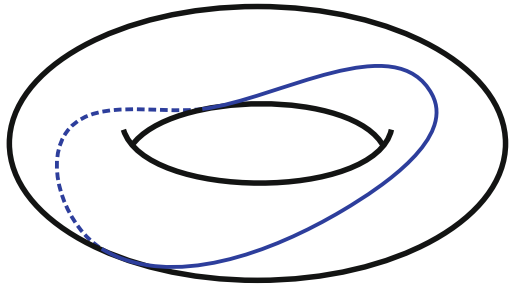

Hybrid Wannier functions

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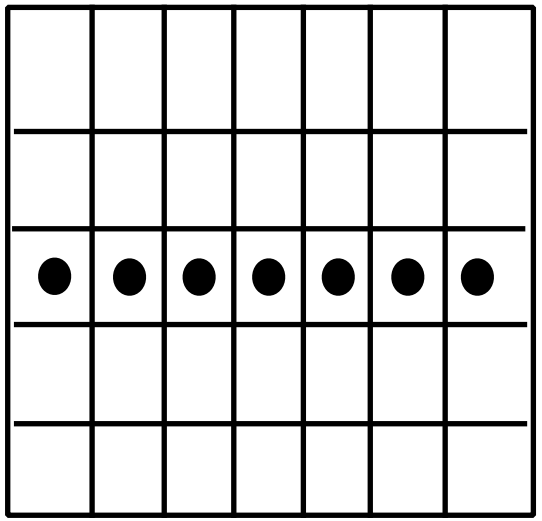
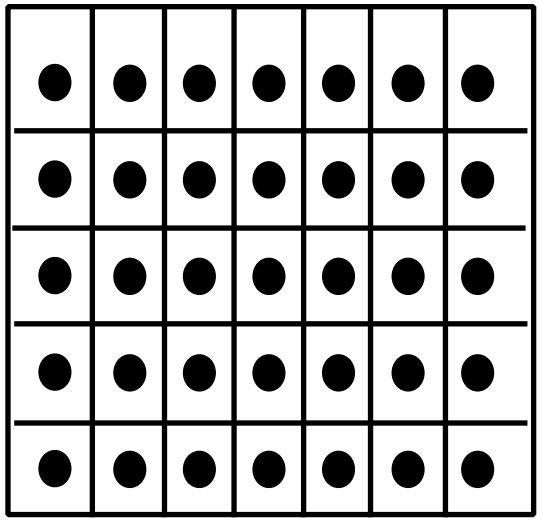
HWF $|h_{k_x}(R_y)\rangle$

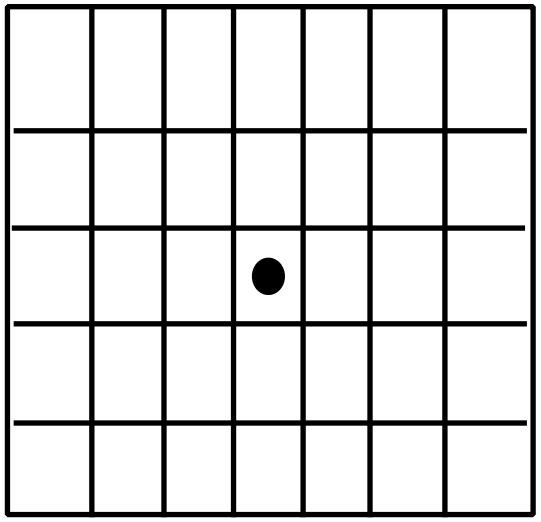


$|\psi(k_x, k_y)\rangle$



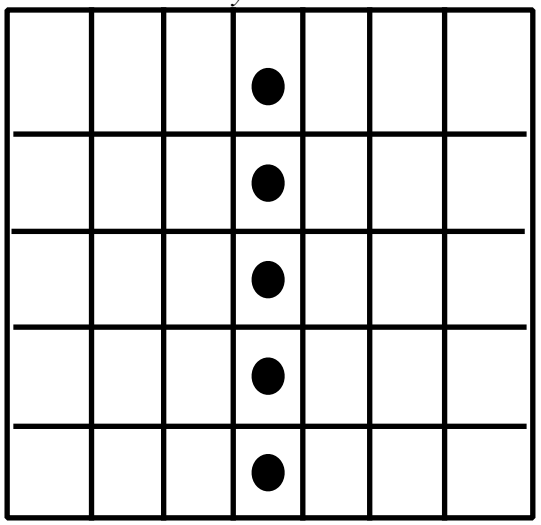
Bloch wavefunction

$|W(R_x, R_y)\rangle$



Wannier function
(Localized in x and y)

HWF $|h_{k_y}(R_x)\rangle$



Topological obstruction

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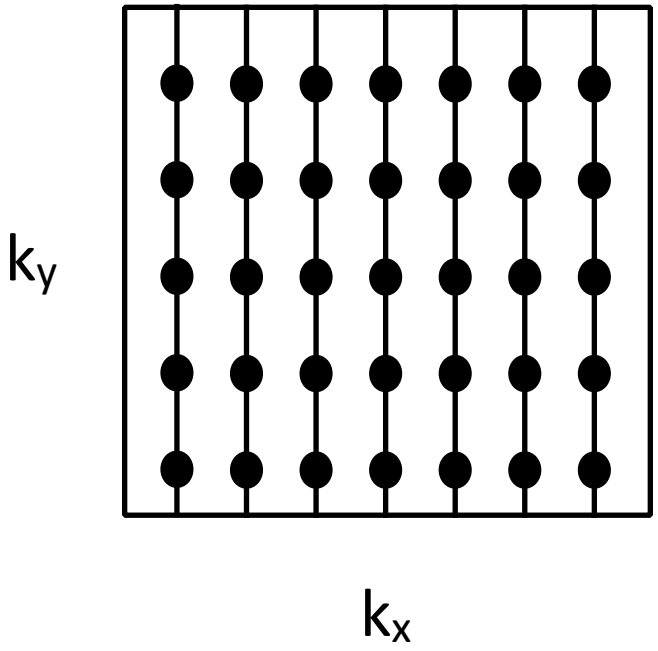
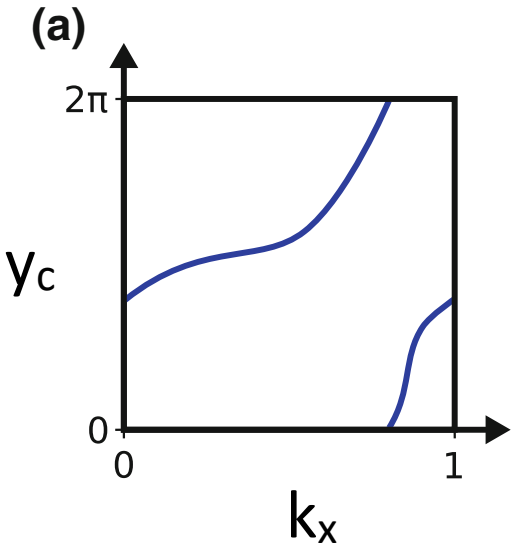
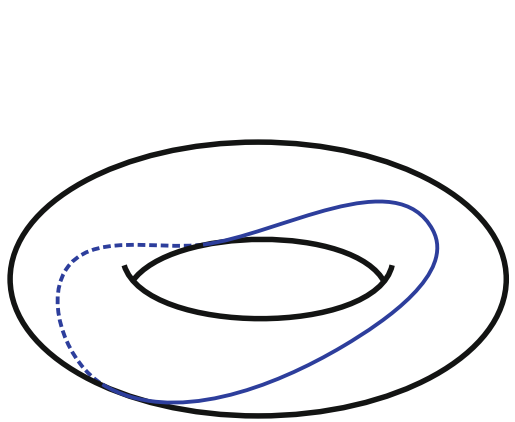
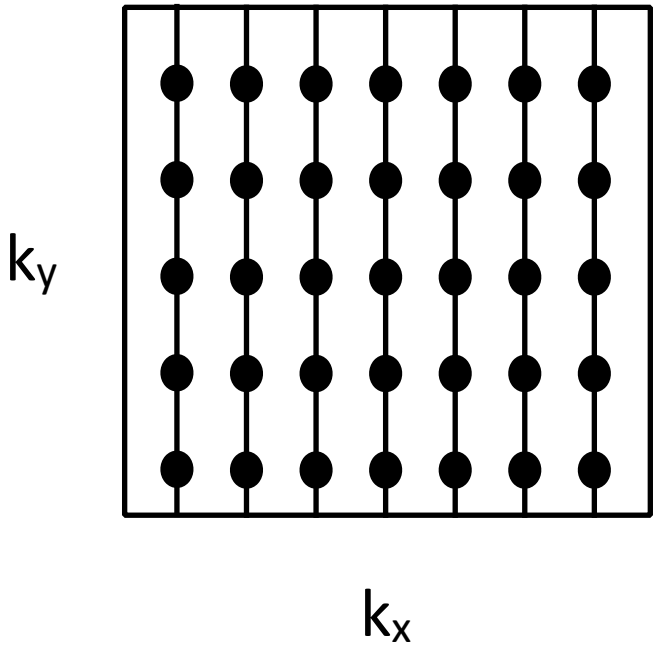


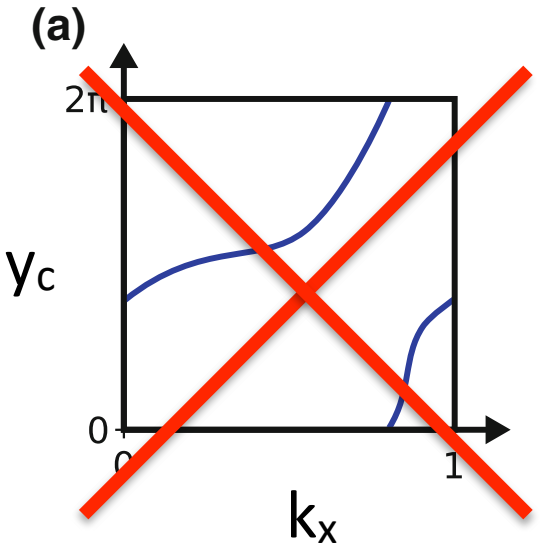


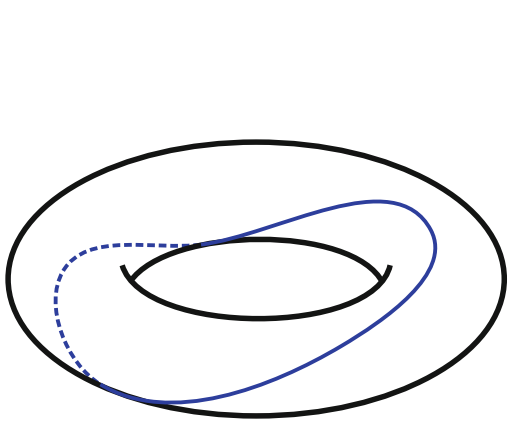


$$\bar{y}_{k_x} = \langle h_{k_x}(0) \,|\, y \,|\, h_{k_x}(0) \rangle = \sum_{R_x} e^{ik_x R_x} \langle w(0,0) \,|\, y \,|\, w(R_x,0) \rangle$$

Topological obstruction







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Atomic Limit

Bloch states $\psi_k(r) = e^{ikr} u_k(r)$ are defined for periodic boundary conditions

Define localized **Wannier States** :

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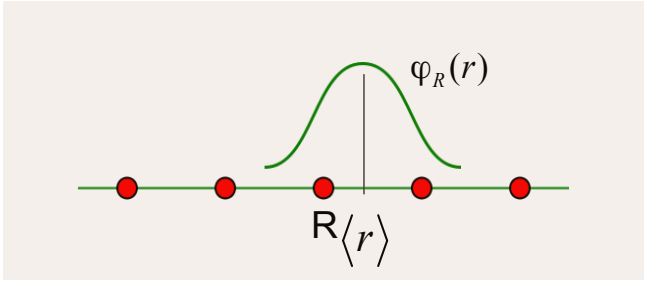
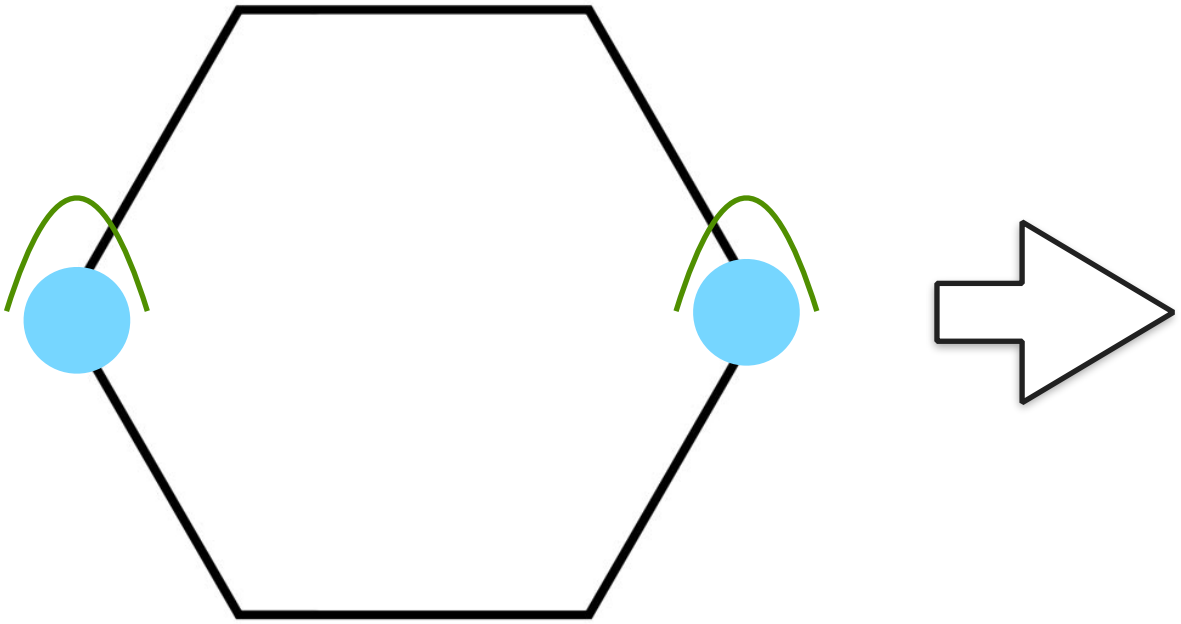
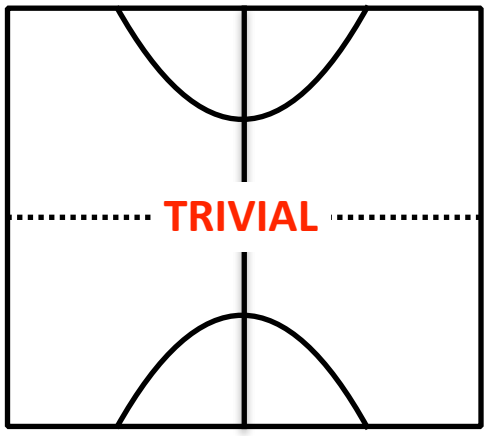




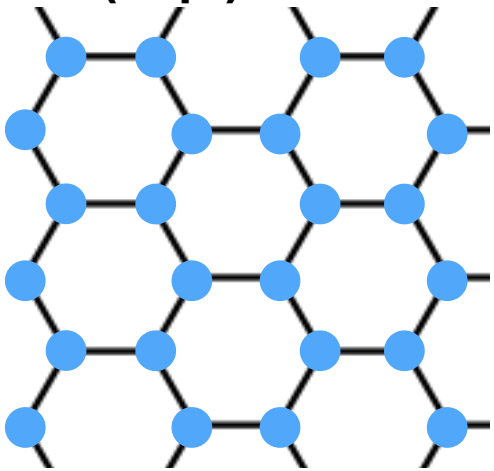


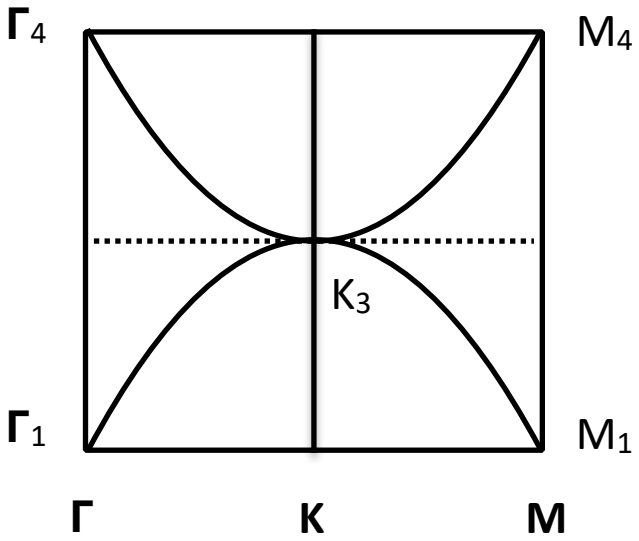
Vanderbilt and Soluyanov PRB (2011)

Elementary Band Representations (EBRs)

orbital + atomic site + lattice
(irrep + wyckoff position + space group)

s (or p_z) orbitals





atomic limit = EBR

An EBR describes a set of Wannierizable bands

J. Zak PRL (1980), Michel and Zak PRB (1999), Michel and Zak Phys. Rep. (2001)

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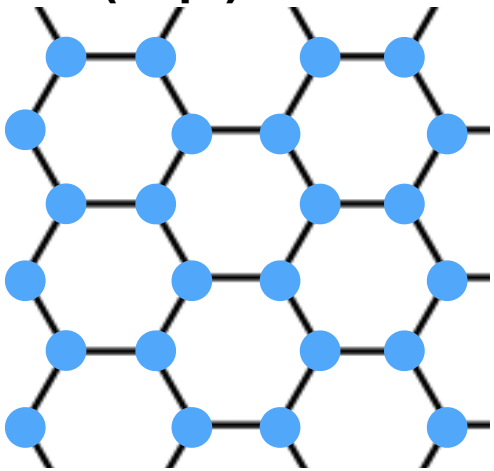

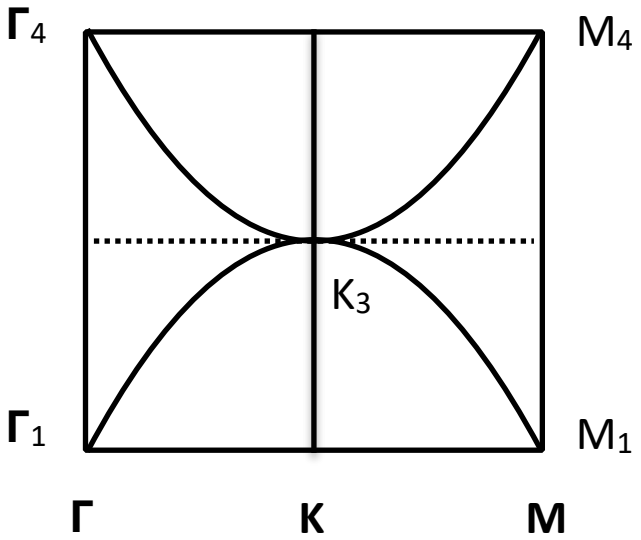

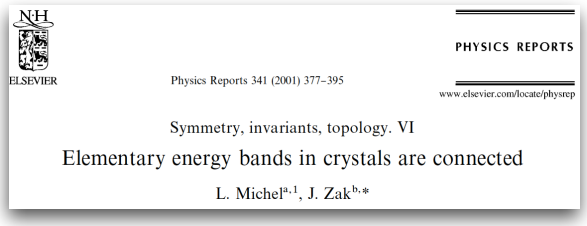
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Physics Reports 341 (2001) 377–395
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Symmetry, invariants, topology. VI

Elementary energy bands in crystals are connected

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

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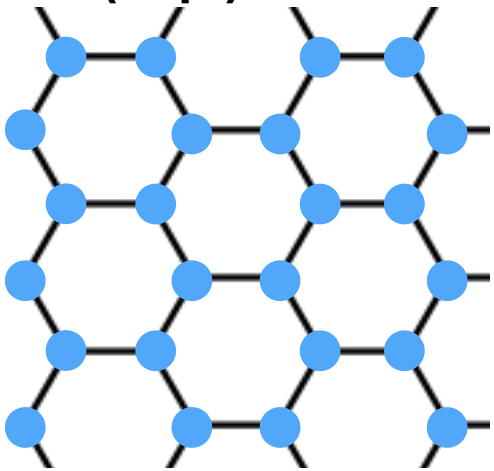

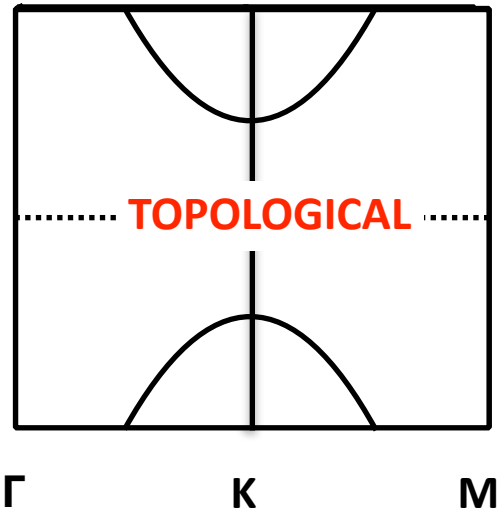

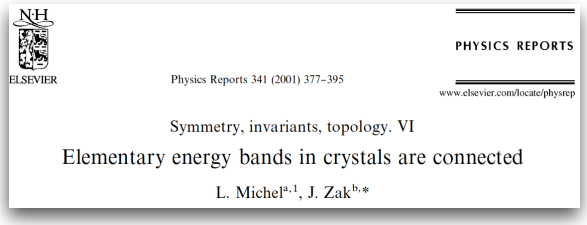
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Crystal Structure

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Space-Groups

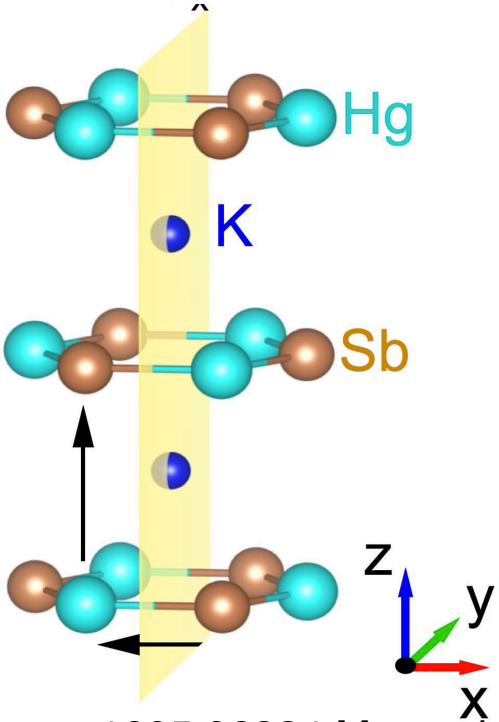

Image: 1605.06824 Ma et al

Ingredients:

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

Elementary band representations (EBRs)

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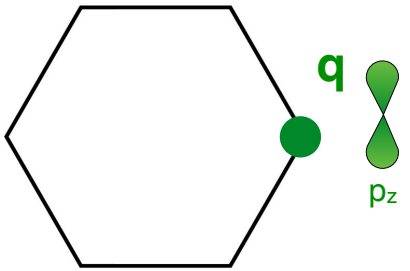
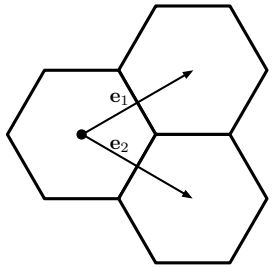
Consider one lattice site:



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

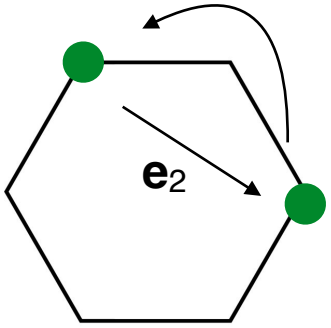
(2) (1)



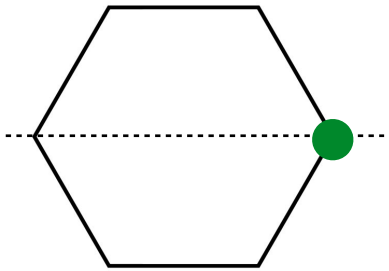
(1) Site-symmetry group, G_q, leaves **q** invariant $\{C_3|01\}, \{m_{1\bar{1}}|00\} \approx C_{3v}$

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

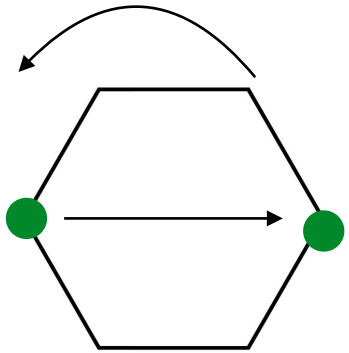
$\{C_3|01\}$



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



$\{C_2|?\}$



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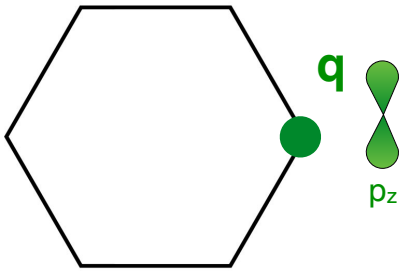

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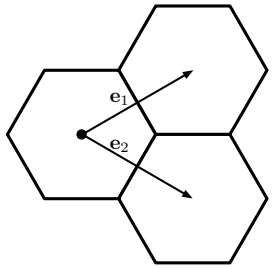
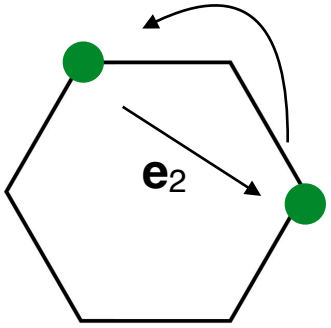


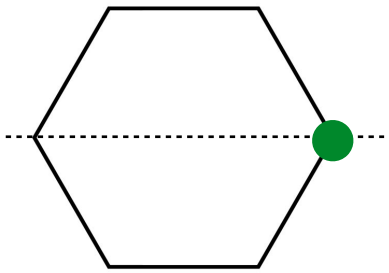
(1) Site-symmetry group, G_q, leaves **q** invariant $\{C_3|01\}, \{m_{1\bar{1}}|00\} \approx C_{3v}$

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

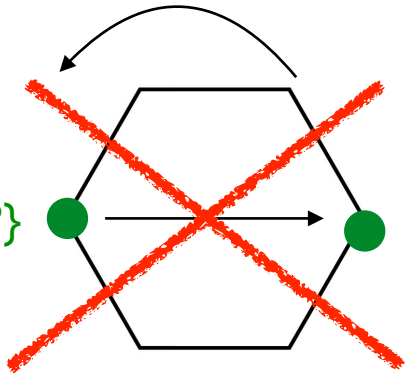
$\{C_3|01\}$



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



$\{C_2|?\}$



Elementary band representations (EBRs)

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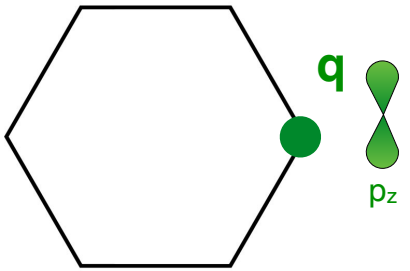
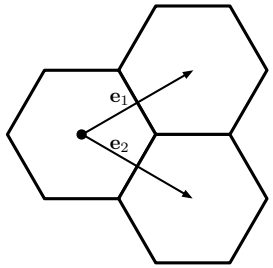
Consider one lattice site:



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

(2) (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

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

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

Elementary band representations (EBRs)

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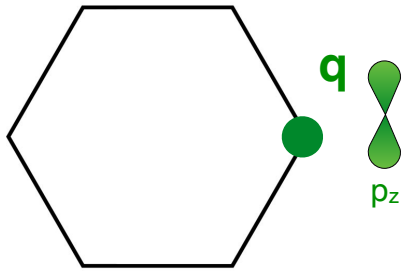
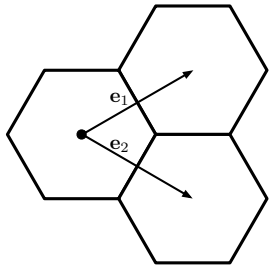
Consider one lattice site:



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

(2) (1)

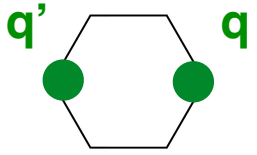


(1) Site-symmetry group, $G_{\mathbf{q}}$, leaves **q** invariant $\{C_3|01\}, \{m_{1\bar{1}}|00\} \approx C_{3v}$

→ Orbitals at **q** transform under a rep, ρ, of $G_{\mathbf{q}}$

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

Wyckoff multiplicity: 2
orbit of q



Elementary band representations (EBRs)

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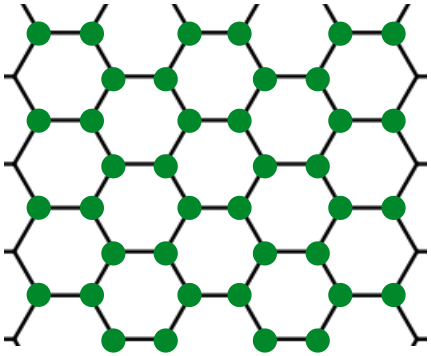
$\bar{\Gamma}_6$ induced in C_{6v}

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

$$\rho_G = \rho \uparrow G$$

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

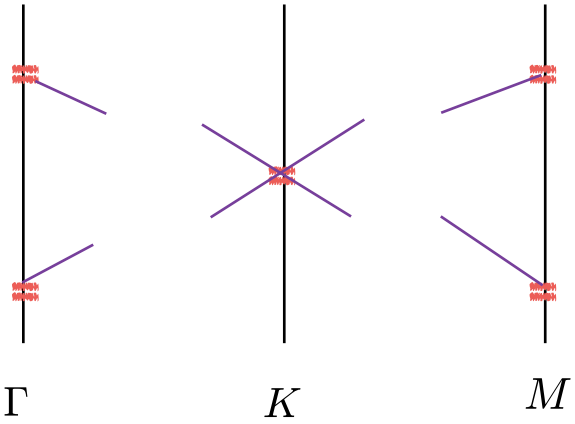
h ∈ G, generators of honeycomb lattice: C_2, C_3, σ



$$\rho_{i\alpha,j\beta}(h) = \rho_{ij}(g_{\alpha\beta})$$
$$g_{\alpha\beta} = g_\alpha^{-1}\{E|t_{\alpha\beta}\}h g_\beta$$

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

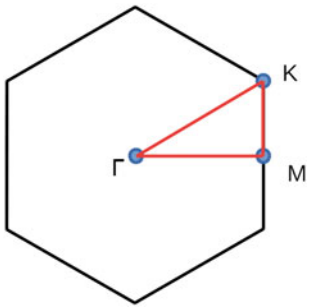
$(\rho \uparrow G) \downarrow G_k$

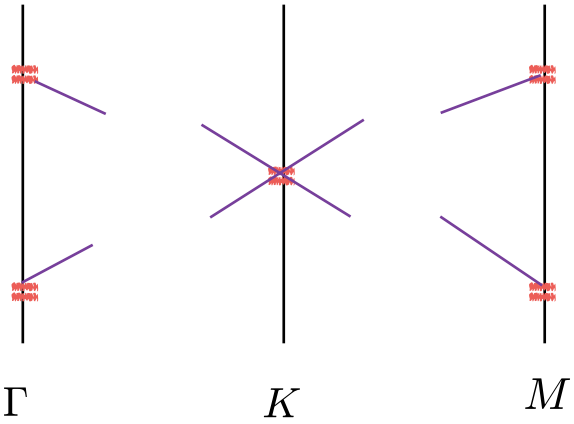


dimension of this band representations = connectivity in the Brillouin zone

Elementary band representations (EBRs)

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





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

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

Compatibility-relations

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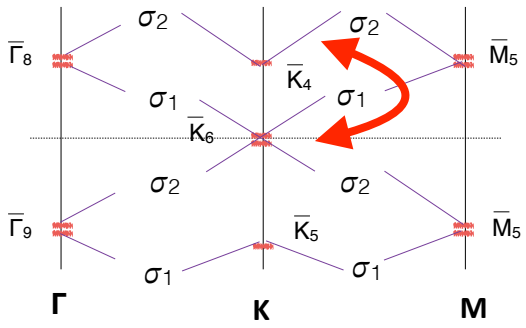
All possible connection between maximal and non-maximal k-vectors

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

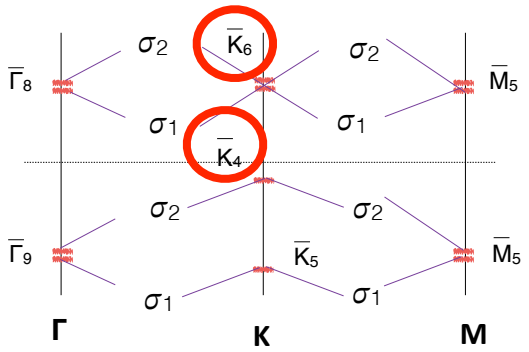
for each max. **k** in ***k** and $\mathbf{k}_i$ non-maximal

E_F



Metal

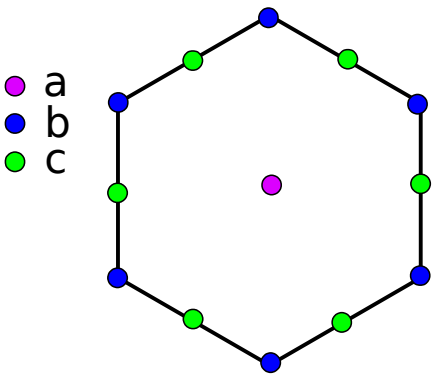
E_F



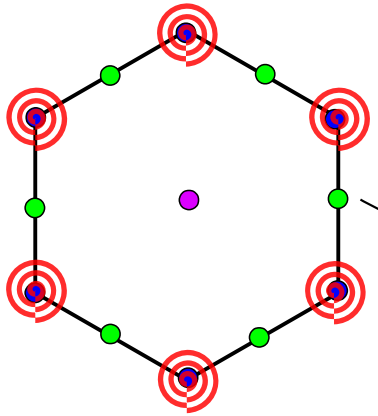
Insulator

B. Bradlyn et al. Nature 547 (2017), M.G. Vergniory et al. Nature 566 (2019), M. G. Vergniory Science (2022

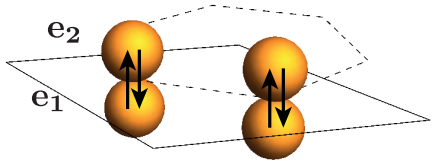
Topological Quantum Chemistry



Maximal symmetry
Wyckoff positions

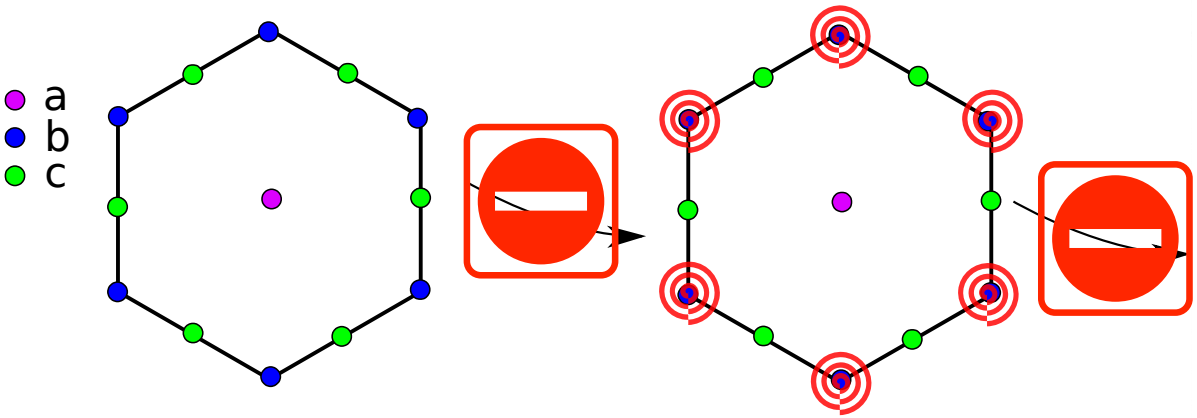


Wannier functions at
some Wyckoff pos.



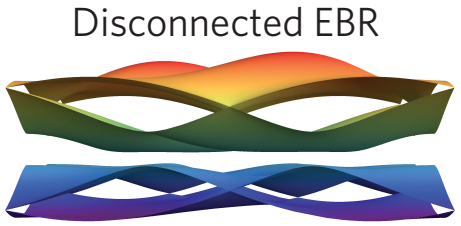
Nature (2017)

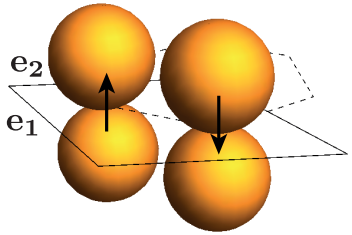
Topological Quantum Chemistry



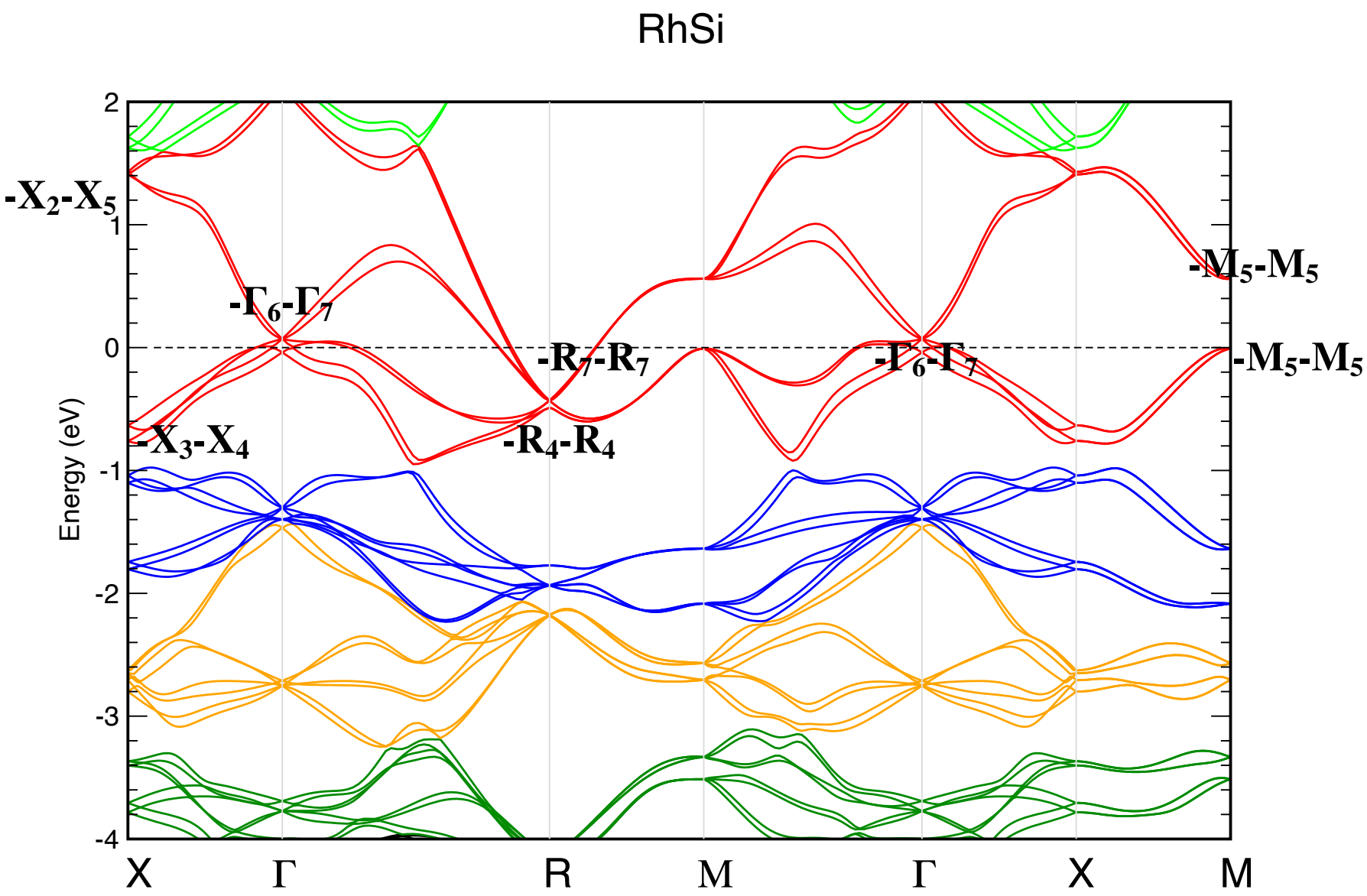
Maximal symmetry
Wyckoff positions

Wannier functions at
some Wyckoff pos.

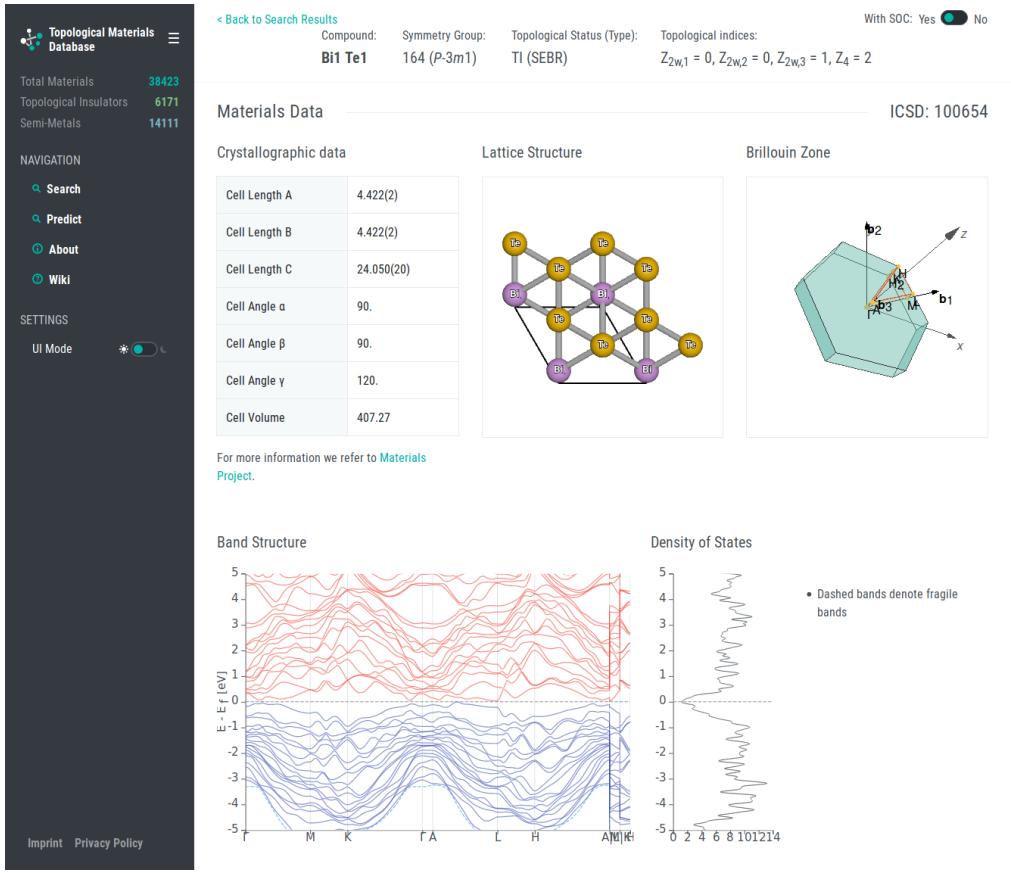


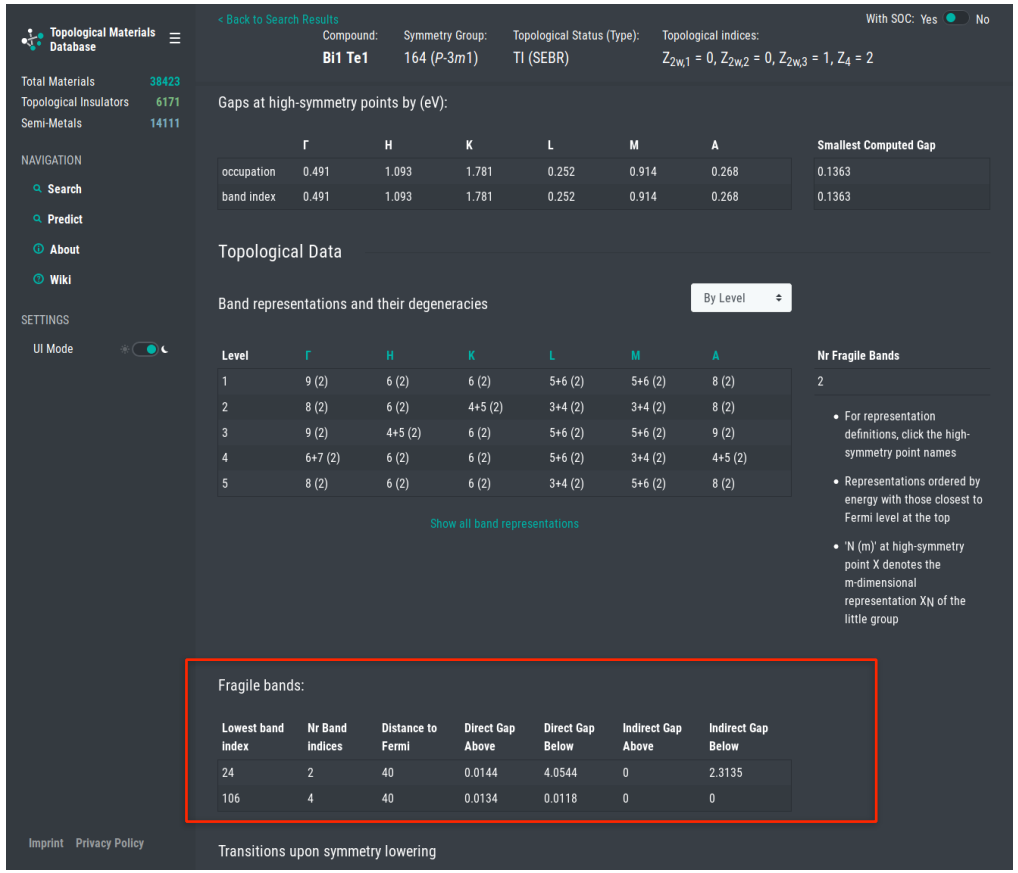


Nature (2017)


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

Topological Quantum Chemistry





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September 2021, Leioa (Spain)

Forthcoming schools and workshops

News:

- **New Article in Nature**
  10/2020: Xu *et al.* "High-throughput calculations of magnetic topological materials" *Nature* (2020) **586**, 702-707.
- New programs: **MBANDREP**, COREPRESENTATIONS, COREPRESENTATIONS PG, MCOMPREL, MSITESYM, **MKVEC**, **Check Topological Magnetic Mat**
  10/2020: new tools in the sections "Magnetic Symmetry and Applications" and "Representations and Applications".
  More info
- New section: **TOPOLOGICAL QUANTUM CHEMISTRY**
  10/2020: tools for the identification of the

Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

Solid State Theory Applications

Topological Quantum Chemistry

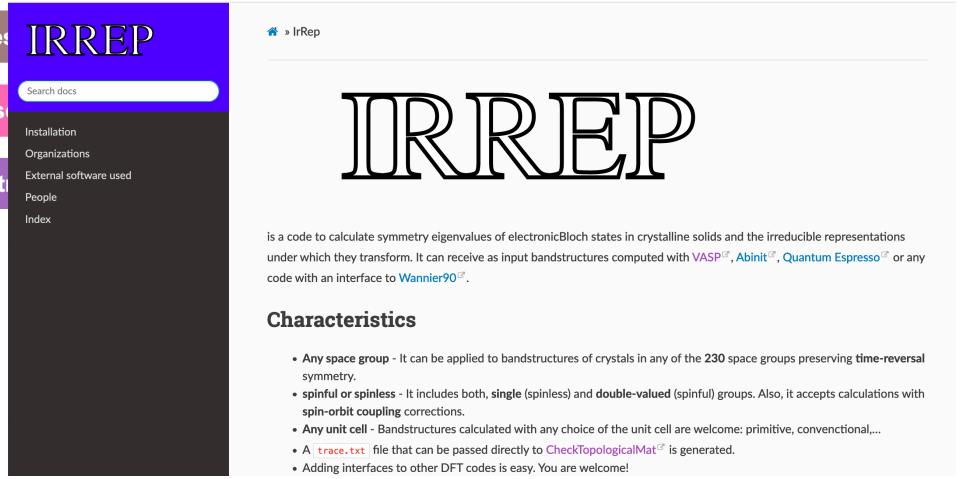
Structure Databases

Raman and Hyper-Raman s

Point-group symmet

Quick access to some tables

Space Groups
Plane Groups
Layer Groups
Rod Groups
Frieze Groups
2D Point Groups
Point Groups
Magnetic Space Groups



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