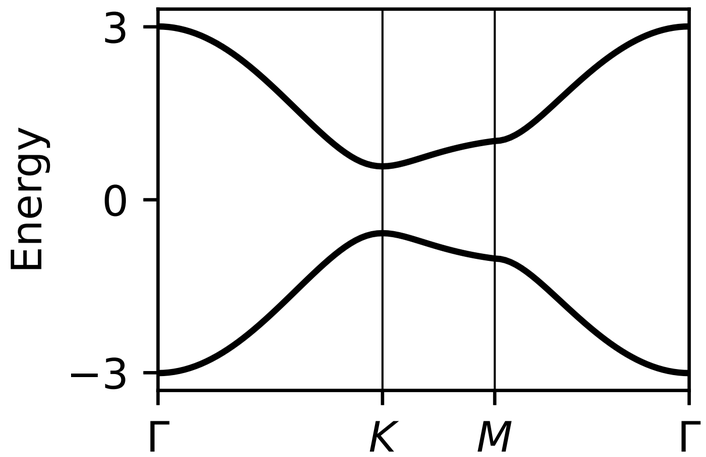
IrRep: hands-on session

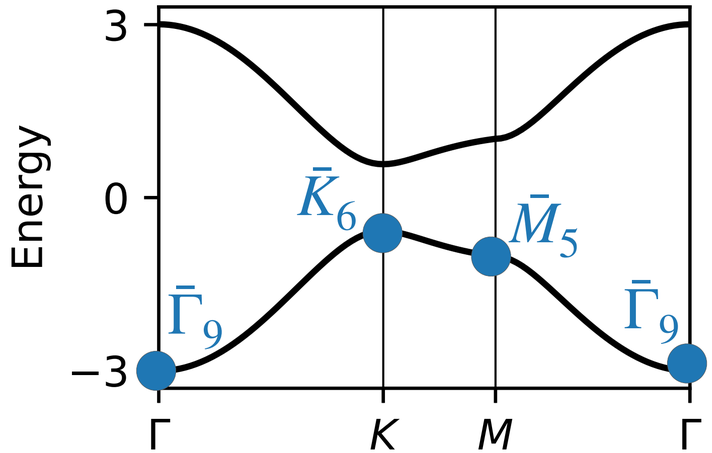
By Maia G. Vergniory
&
Mikel Iraola

Diagnosing topology within TQC

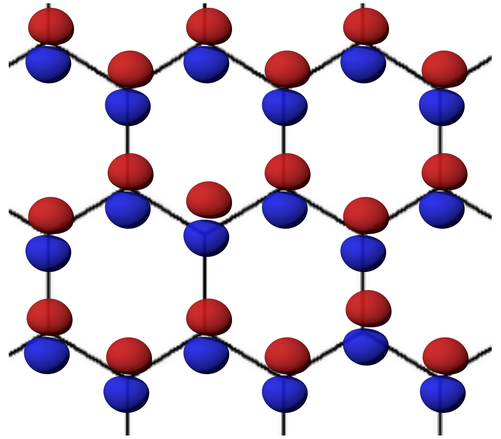
1 **Calculate the band structure**



2 **Determine the IRs of valence bands**



3 **Check if they coincide with an atomic limit ?**



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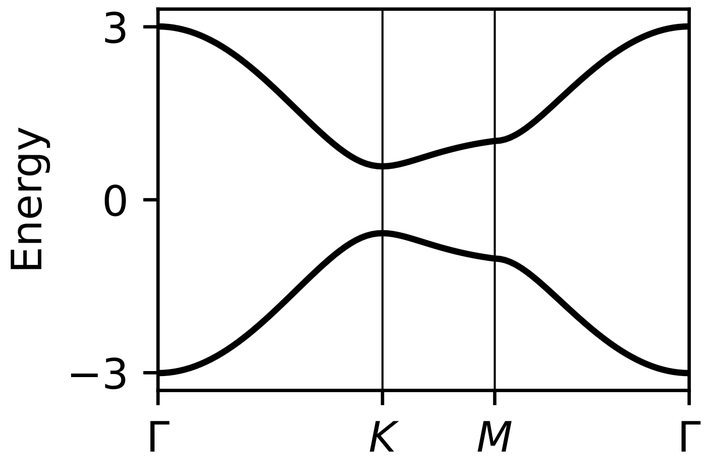

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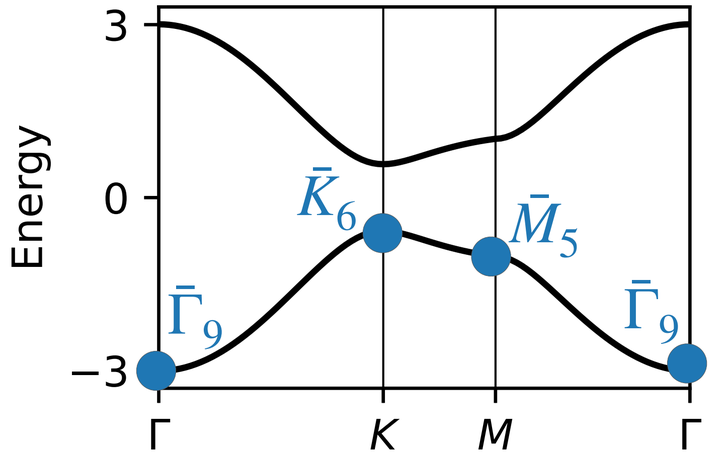

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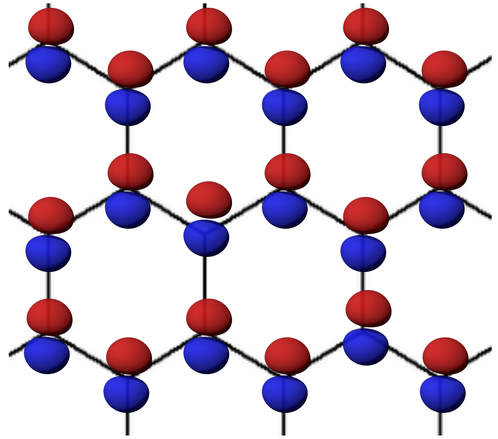

$$H(\boldsymbol{k}) \longrightarrow \begin{cases} \epsilon_{\boldsymbol{k},1} \; |\psi_{\boldsymbol{k},1}\rangle \longrightarrow \bar{\Gamma}_9 \\ \epsilon_{\boldsymbol{k},2} \; |\psi_{\boldsymbol{k},2}\rangle \longrightarrow \bar{K}_6 \\ \epsilon_{\boldsymbol{k},3} \; |\psi_{\boldsymbol{k},3}\rangle \longrightarrow \bar{M}_5 \end{cases} \longrightarrow \{\bar{\Gamma}_9, \bar{K}_6, \bar{M}_5\} = \sum_i n_i \, EBR_i$$

$$n_i \in \mathbb{N} \cup \{0\}$$

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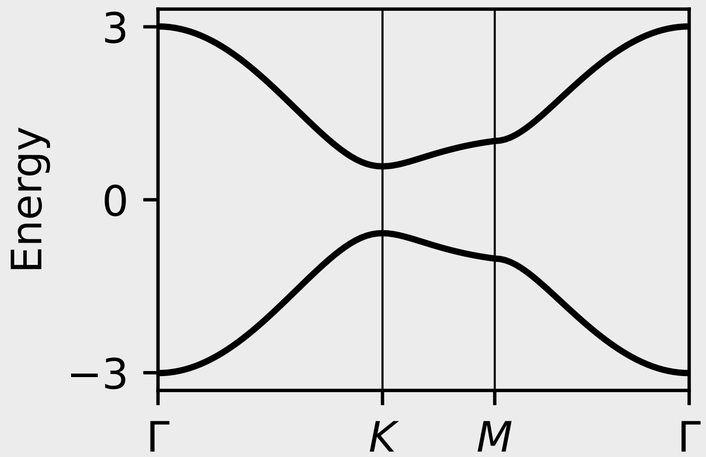

Density Functional Theory

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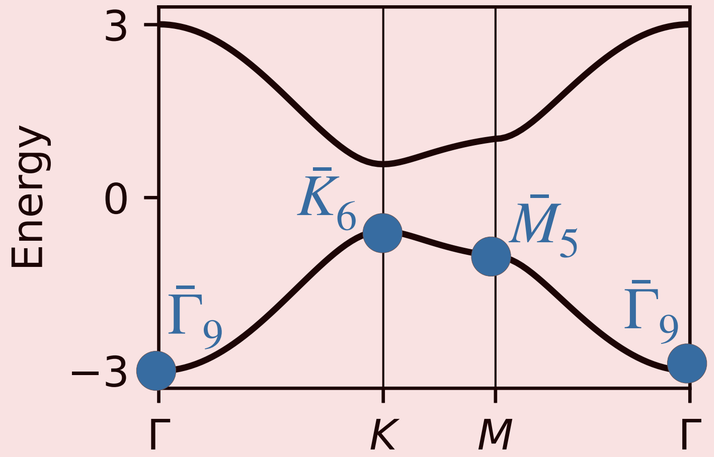

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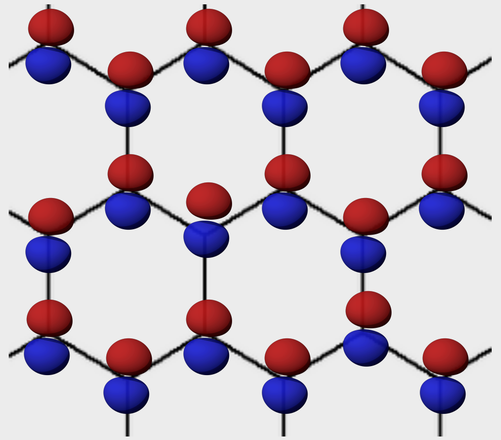

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Bilbao Crystallographic Server

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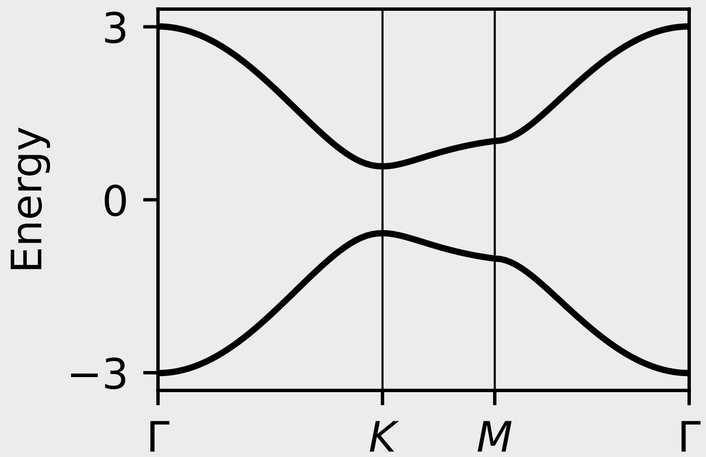

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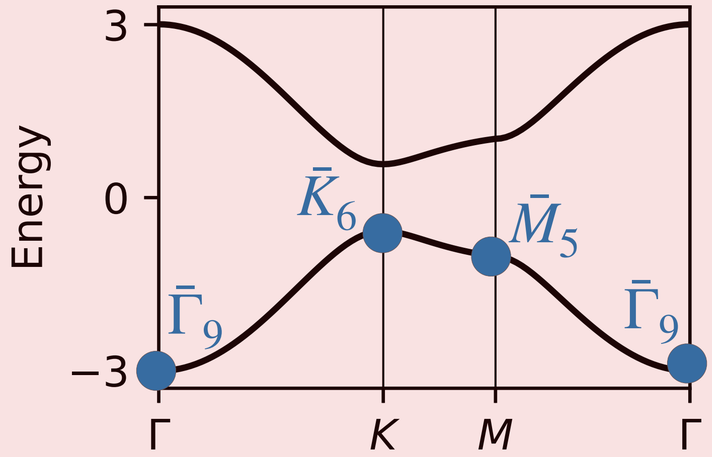

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IrRep

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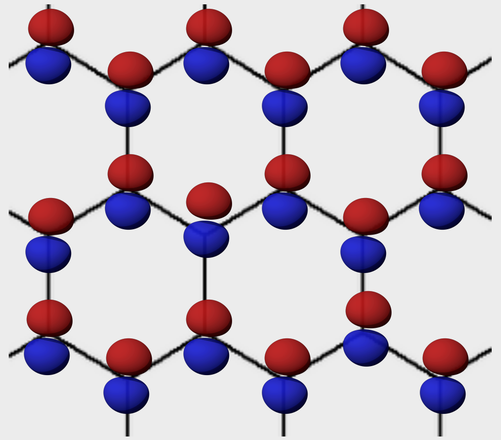

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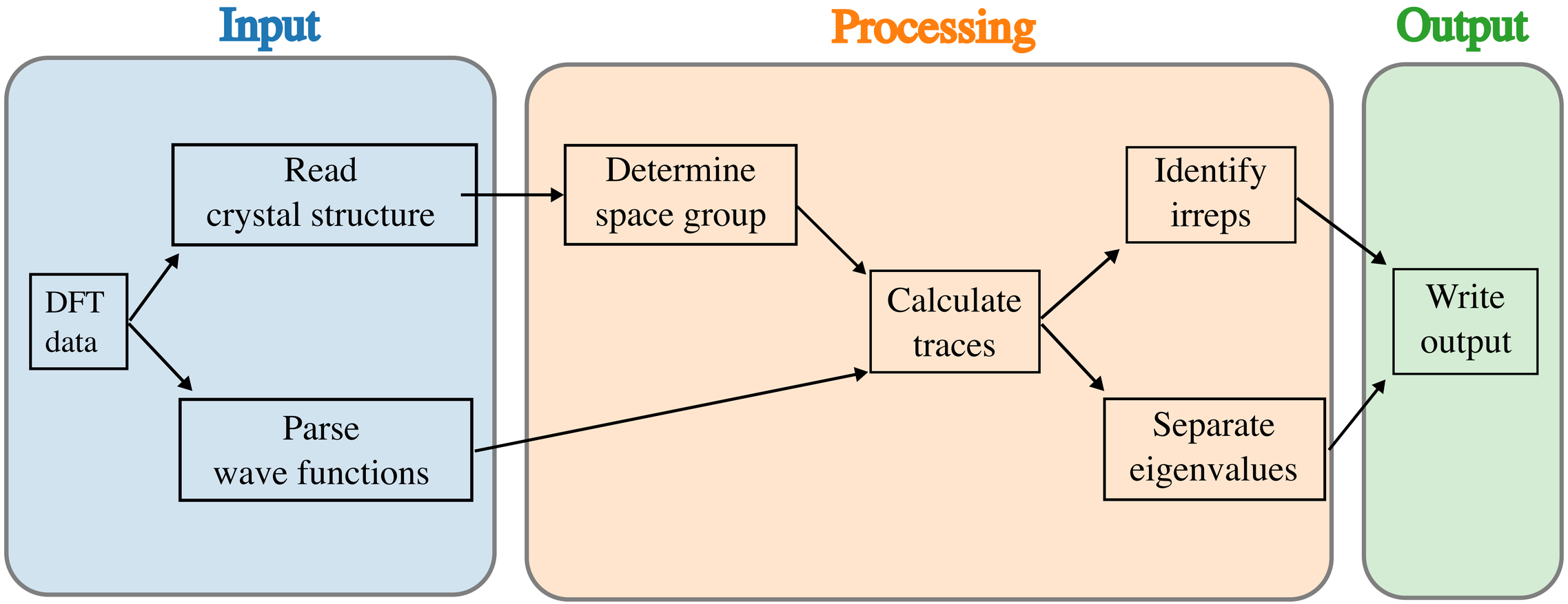

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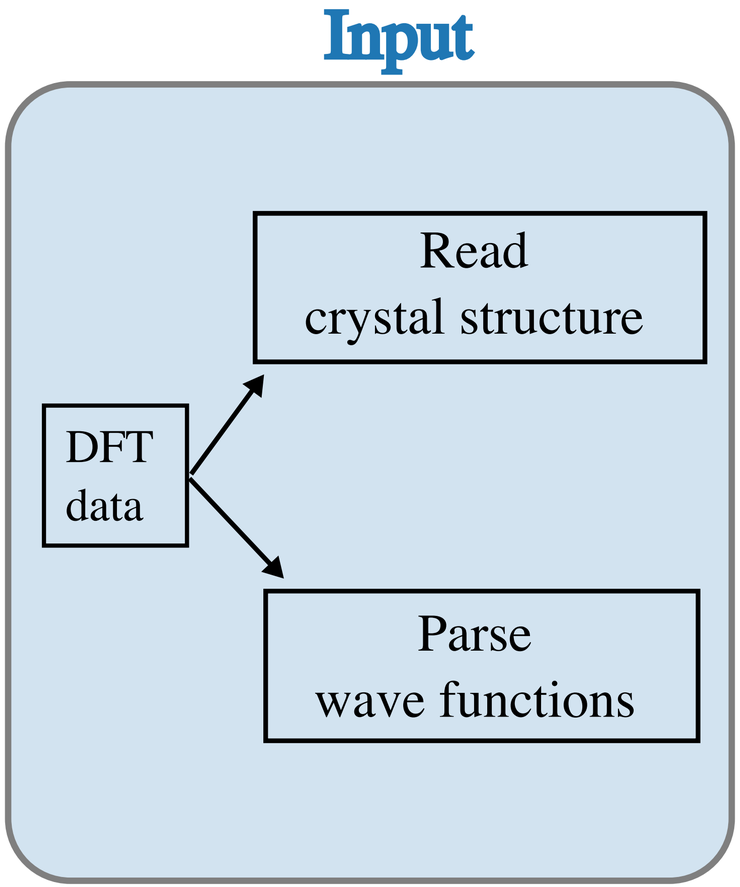

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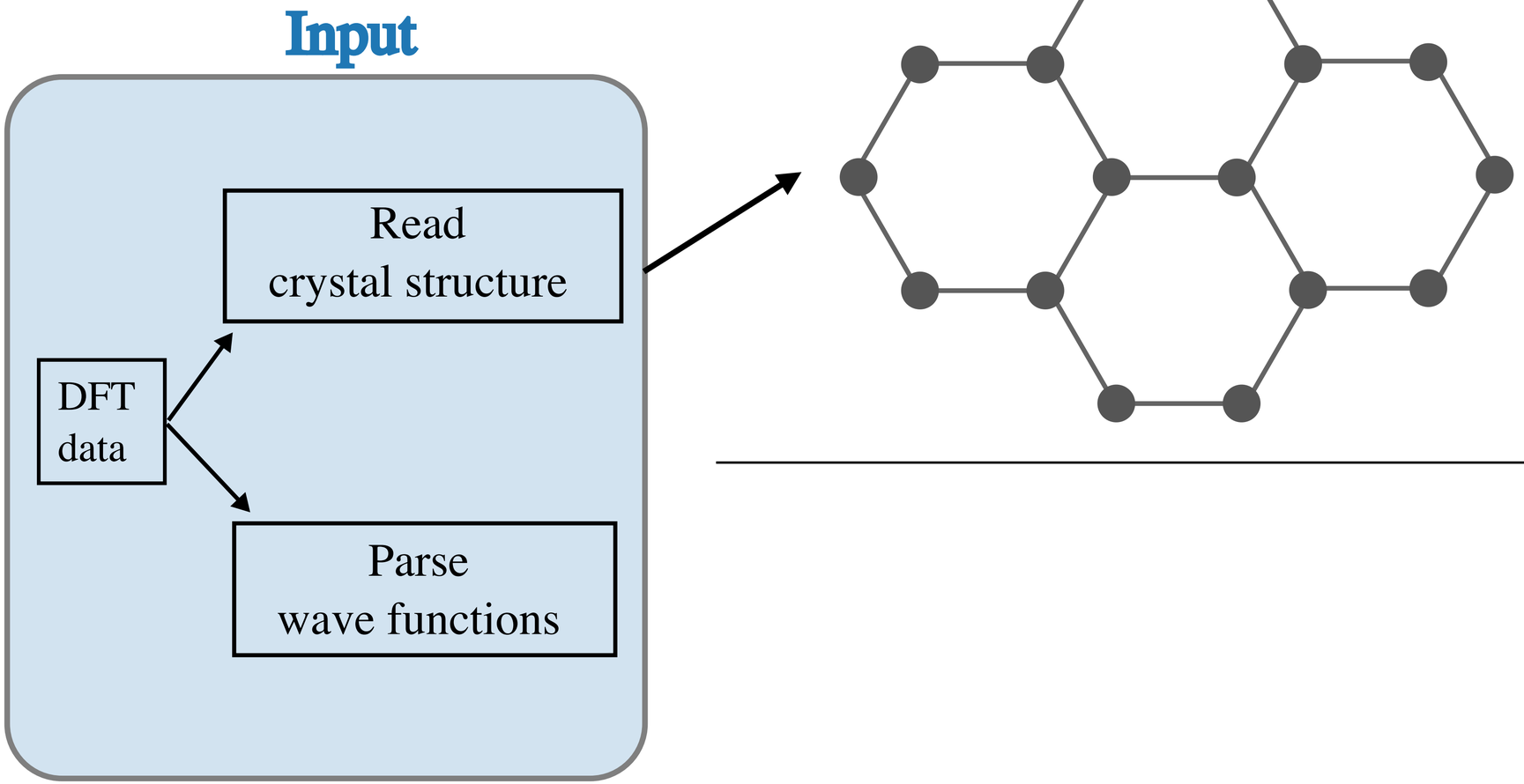

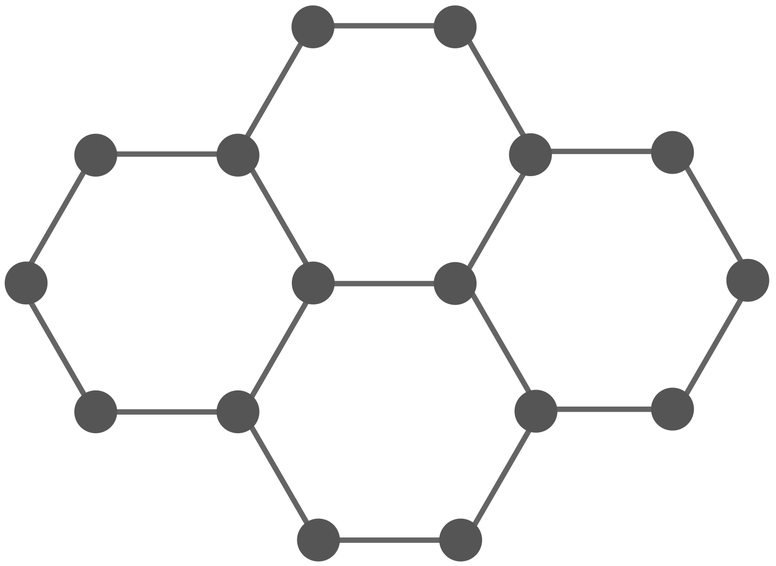

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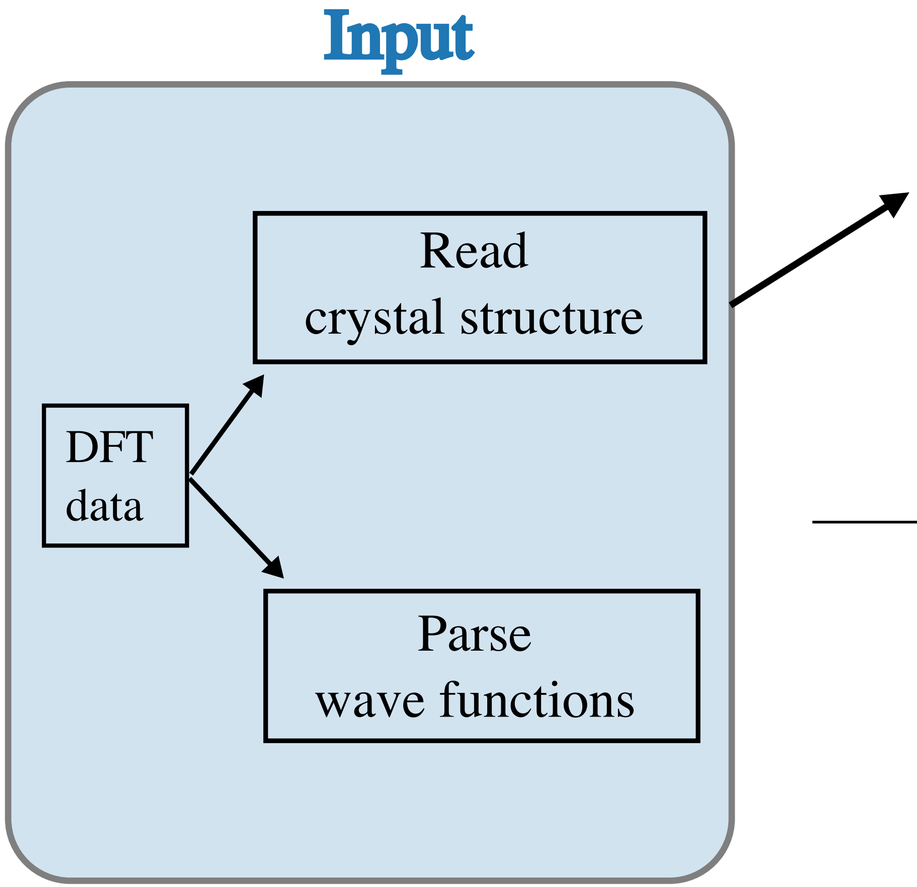

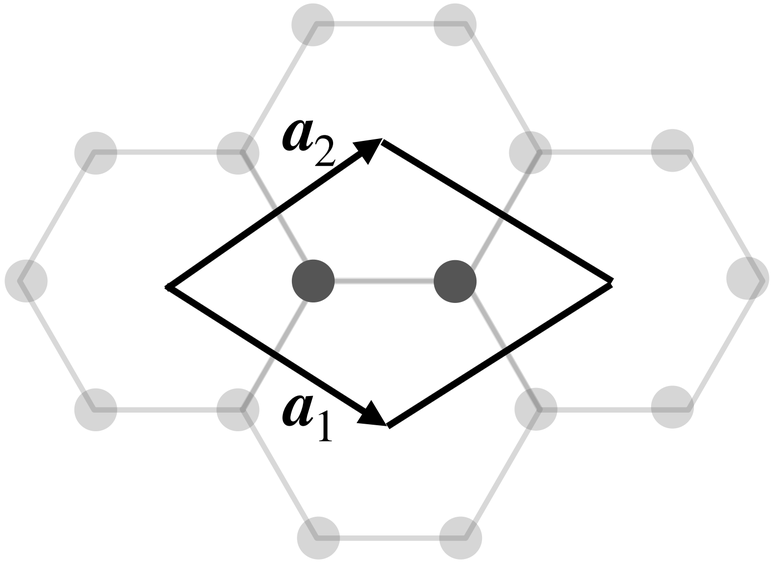

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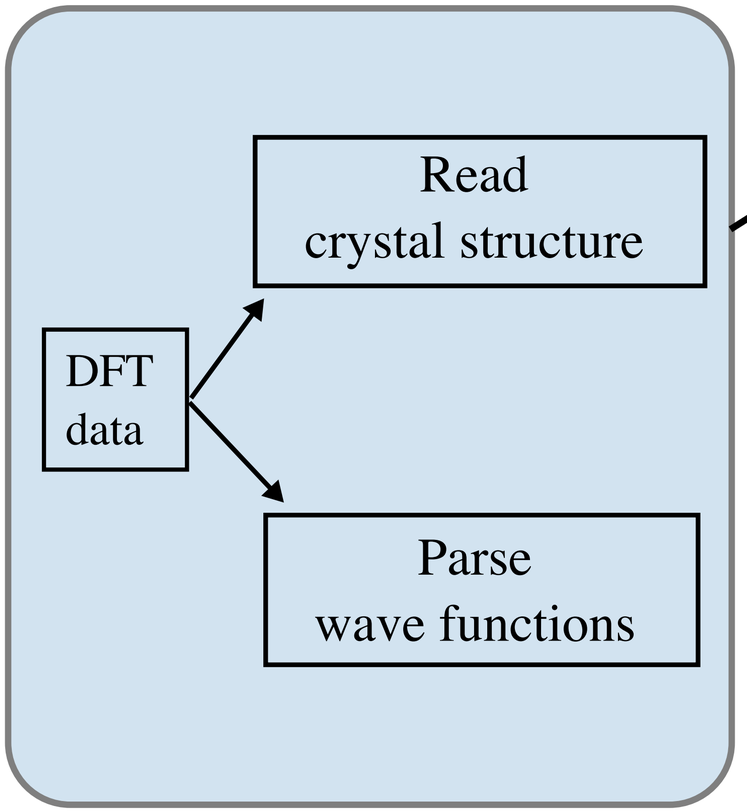

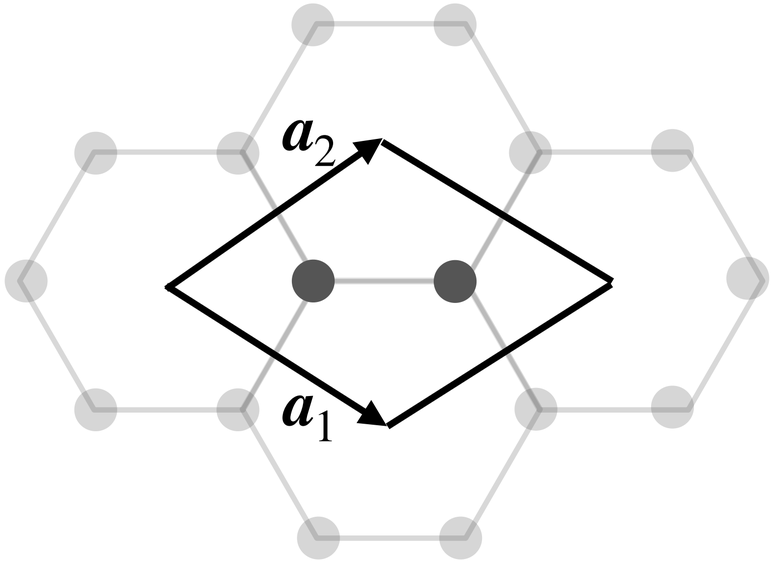

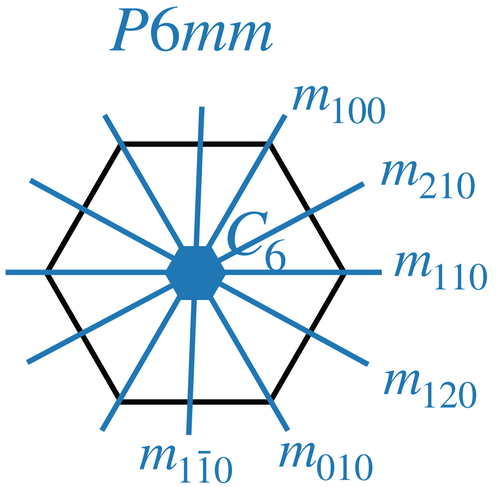

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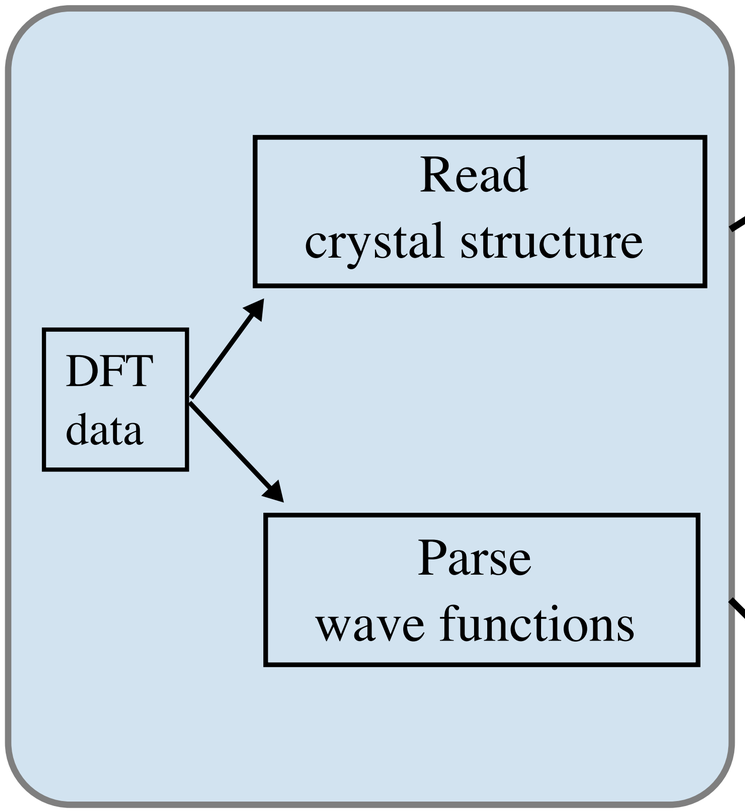

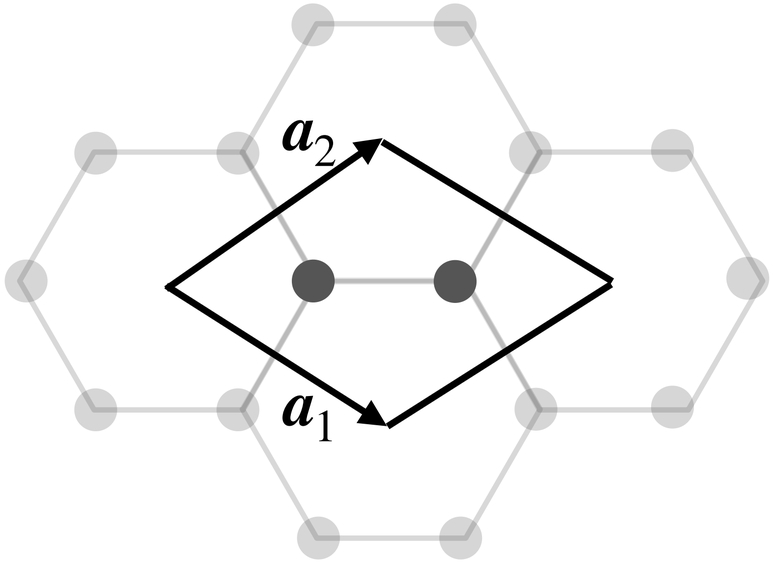

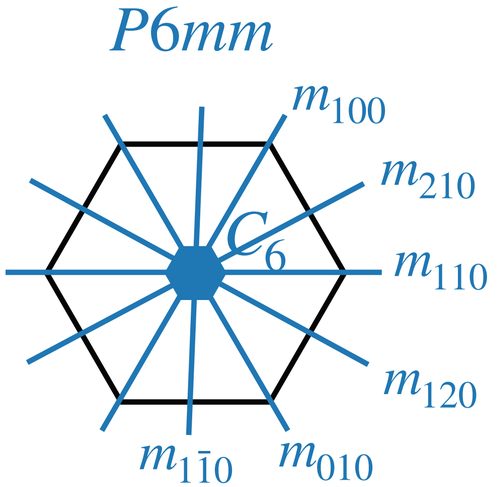

Wave functions are expanded in terms of plane waves

$$\psi_{kn}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} C_{kn}(\boldsymbol{G})\ e^{i(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}} \longrightarrow |\psi_{kn}\rangle = \sum_{\boldsymbol{G}} C_{kn}(\boldsymbol{G})\,|\boldsymbol{k}+\boldsymbol{G}\rangle$$

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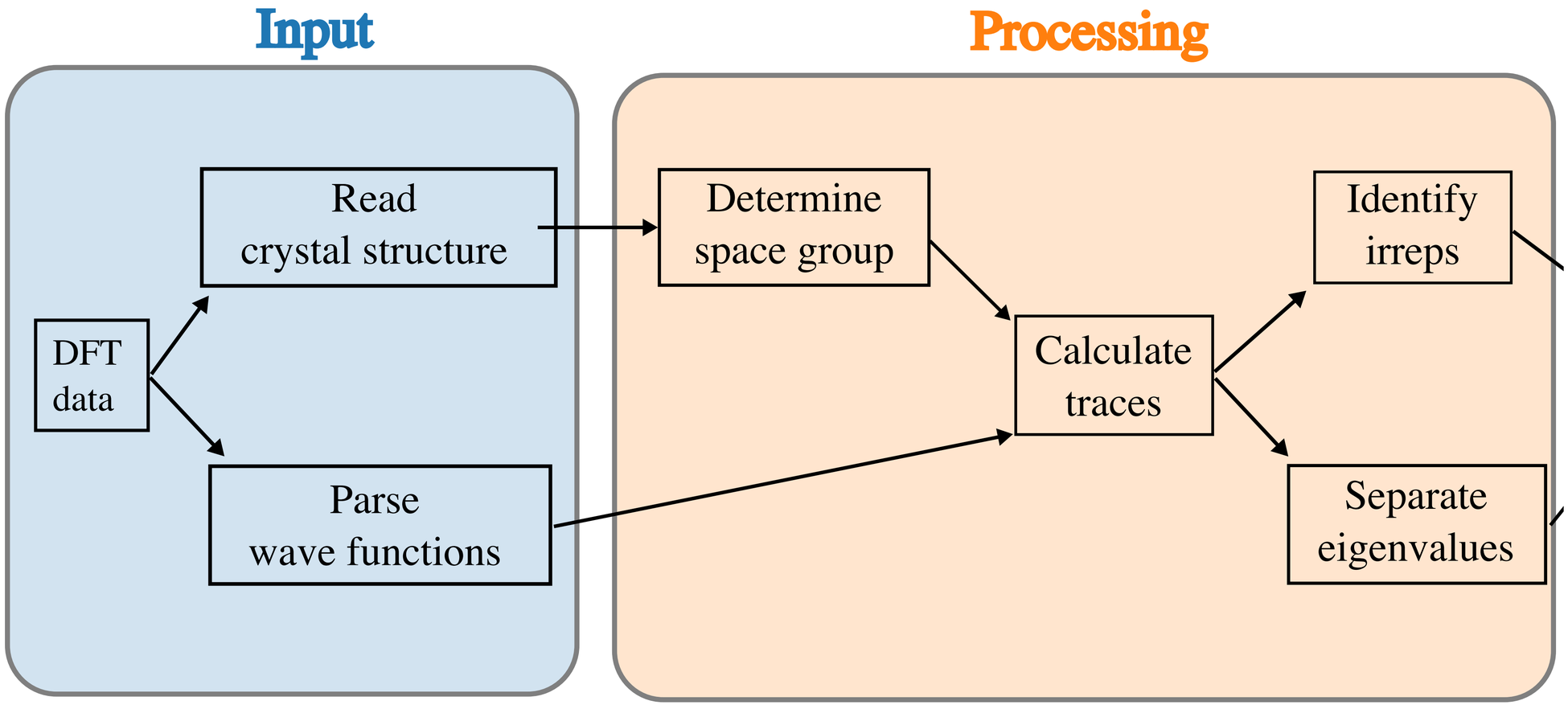

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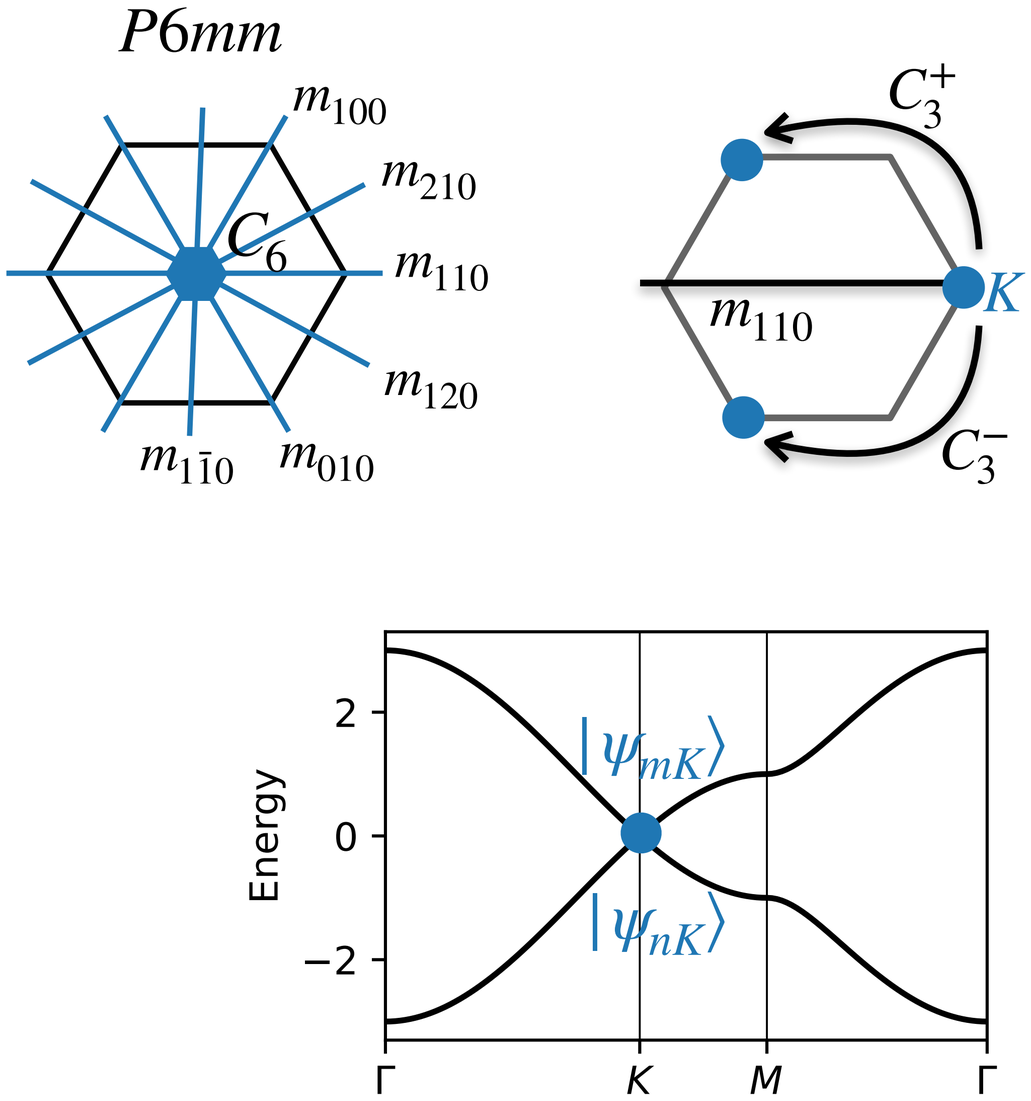

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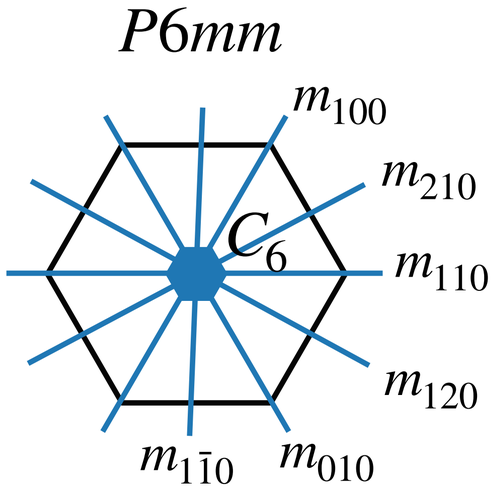

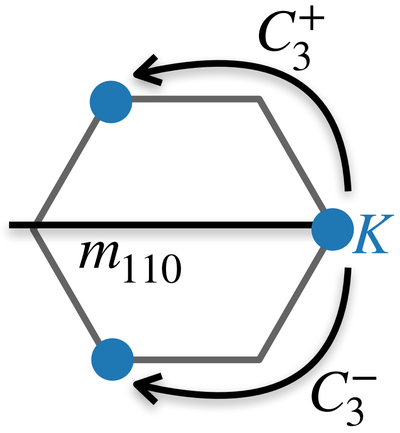

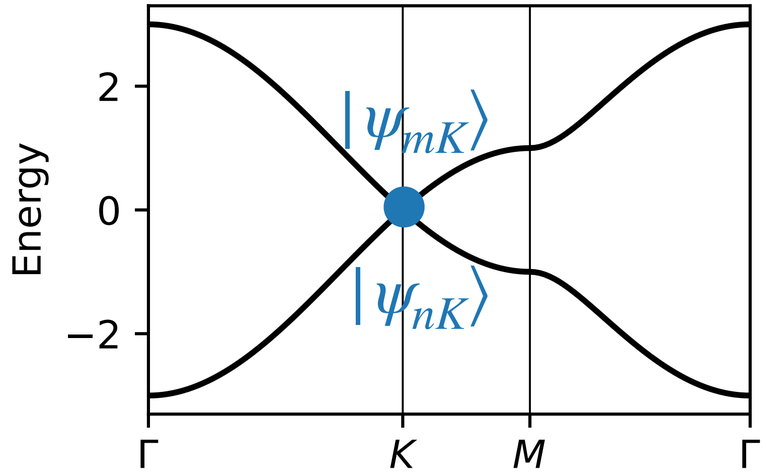

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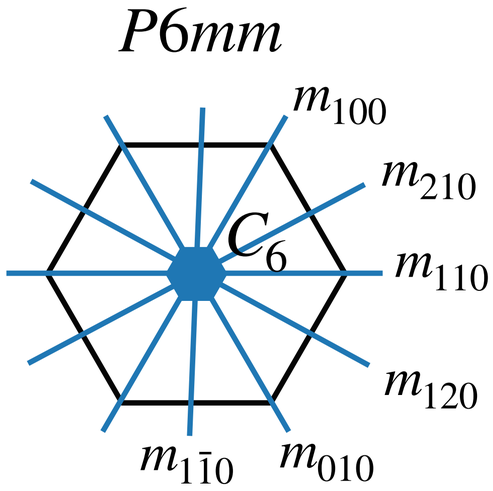

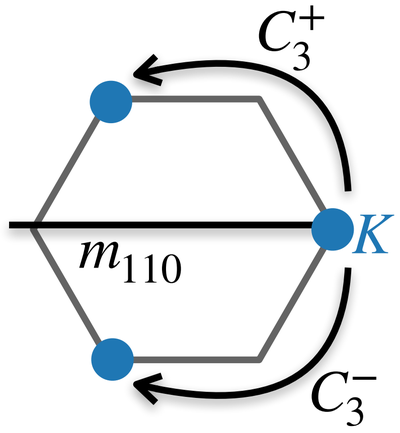

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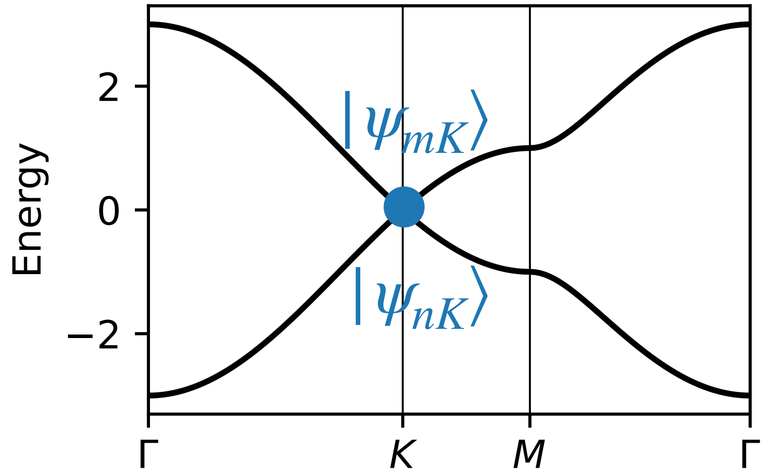

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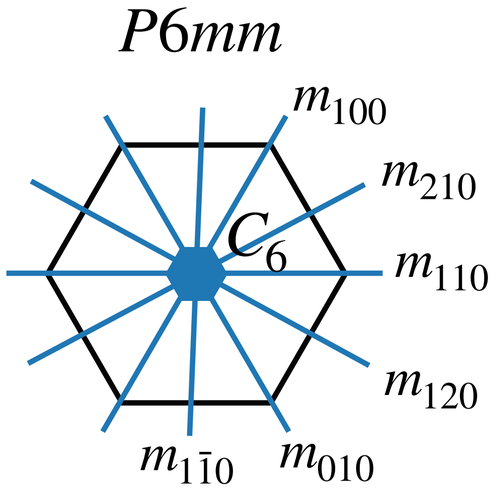

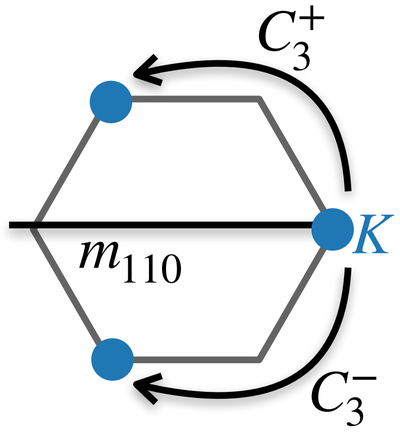

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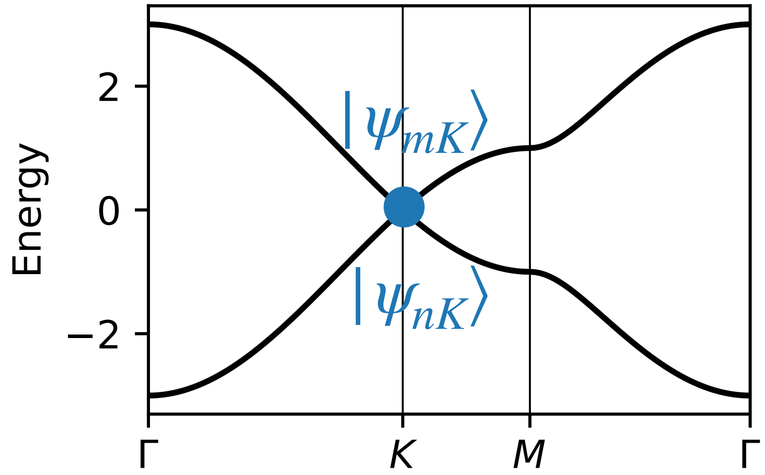

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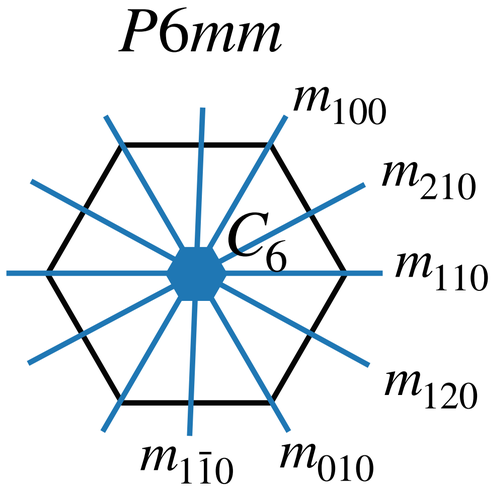

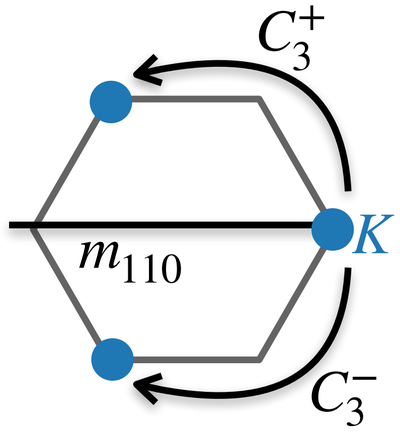

2. Pick $g = \{R \,|\, \boldsymbol{v}\}$ and calculate the expected values $\langle \psi_{Kn} | g | \psi_{Kn} \rangle$ and $\langle \psi_{Km} | g | \psi_{Km} \rangle$

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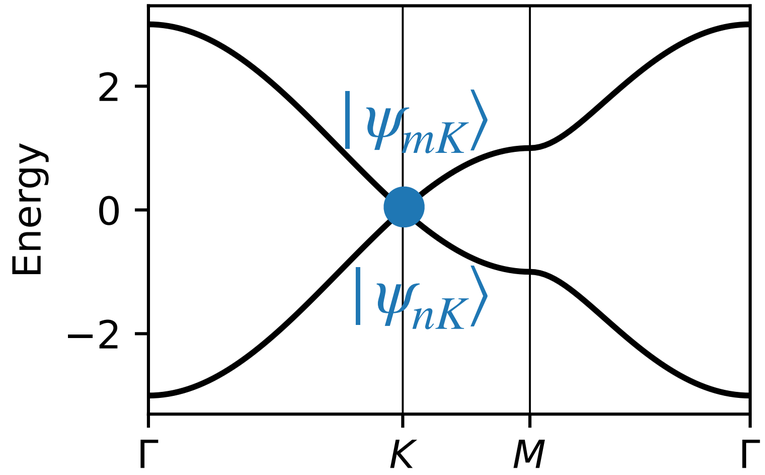
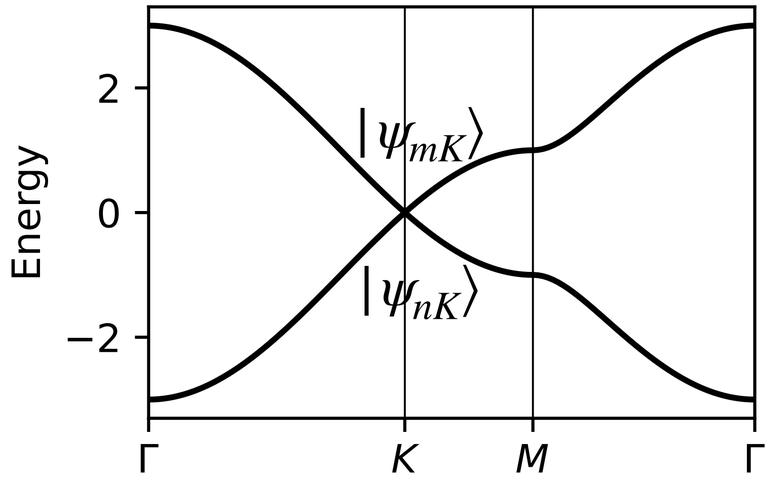


3. Compute the trace of the symmetry

$$g : \begin{pmatrix} \langle \psi_{nK} | g | \psi_{nK} \rangle & \langle \psi_{nK} | g | \psi_{mK} \rangle \\ \langle \psi_{mK} | g | \psi_{nK} \rangle & \langle \psi_{mK} | g | \psi_{mK} \rangle \end{pmatrix} \longrightarrow \mathrm{Tr}\,(g) = 1$$

IrRep: how does it work?

states	C_3^+	C_3^-	M_y
$\|\psi_{1K}\rangle$ $\|\psi_{2K}\rangle$	1	1	0



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4 Identify the IR by matching the traces with the character of the IR

irreps	C_3^+	C_3^-	M_y
	Bilbao Crystallographic Server		
$\bar{K}_4$	-1	-1	$-i$
$\bar{K}_5$	-1	-1	i
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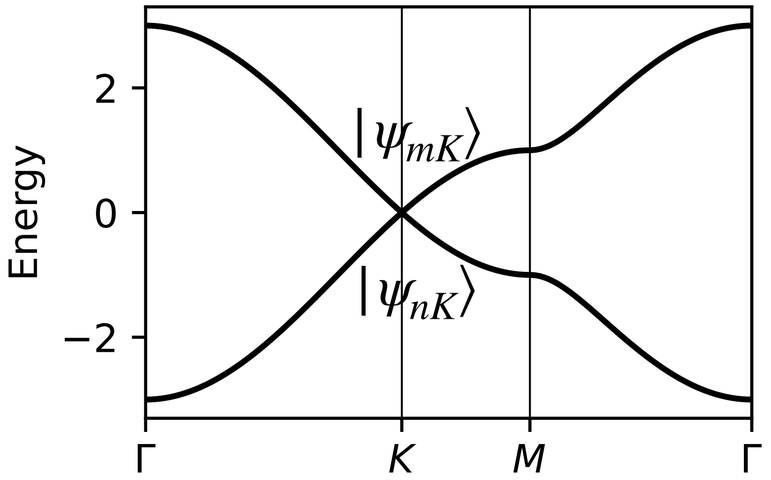

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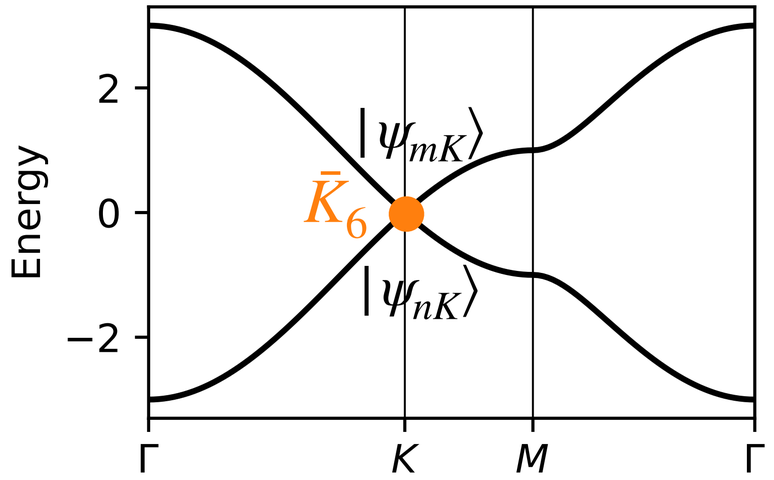
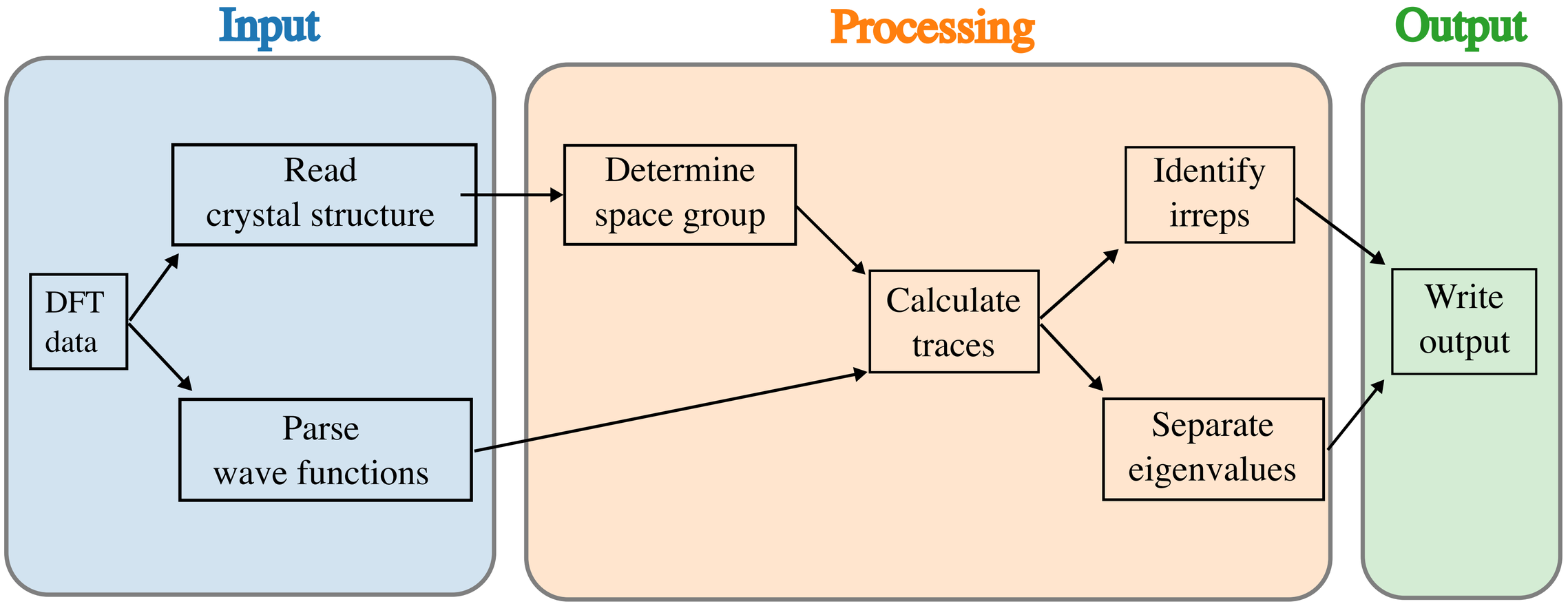


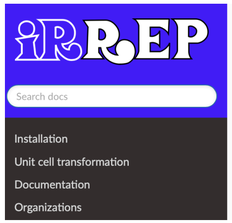
IrRep: how does it work?



IrRep

M. Iraola, S. Tsirkin, *et al.* Comput. Phys. Commun. 272, 108226 (2022)

- ✓ Interfaces to 4 DFT codes (more to come…)
- ✓ You can use the cell that you want for the DFT calculation
- ✓ Uses the notation of the Bilbao Cryst. Server
- ✓ It has an extensive documentation on its web page
- ✓ It’s for free !



GitHub

https://github.com/stepan-tsirkin/irrep