



Topological Quantum Chemistry

Hands-on-session

Aussois GDR School, May 2024

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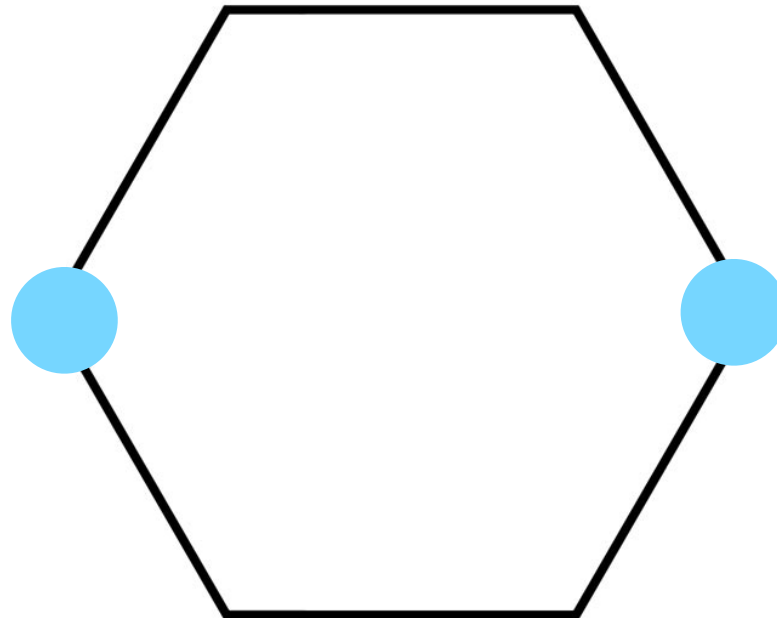
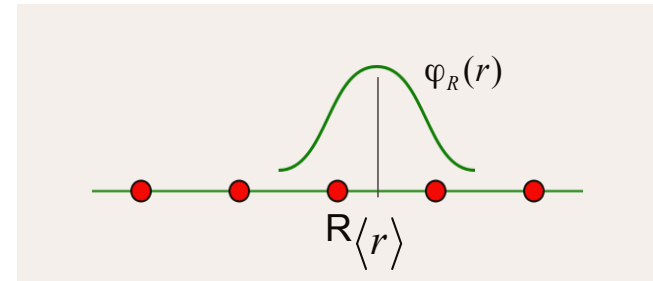


Wannier functions

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

Define localized **Wannier States** :

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





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



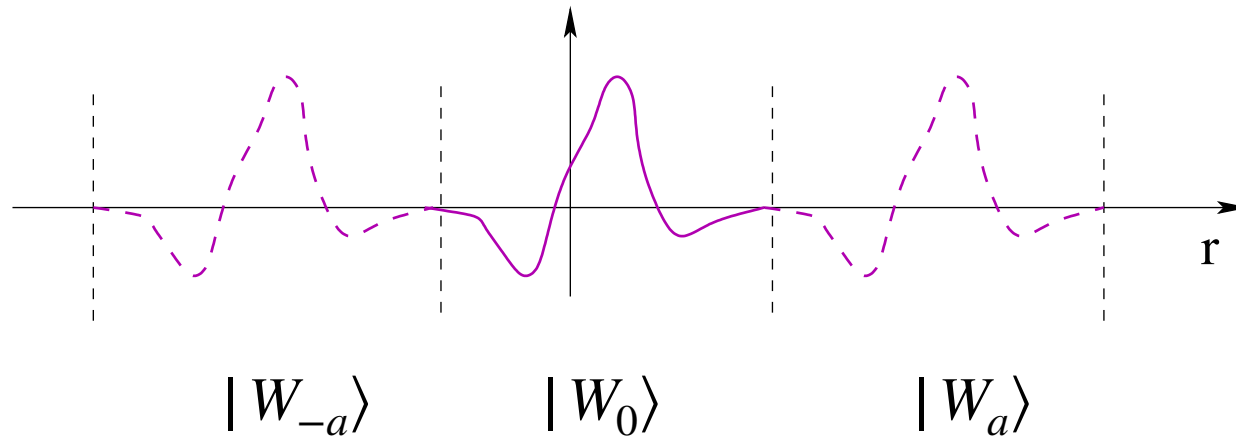
Wannier functions

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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

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

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

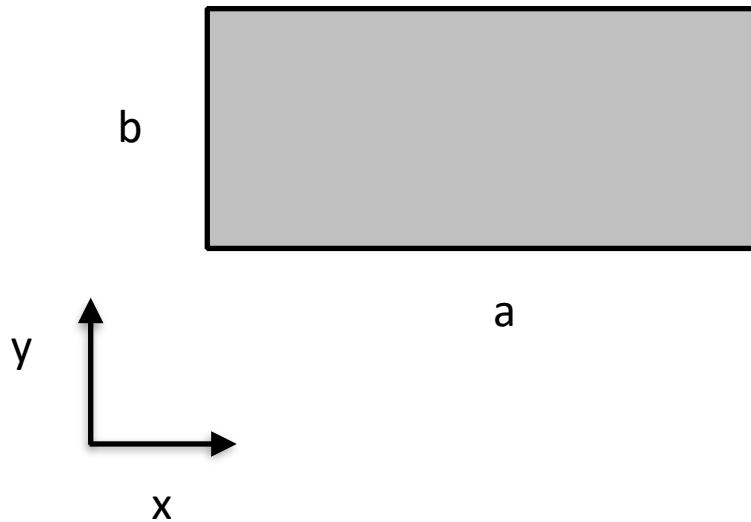


Hybrid Wannier functions

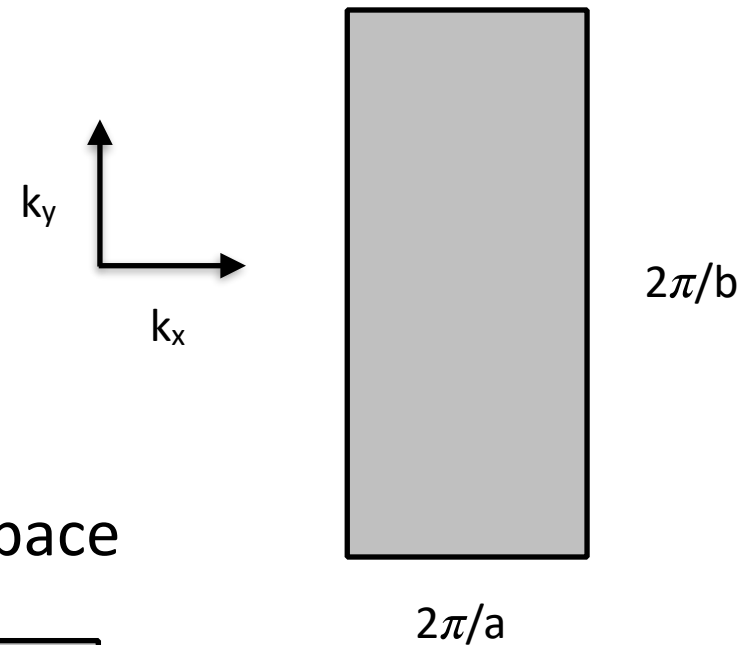
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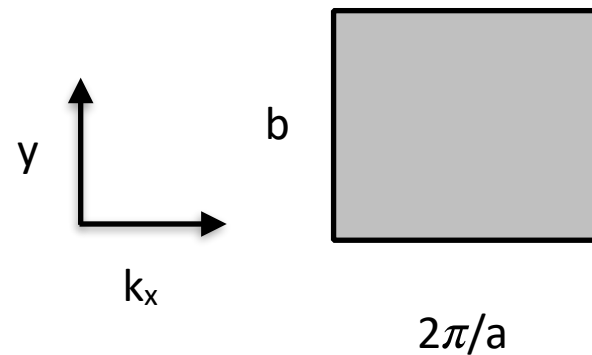
Real-space unit cell



Reciprocal-space unit cell



Hybrid space





Hybrid Wannier functions

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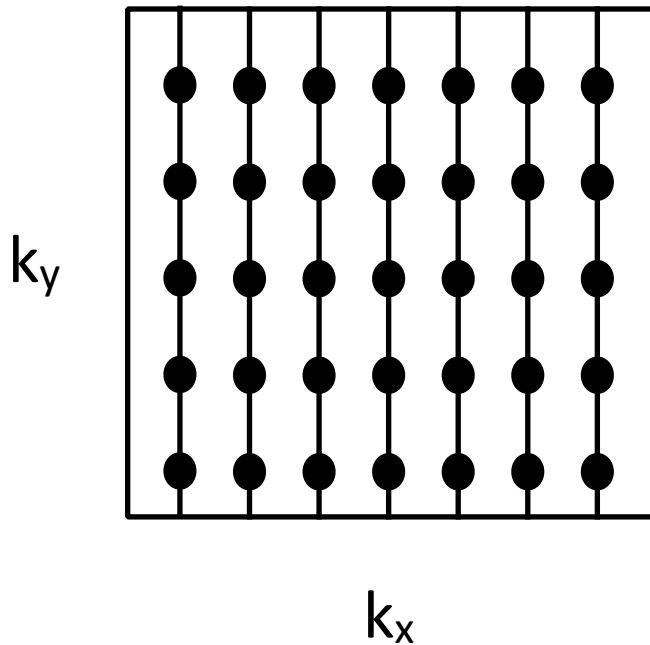
At each k_x find 1D WF along y , and their centers

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

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



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





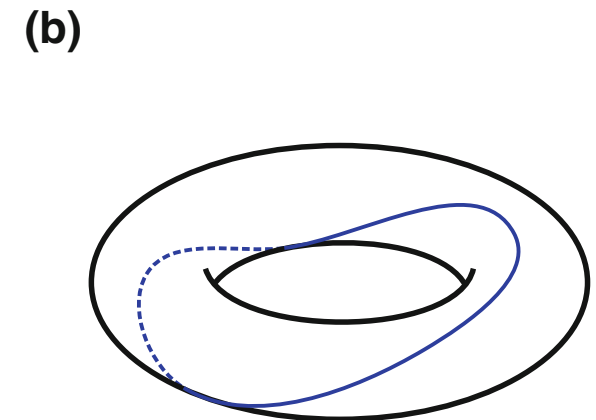
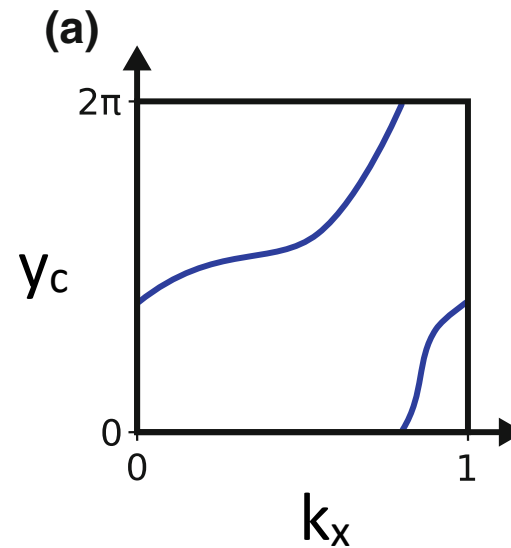
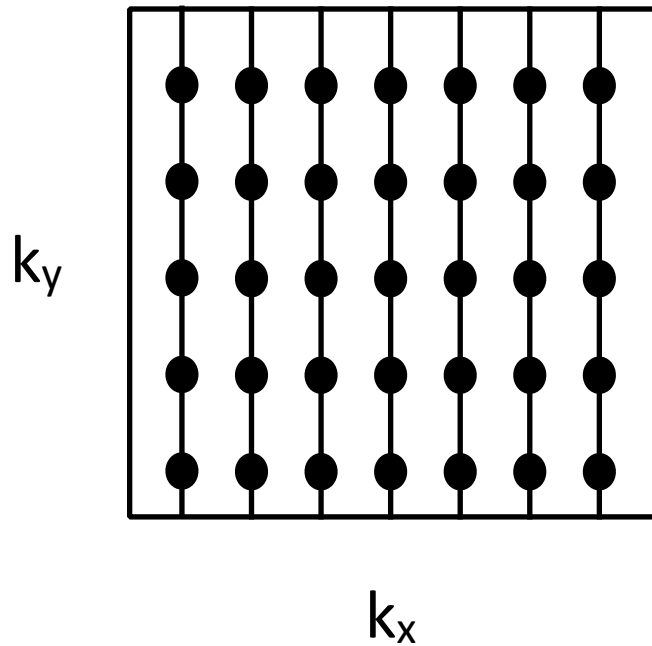
Hybrid Wannier functions

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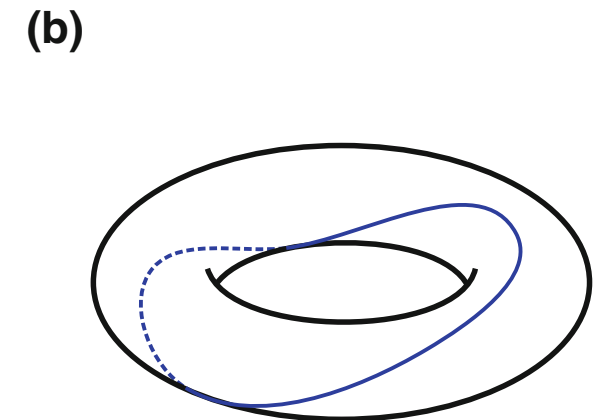
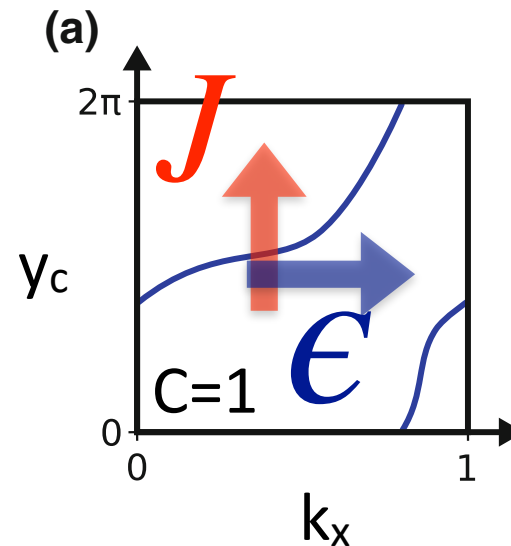
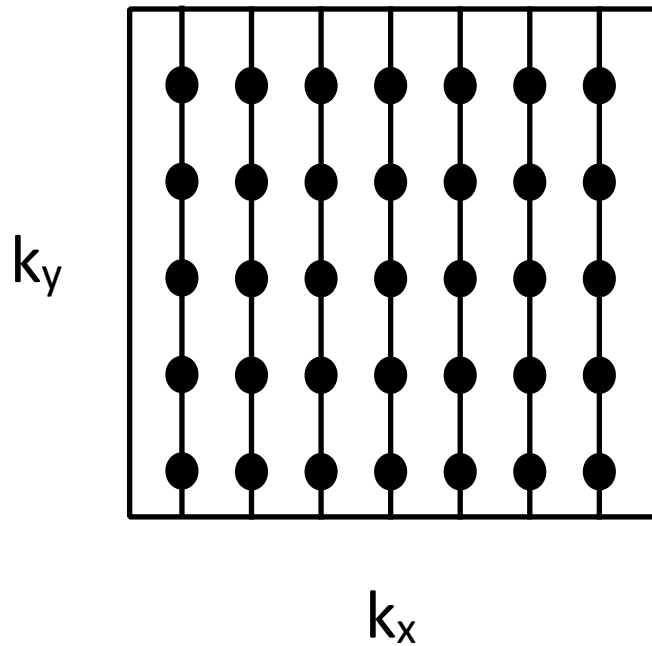


Hybrid Wannier functions



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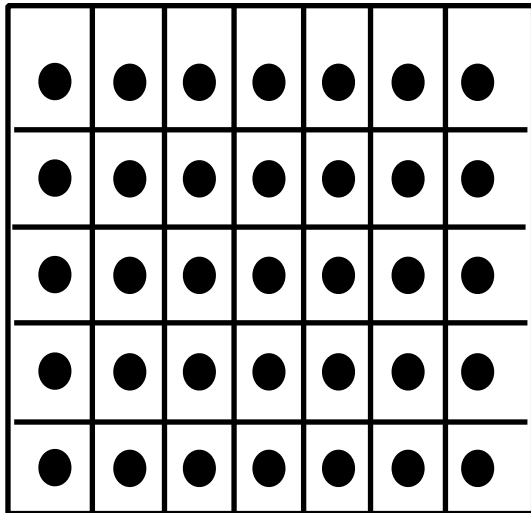




Hybrid Wannier functions



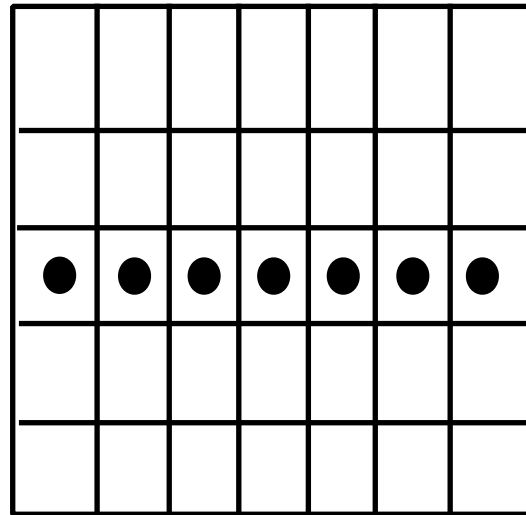
$$|\psi(k_x, k_y)\rangle$$



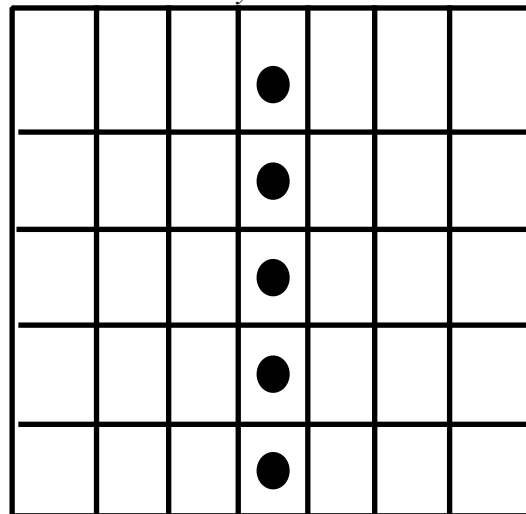
Bloch wavefunction

HWF

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

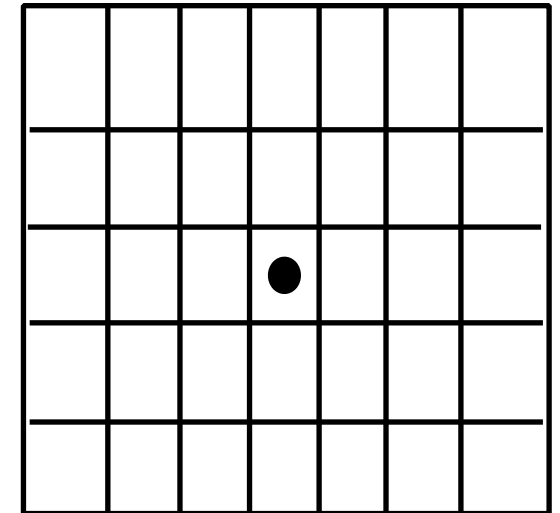


$$|h_{k_y}(R_x)\rangle$$



HWF

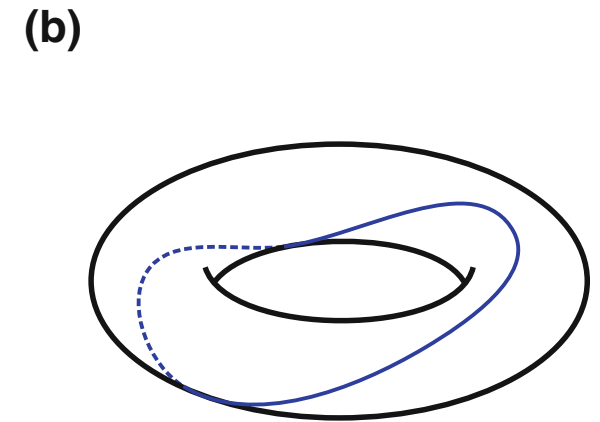
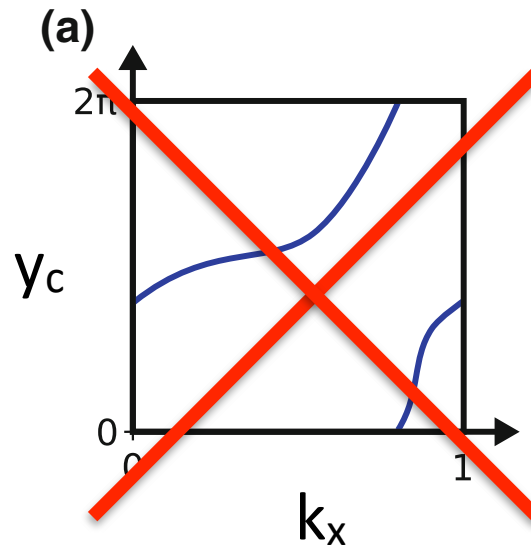
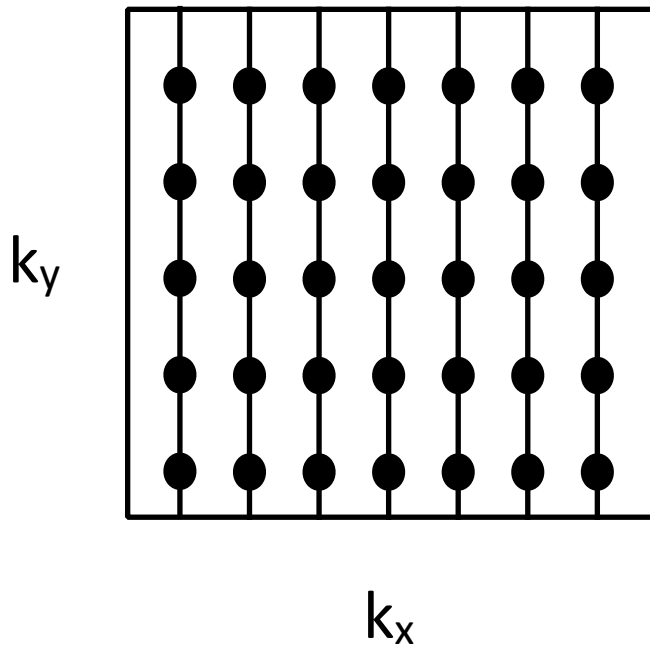
$$|W(R_x, R_y)\rangle$$



Wannier function
(Localized in x and y)



Topological obstruction



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

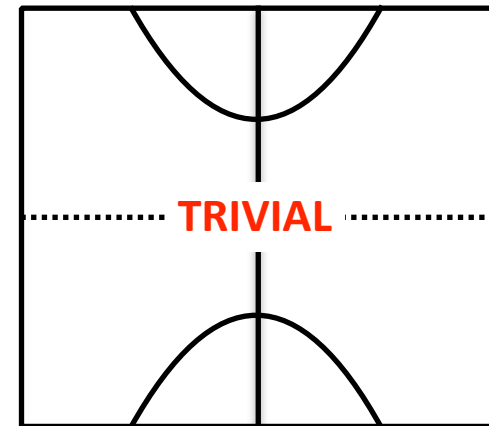
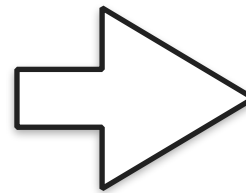
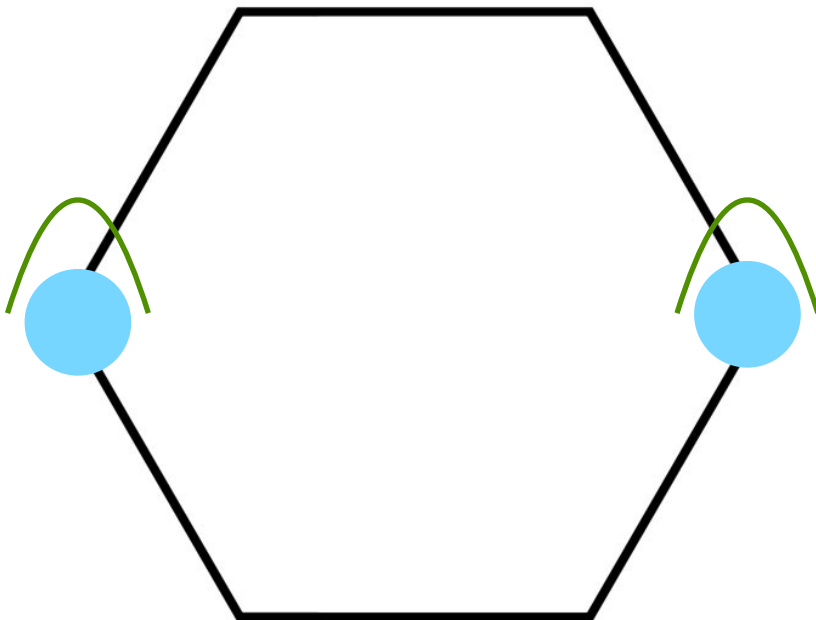
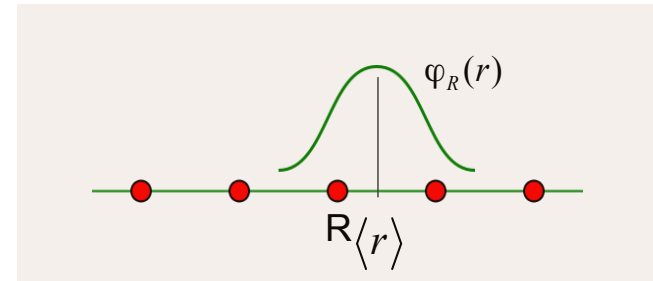


Atomic Limit

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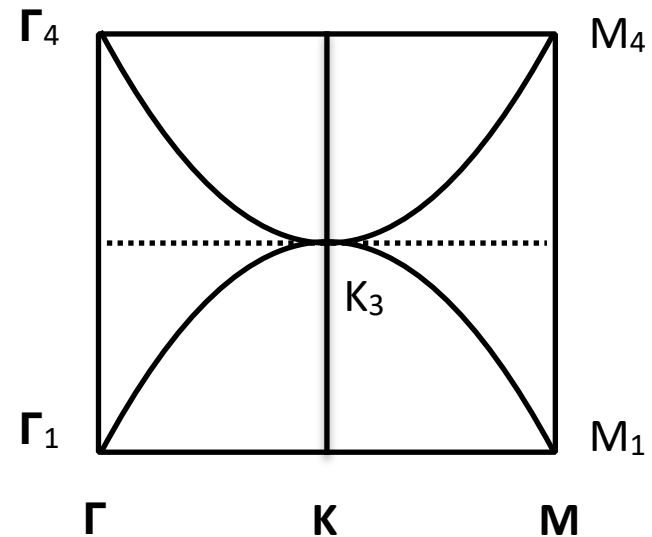
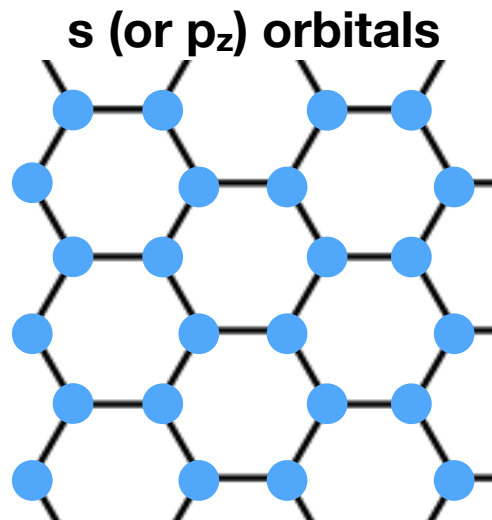
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Elementary Band Representations (EBRs)

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



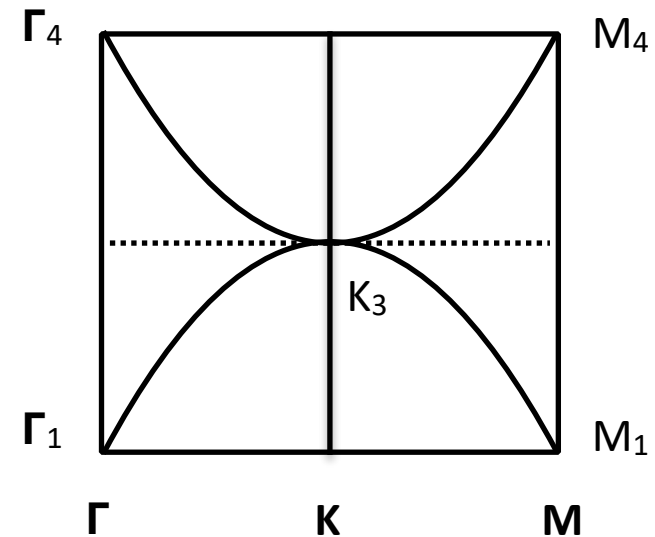
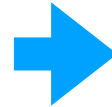
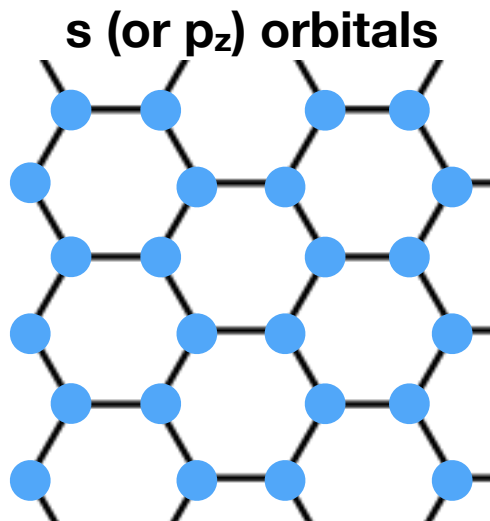
atomic limit = EBR

An EBR describes a set of Wannierizable bands



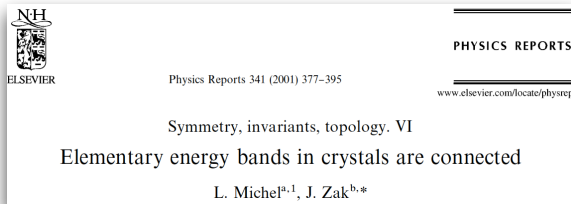
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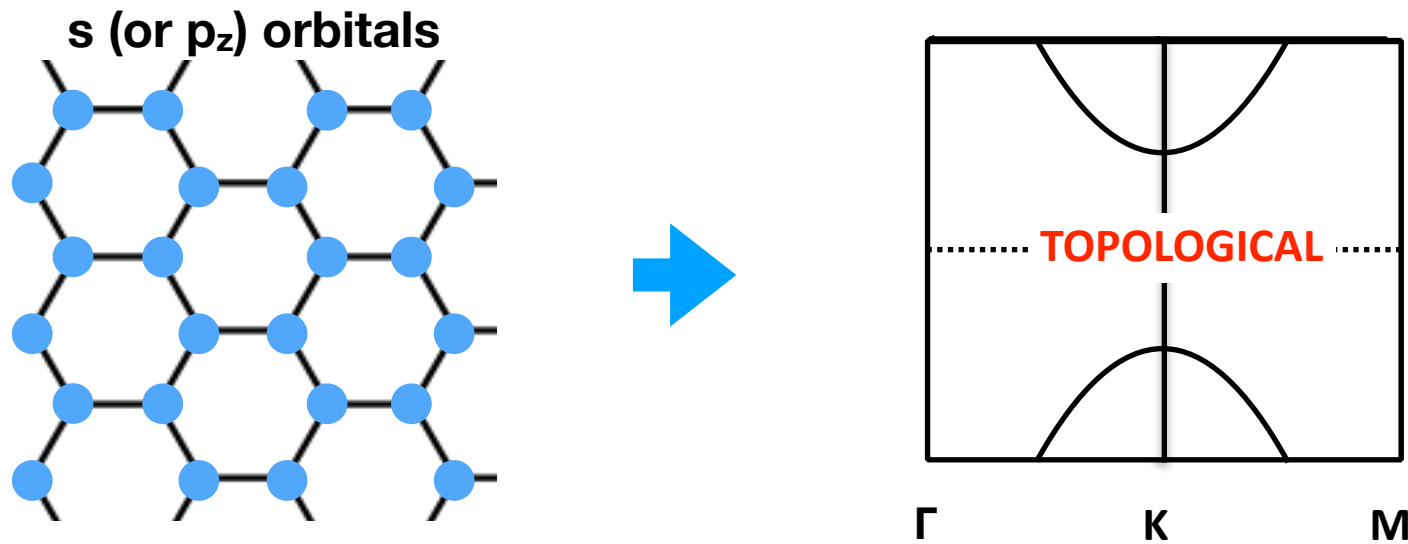
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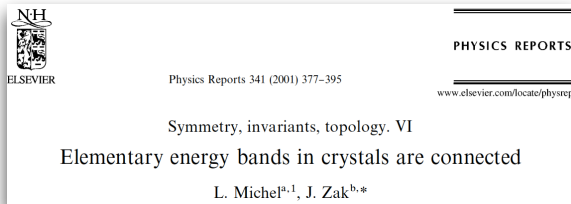
Elementary Band Representations (EBRs)

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atomic limit = EBR

An EBR describes a set of Wannierizable bands





Crystal Structure

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230 Space-Groups

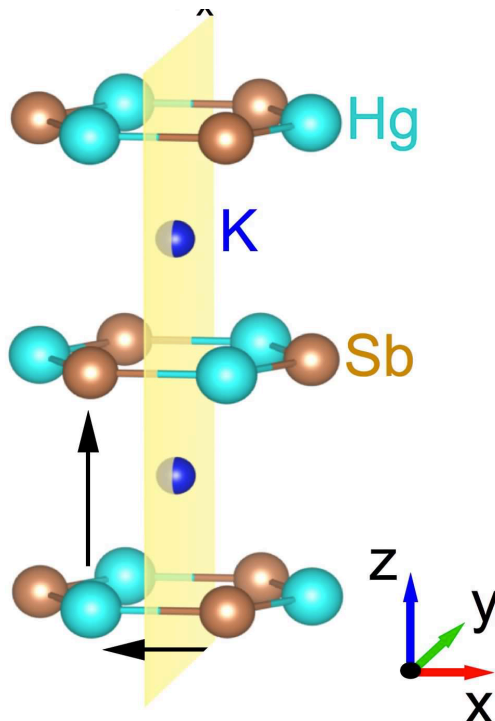


Image: 1605.06824 Ma et al

Ingredients:

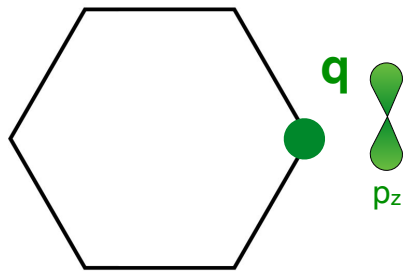
- unit lattice translations (Z^3)
- point group operations (rotations, reflections)
- non-symmorphic (screw, glide)
- orbitals
- atoms in some lattice positions



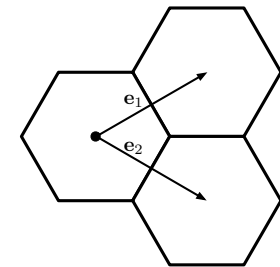
Elementary band representations (EBRs)



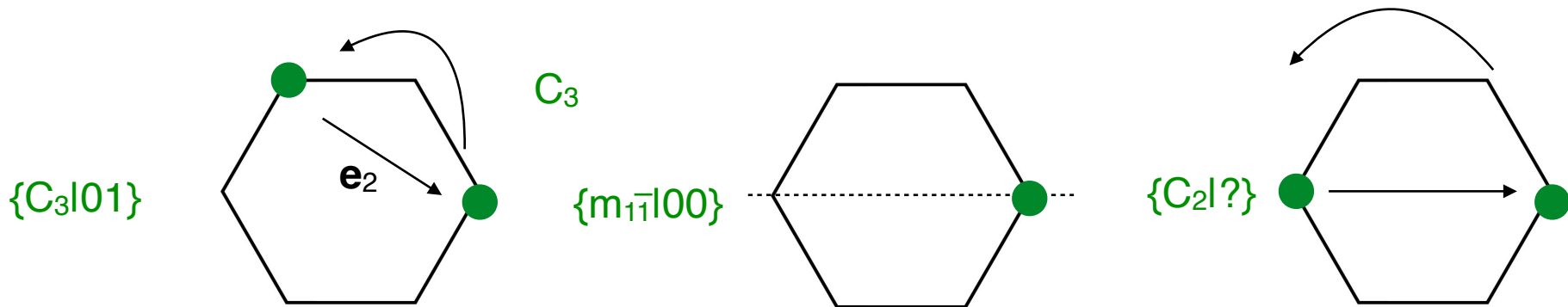
Consider one lattice site:



$$G = \underbrace{U(g_\alpha)}_{(2)} \underbrace{(G_q \rtimes \mathbf{Z}^3)}_{(1)}$$



- (1) Site-symmetry group, G_q , leaves \mathbf{q} invariant $\{C_3|01\}, \{m_{1\bar{1}}|00\} \approx C_{3v}$
 → Orbitals at \mathbf{q} transform under a rep, ρ , of G_q

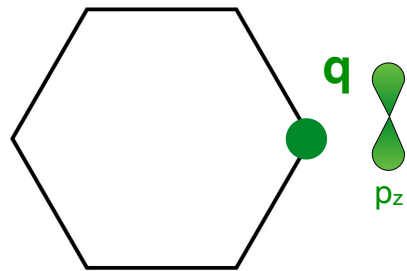




Elementary band representations (EBRs)

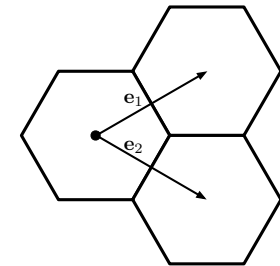


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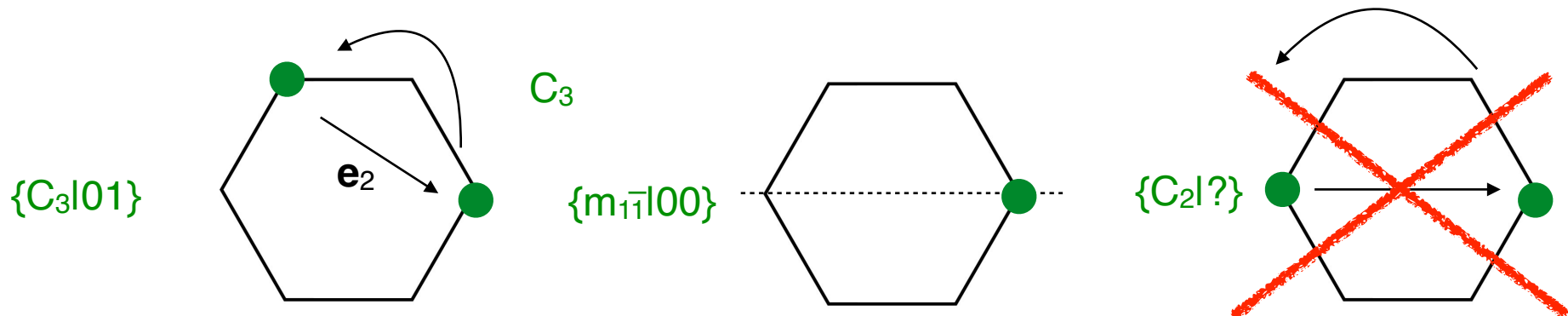


$$G = \bigcup_{\alpha} (g_{\alpha}) \quad (G_q \times \mathbf{Z}^3)$$

(2) (1)



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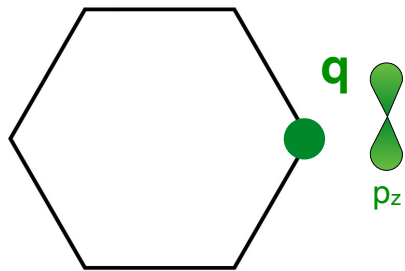




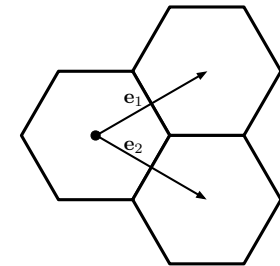
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Rep	E	C_3	M	\bar{E}
→ $\bar{\Gamma}_6$	2	1	0	-2

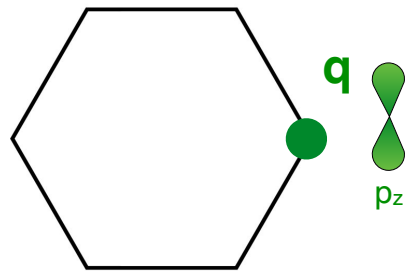
Character table for the double-valued representation of C_{3v}



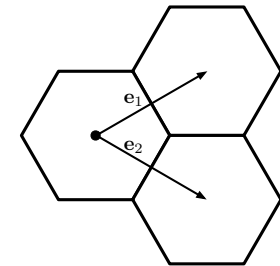
Elementary band representations (EBRs)



Consider one lattice site:




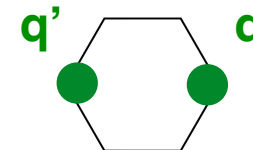
$$G = \underbrace{U(g_\alpha)}_{(2)} \underbrace{(G_q \times \mathbf{Z}^3)}_{(1)}$$



- (1) Site-symmetry group, G_q , leaves \mathbf{q} invariant $\{C_3|01\}, \{m_{1\bar{1}}|100\} \approx C_{3v}$
 → Orbitals at \mathbf{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” $\{C_2|100\}, \{E|100\}$


 Wyckoff multiplicity: 2
 orbit of \mathbf{q}



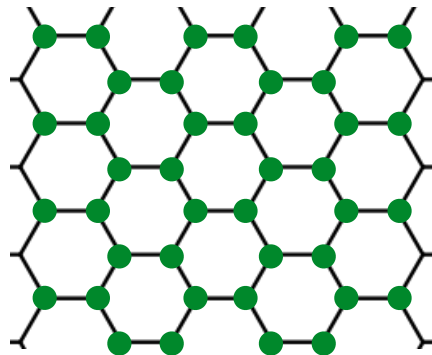
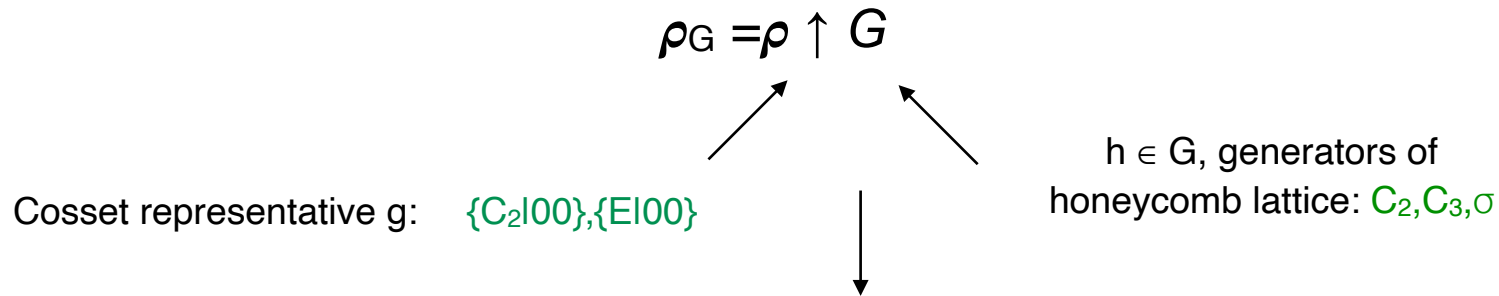


Elementary band representations (EBRs)



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

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

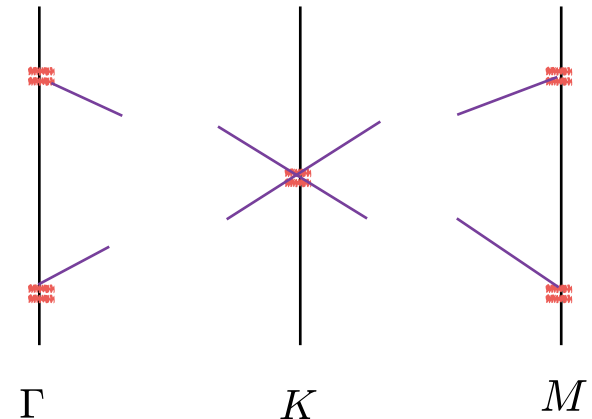


$$\rho_{i\alpha, j\beta}(h) = \rho_{ij}(g_{\alpha\beta})$$

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

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

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



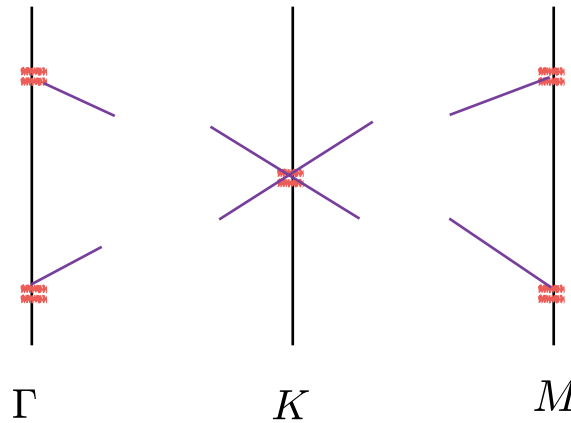
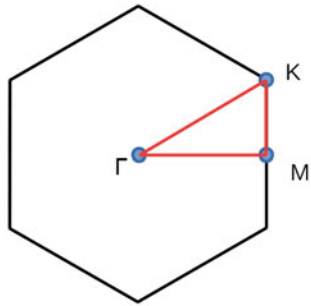
dimension of this band representations = connectivity in the Brillouin zone



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

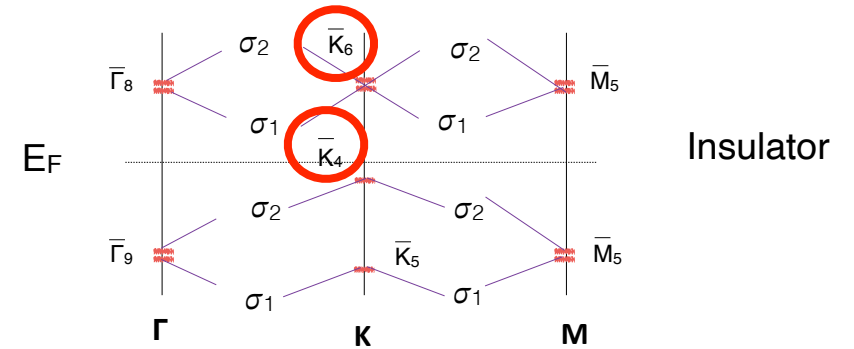
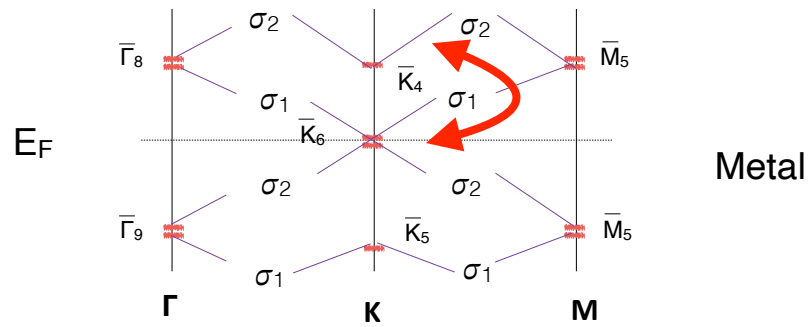


All possible connection between maximal and non-maximal k-vectors

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

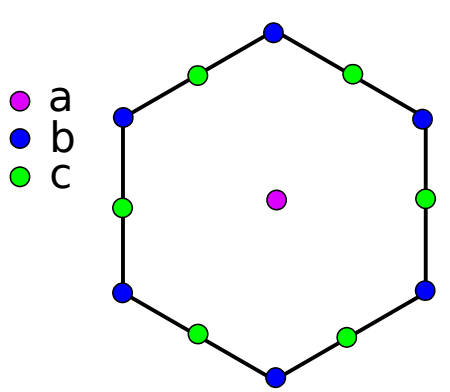
$$\mathbf{k}_i(\mathbf{u}_2) = \mathbf{k}_2$$

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

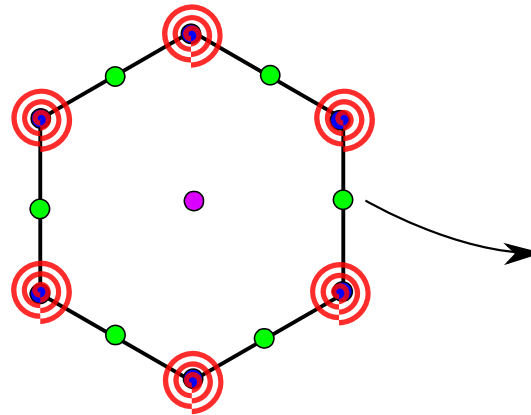




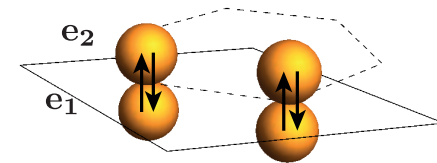
Topological Quantum Chemistry



Maximal symmetry
Wyckoff positions



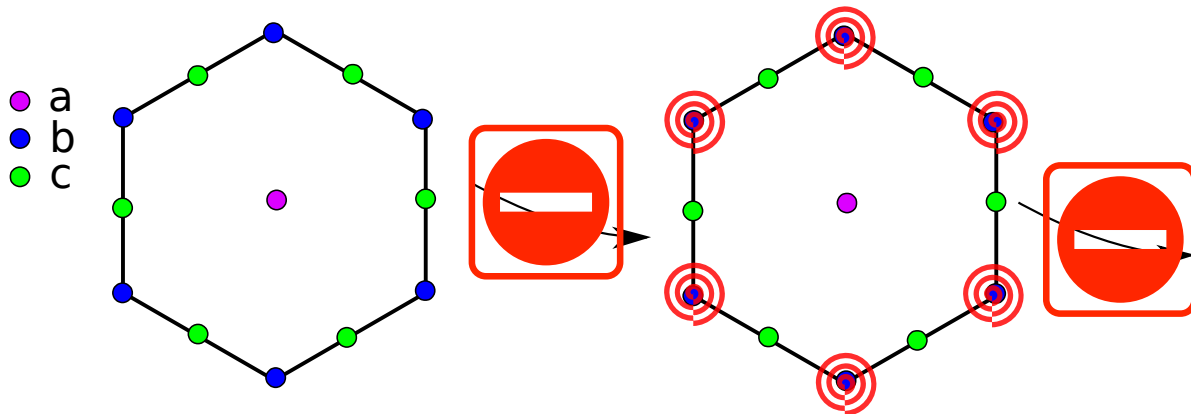
Wannier functions at
some Wyckoff pos.



Nature (2017)

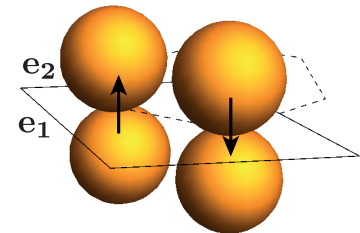
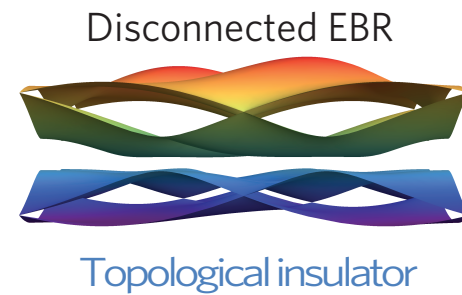


Topological Quantum Chemistry



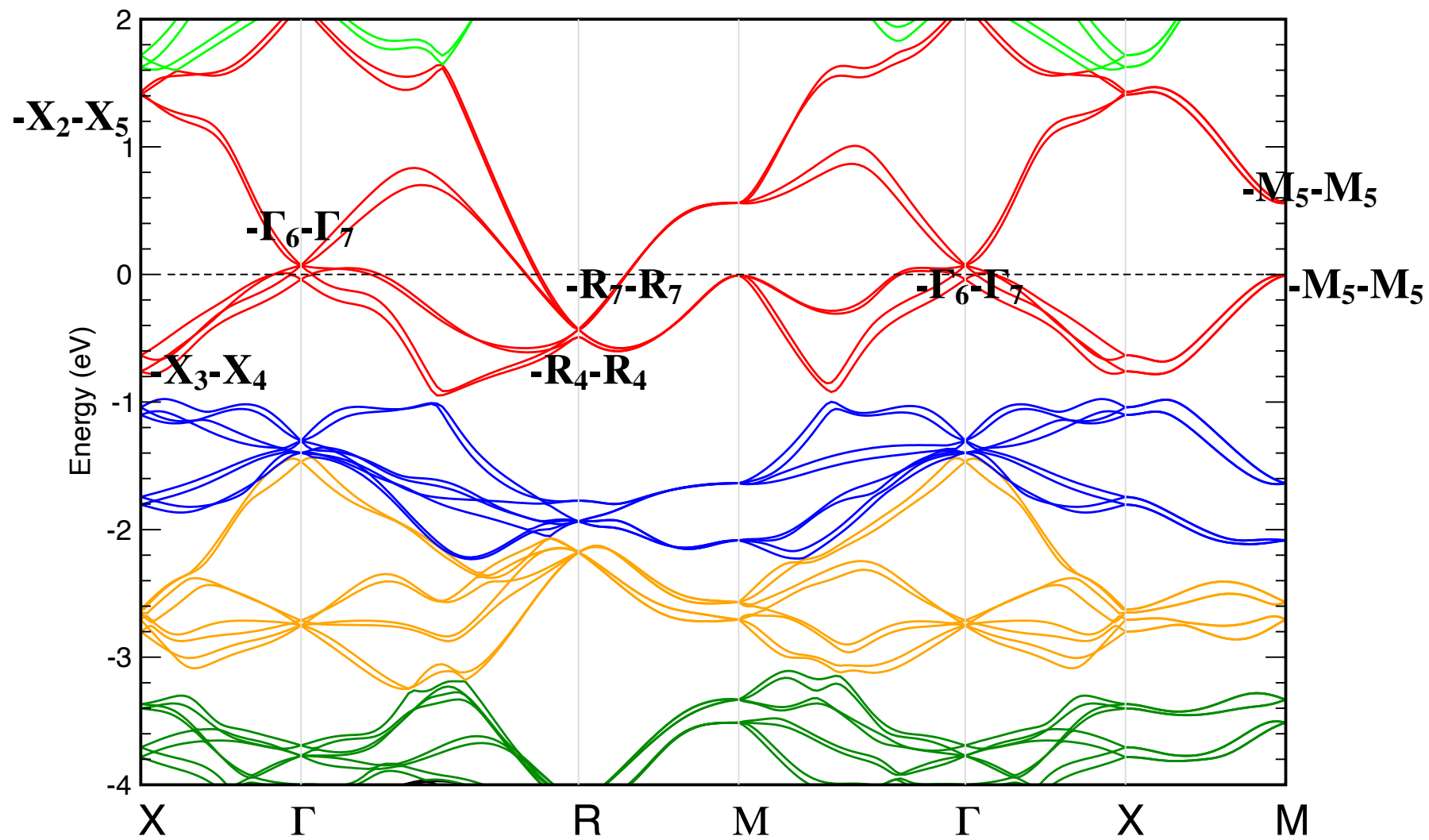
Maximal symmetry
Wyckoff positions

Wannier functions at
some Wyckoff pos.



Nature (2017)

RhSi





Topological Quantum Chemistry

Topological Materials Database

Total Materials: 38423
Topological Insulators: 6171
Semi-Metals: 14111

NAVIGATION: Search, Predict, About, Wiki
SETTINGS: UI Mode

[Back to Search Results](#) | Compound: **Bi1 Te1** | Symmetry Group: 164 (P-3m1) | Topological Status (Type): TI (SEBR) | Topological indices: $Z_{2W,1} = 0, Z_{2W,2} = 0, Z_{2W,3} = 1, Z_4 = 2$ | With SOC: Yes No

ICSD: 100654

Materials Data

Crystallographic data

Cell Length A	4.422(2)
Cell Length B	4.422(2)
Cell Length C	24.050(20)
Cell Angle α	90.
Cell Angle β	90.
Cell Angle γ	120.
Cell Volume	407.27

Lattice Structure:

Brillouin Zone:

For more information we refer to [Materials Project](#).

Band Structure

Density of States

• Dashed bands denote fragile bands

Topological Materials Database

Total Materials: 38423
Topological Insulators: 6171
Semi-Metals: 14111

NAVIGATION: Search, Predict, About, Wiki
SETTINGS: UI Mode

[Back to Search Results](#) | Compound: **Bi1 Te1** | Symmetry Group: 164 (P-3m1) | Topological Status (Type): TI (SEBR) | Topological indices: $Z_{2W,1} = 0, Z_{2W,2} = 0, Z_{2W,3} = 1, Z_4 = 2$ | With SOC: Yes No

Gaps at high-symmetry points by (eV):

	Γ	H	K	L	M	A	Smallest Computed Gap
occupation	0.491	1.093	1.781	0.252	0.914	0.268	0.1363
band index	0.491	1.093	1.781	0.252	0.914	0.268	0.1363

Topological Data

Band representations and their degeneracies

By Level

Level	Γ	H	K	L	M	A	Nr Fragile Bands
1	9 (2)	6 (2)	6 (2)	5+6 (2)	5+6 (2)	8 (2)	2
2	8 (2)	6 (2)	4+5 (2)	3+4 (2)	3+4 (2)	8 (2)	
3	9 (2)	4+5 (2)	6 (2)	5+6 (2)	5+6 (2)	9 (2)	
4	6+7 (2)	6 (2)	6 (2)	5+6 (2)	3+4 (2)	4+5 (2)	
5	8 (2)	6 (2)	6 (2)	3+4 (2)	5+6 (2)	8 (2)	

Show all band representations

- For representation definitions, click the high-symmetry point names
- Representations ordered by energy with those closest to Fermi level at the top
- 'N (m)' at high-symmetry point X denotes the m-dimensional representation X_N of the little group

Fragile bands:

Lowest band index	Nr Band indices	Distance to Fermi	Direct Gap Above	Direct Gap Below	Indirect Gap Above	Indirect Gap Below
24	2	40	0.0144	4.0544	0	2.3135
106	4	40	0.0134	0.0118	0	0

Transitions upon symmetry lowering

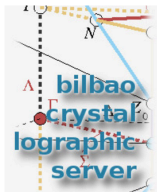


<http://www.cryst.ehu.es/>

MAX PLANCK INSTITUTE
FOR CHEMICAL PHYSICS OF SOLIDS



bilbao crystallographic server



Crystallography Online: Workshop on the use of the structural and magnetic tools of the Bilbao Crystallographic Server
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

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Quick access to some tables

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

Space Groups

Plane Groups

Layer Groups

Rod Groups

Frieze Groups

2D Point Groups

Point Groups

Magnetic Space Groups

<https://irrep.dipc.org>

IRREP

Search docs

- Installation
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IrRep

IRREP

is a code to calculate symmetry eigenvalues of electronic Bloch states in crystalline solids and the irreducible representations under which they transform. It can receive as input bandstructures computed with [VASP](#), [Abinit](#), [Quantum Espresso](#) or any code with an interface to [Wannier90](#).

Characteristics

- **Any space group** - It can be applied to bandstructures of crystals in any of the 230 space groups preserving time-reversal symmetry.
- **spinful or spinless** - It includes both, single (spinless) and double-valued (spinful) groups. Also, it accepts calculations with spin-orbit coupling corrections.
- **Any unit cell** - Bandstructures calculated with any choice of the unit cell are welcome: primitive, conventional,...
- A `trace.txt` file that can be passed directly to [CheckTopologicalMat](#) is generated.
- Adding interfaces to other DFT codes is easy. You are welcome!

Thank you!