

26 March, 2020  
Wannier90 School

# Symmetry-adapted Wannier functions lecture and tutorials

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Collaborators (SAWF part): Yoshiro Nohara, Takashi Koretsune, and Ryotaro Arita



PHYSICAL REVIEW B 87, 235109 (2013)

## Symmetry-adapted Wannier functions in the maximal localization procedure

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(Received 25 March 2013; published 10 June 2013)

A procedure to construct symmetry-adapted Wannier functions in the framework of the maximally localized Wannier function approach [Marzari and Vanderbilt, *Phys. Rev. B* **56**, 12847 (1997); Souza, Marzari, and Vanderbilt, *ibid.* **65**, 035109 (2001)] is presented. In this scheme, the minimization of the spread functional of the Wannier functions is performed with constraints that are derived from symmetry properties of the specified set of the Wannier functions and the Bloch functions used to construct them, therefore one can obtain a solution that does not necessarily yield the global minimum of the spread functional. As a test of this approach, results of atom-centered Wannier functions for GaAs and Cu are presented.

DOI: [10.1103/PhysRevB.87.235109](https://doi.org/10.1103/PhysRevB.87.235109)

PACS number(s): 71.15.Ap

Symmetry-adapted Wannier functions = “maxloc” procedure + **symmetry constraint**  
→ obtain irreducible representations of a subgroup of full symmetry group  
(irreducible representations of site-symmetry group)

Now available in Wannier90

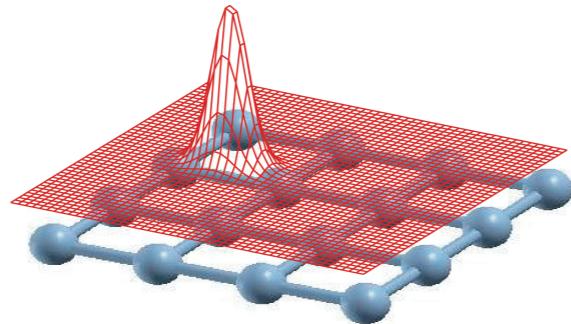
※ Please use version 3.1.0 !!!

# Maximally localized Wannier function

N. Marzari and D. Vanderbilt, Phys. Rev. B. 56 12847 (1997)  
I. Souza et al., ibid. 65, 035109 (2001)

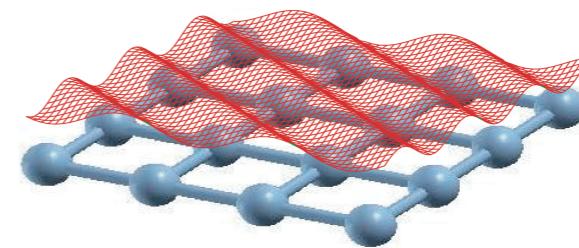
$$|w_{n\mathbf{R}}\rangle = a_{n\mathbf{R}}^\dagger |0\rangle$$

Wannier State



$$|\psi_{\alpha\mathbf{k}}\rangle = c_{\alpha\mathbf{k}}^\dagger |0\rangle$$

Bloch state



$$|w_{n\mathbf{R}}\rangle = \frac{1}{\sqrt{N}} \sum_{\alpha\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} U_{\alpha n, \mathbf{k}} |\psi_{\alpha\mathbf{k}}\rangle$$

The unitary matrix  $U$  is decided to minimize the spread functional  $\Omega$ :

$$\Omega = \sum_n \left[ \langle r^2 \rangle_n - \bar{\mathbf{r}}_n^2 \right]$$

where,

$$\bar{\mathbf{r}}_n = \langle w_{n\mathbf{0}} | \mathbf{r} | w_{n\mathbf{0}} \rangle$$

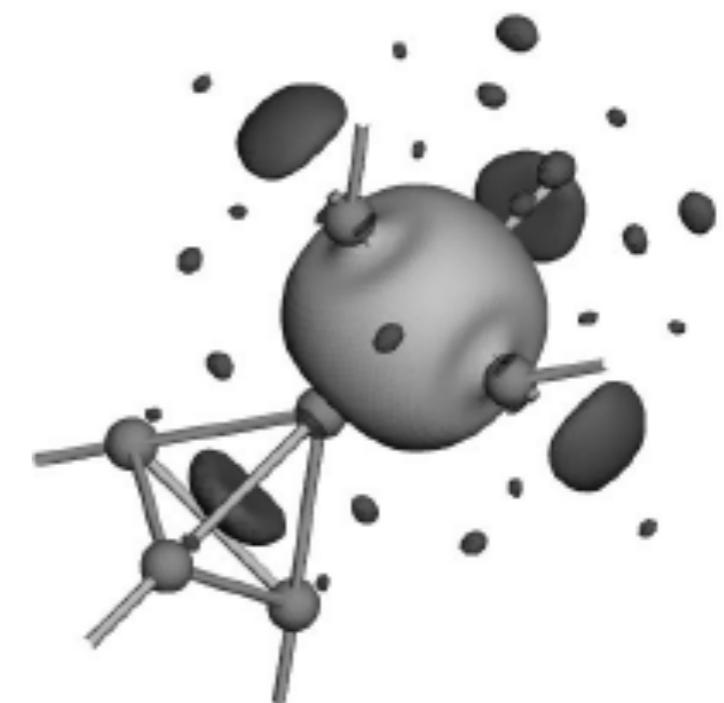
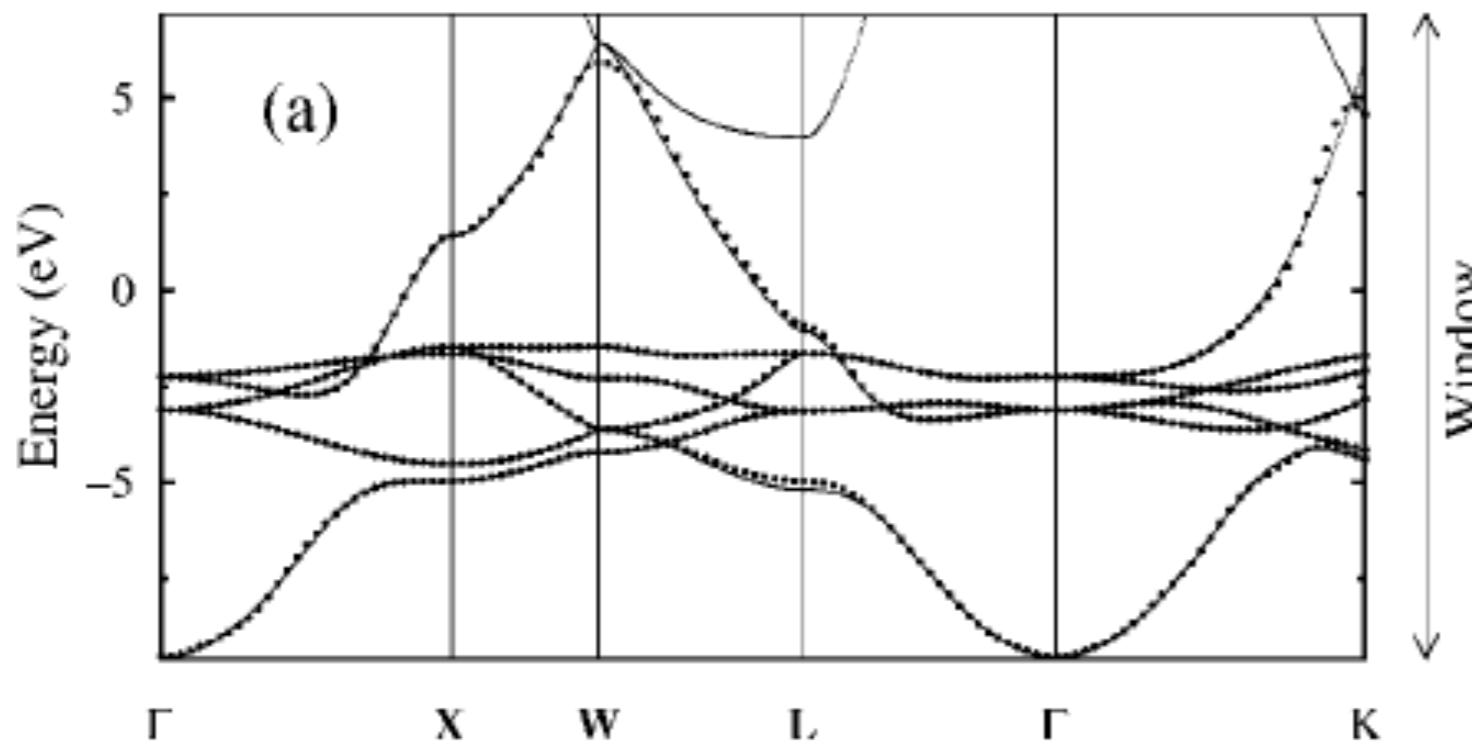
$$\langle r^2 \rangle_n = \langle w_{n\mathbf{0}} | r^2 | w_{n\mathbf{0}} \rangle$$

# Symmetry breaking of “maxloc” Wannier functions : Copper

I. Souza et al., Phys. Rev. B 65 035109 (2001)

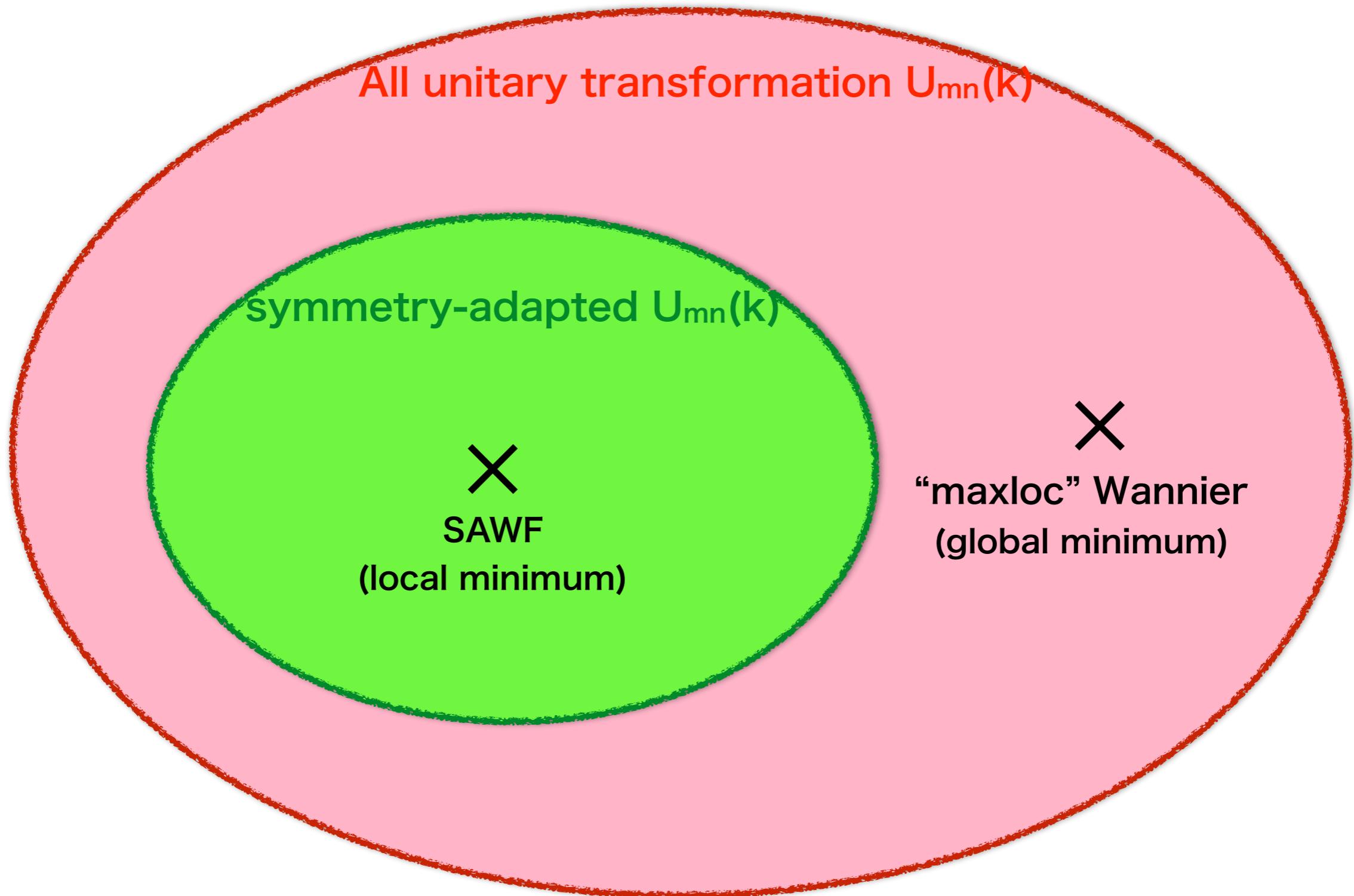
initial projections with atom-centered s and d orbitals, i.e., 6 orbital model  
→ results in interstitial-centered s-like “maxloc”

(“maxloc” procedure does not care about symmetry at all)



# Concept of Symmetry-adapted Wannier functions (SAWF)

SAWF = “maxloc” procedure + **symmetry constraint**  
→ obtain irreducible representations of site-symmetry group



# Symmetry-adapted Wannier functions

R. Sakuma, Phys. Rev. B **87** 235109 (2013)

- Symmetry-adapted Wannier functions = maxloc procedure + **symmetry constraint**
  - obtain irreducible representations of a subgroup of full symmetry group  
(irreducible representations of site-symmetry group)

$$w_{n\mathbf{R}}(\mathbf{r}) = \frac{V}{(2\pi)^3} \int_{\text{BZ}} \left[ \sum_m U_{mn}^{(\mathbf{k})} \psi_{m\mathbf{k}}(\mathbf{r}) \right] e^{-i\mathbf{k}\cdot\mathbf{R}} d\mathbf{k}$$

- ✓ Constraint on  $U(\mathbf{k})$  for  $\mathbf{k} \in$  Irreducible BZ

$$U(\mathbf{k}) = \frac{\tilde{d}(g_{\mathbf{k}}, \mathbf{k})}{\text{matrices related to symmetry}} \underline{U(\mathbf{k})} \underline{D^{\dagger}(g_{\mathbf{k}}, \mathbf{k})}$$

$$g_{\mathbf{k}} \mathbf{k} = \mathbf{k}$$

$$\begin{aligned}\hat{g}\psi_{\mathbf{k}I}(\mathbf{r}) &= \sum_{I'} D_{I'I}(g, \mathbf{k}) \psi_{R\mathbf{k}I'}(\mathbf{r}) \\ \hat{g}\psi_{\mathbf{k}\mu}^{\text{KS}}(\mathbf{r}) &= \sum_{\mu'} \tilde{d}_{\mu'\mu}(g, \mathbf{k}) \psi_{R\mathbf{k}\mu'}^{\text{KS}}(\mathbf{r})\end{aligned}$$

- ✓ Unitary matrix for other  $\mathbf{k}$  points

$$U(R\mathbf{k}) = \tilde{d}(g, \mathbf{k}) \underline{U(\mathbf{k})} \underline{D^{\dagger}(g, \mathbf{k})}$$

Acknowledgements: Yoshiro Nohara for implementation

# Important quantities: D and $\tilde{d}$ matrices

$D(g, \mathbf{k})$  num\_wann×num\_wann matrix

$$\hat{g}\psi_{\mathbf{k}I}(\mathbf{r}) = \sum_{I'} D_{I'I}(g, \mathbf{k})\psi_{R\mathbf{k}I'}(\mathbf{r})$$

Transformation of symmetry-adapted (Wannier-gauge)  
Bloch functions by sym. ops.

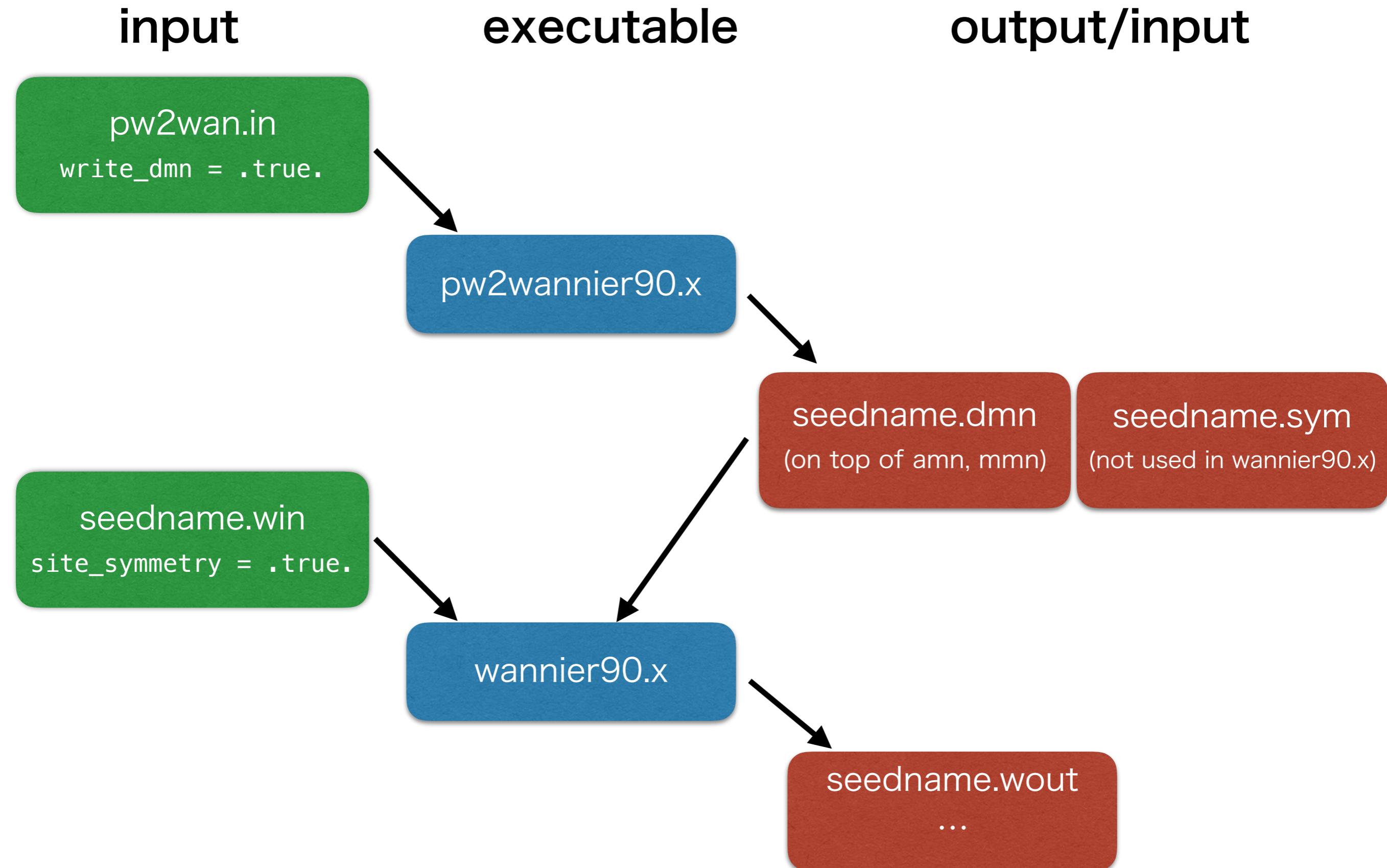
$\tilde{d}(g_{\mathbf{k}}, \mathbf{k})$  num\_bands×num\_bands matrix

$$\hat{g}\psi_{\mathbf{k}\mu}^{\text{KS}}(\mathbf{r}) = \sum_{\mu'} \tilde{d}_{\mu'\mu}(g, \mathbf{k})\psi_{R\mathbf{k}\mu'}^{\text{KS}}(\mathbf{r})$$

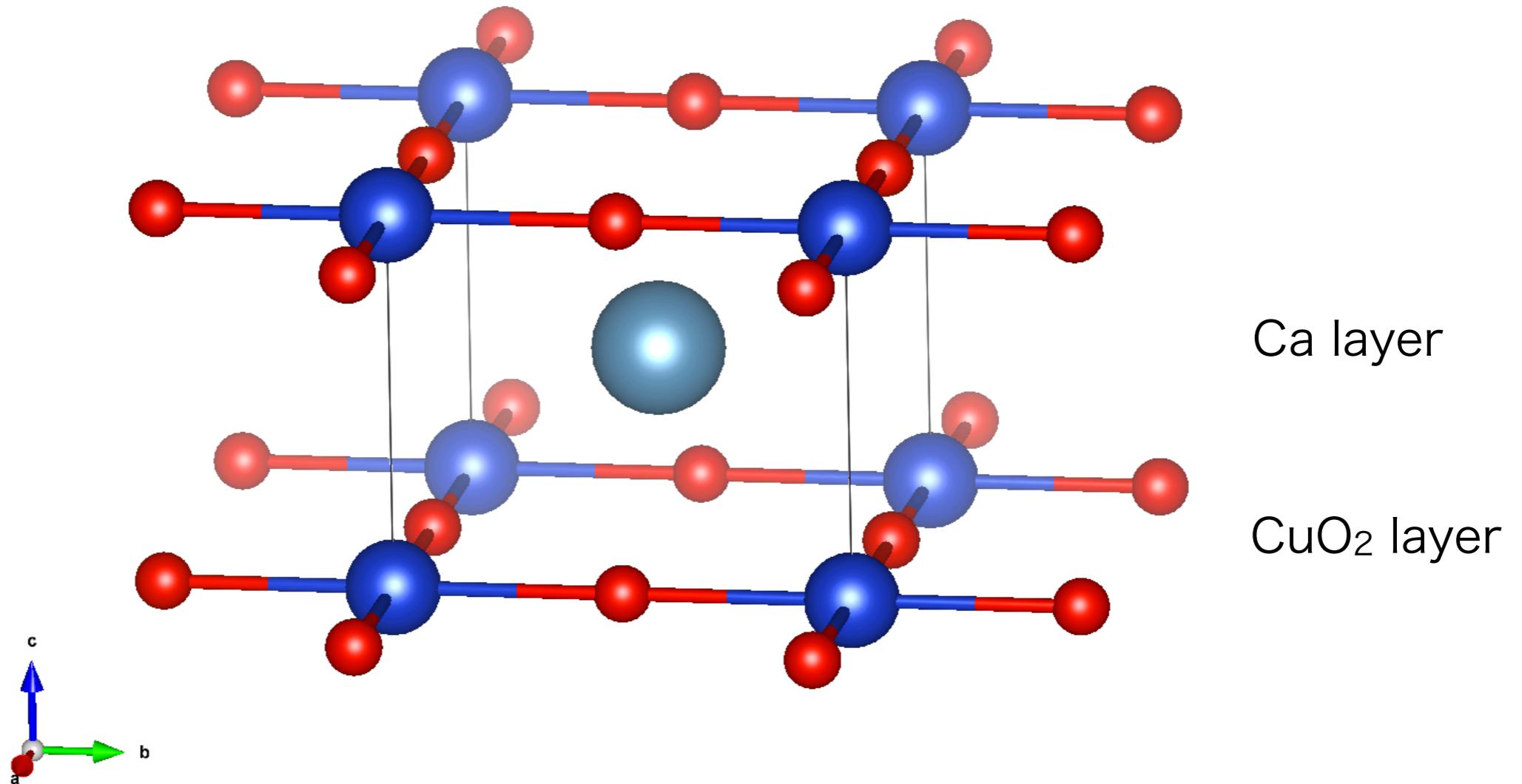
Transformation of Kohn-Sham Bloch functions by sym. ops.

written in seedname.dmn file

# Flow of calculation (after nscf calculations and creating .nnkp file)

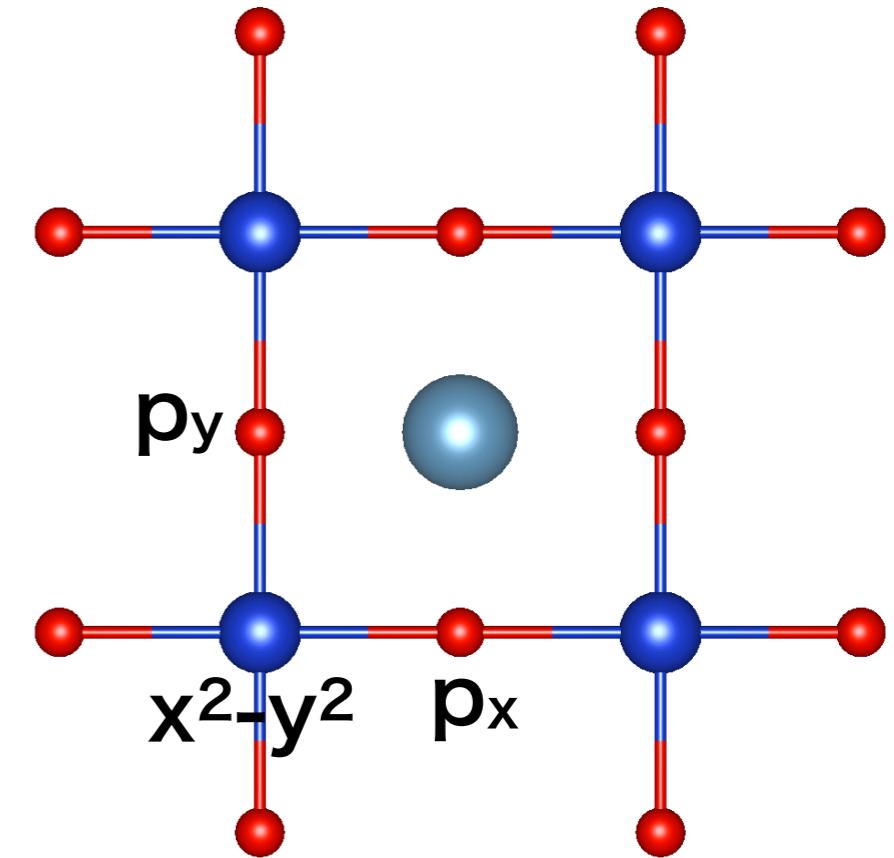
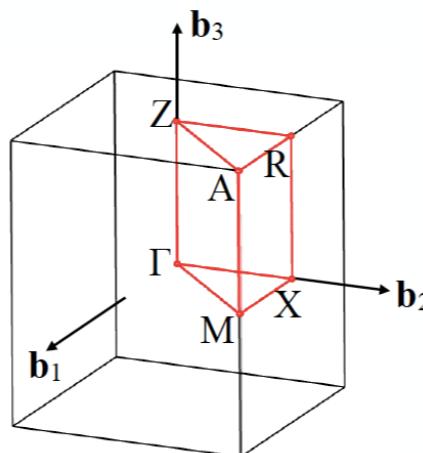
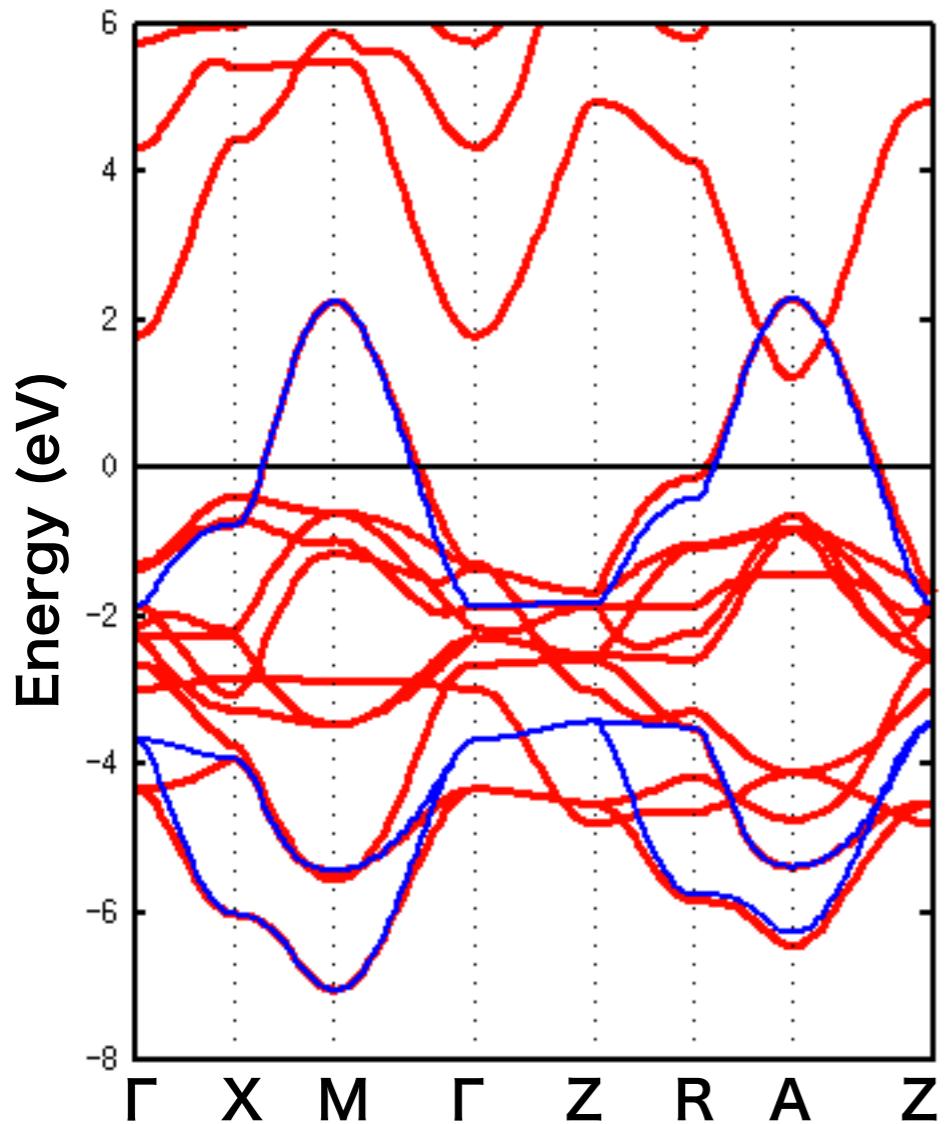


# Example of $D_{mn}$ : $\text{CaCuO}_2$ d-p model



- ✿ Famous family of high-T<sub>c</sub> cuprates
- ✿ Quasi-2D (layered) material
- ✿ 16 symmetry operations ( $P4/mmm$ )

# Example of $D_{mn}$ : CaCuO<sub>2</sub> d-p model



$$\hat{g} \psi_{\mathbf{k}I}(\mathbf{r}) = \sum_{I'} D_{I'I}(g, \mathbf{k}) \psi_{R\mathbf{k}I'}(\mathbf{r})$$

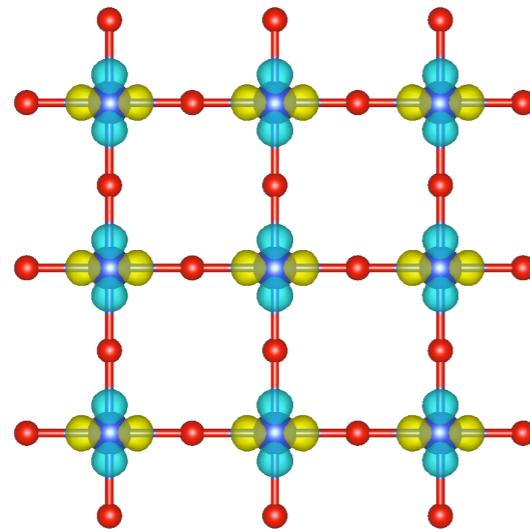
⌚ D matrix → how does the SAWF transform by sym. ops.

# Example of $D_{mn}$ ( $90^\circ$ rotation, $\Gamma$ ): CaCuO<sub>2</sub> d-p model

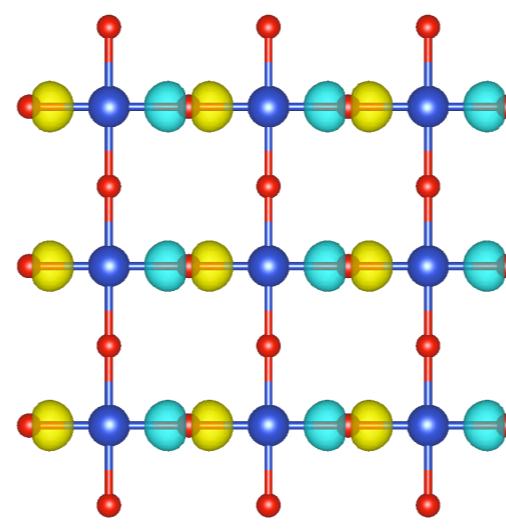
$$\hat{R}_{\pi/2} \Psi_{\Gamma n}(\mathbf{r}) = \sum_m D_{mn} \Psi_{\Gamma m}(\mathbf{r})$$

Wannier-gauge Bloch at  $\Gamma$

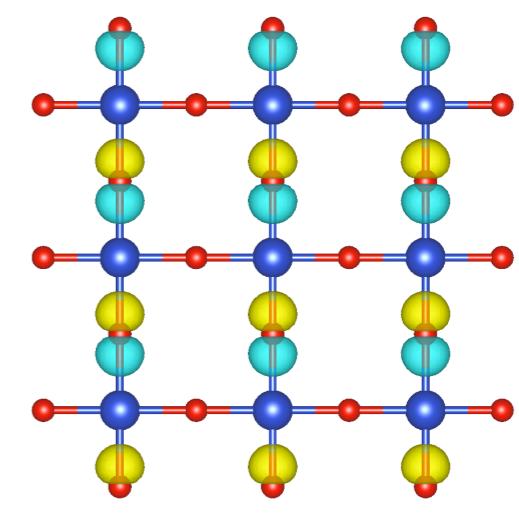
$$\Psi_{\Gamma, x^2-y^2, (0,0,0)}$$



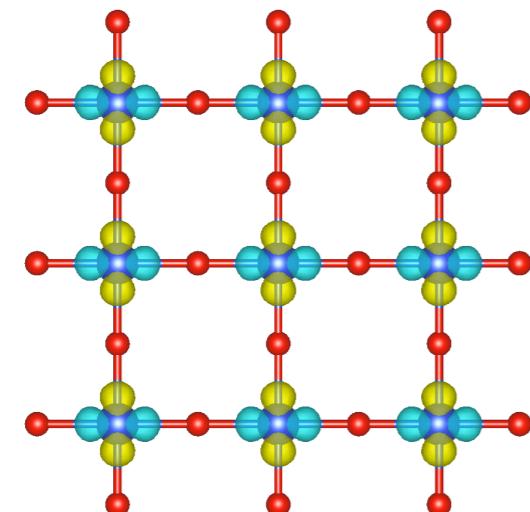
$$\Psi_{\Gamma, p_x, (1/2,0,0)}$$



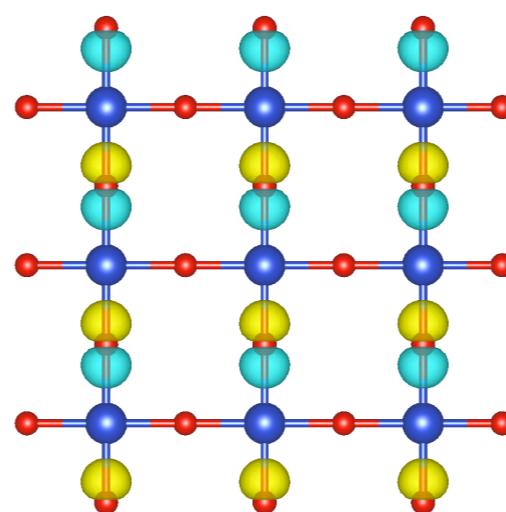
$$\Psi_{\Gamma, p_y, (0,1/2,0)}$$



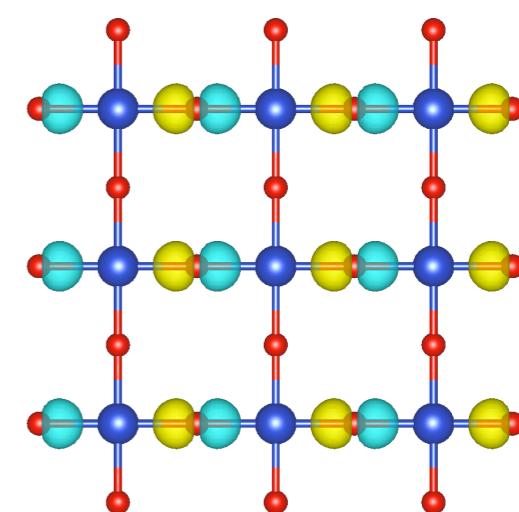
after  $90^\circ$  rotation



$$\rightarrow (-1) \Psi_{\Gamma, x^2-y^2, (0,0,0)}$$



$$\rightarrow \Psi_{\Gamma, p_y, (0,1/2,0)}$$



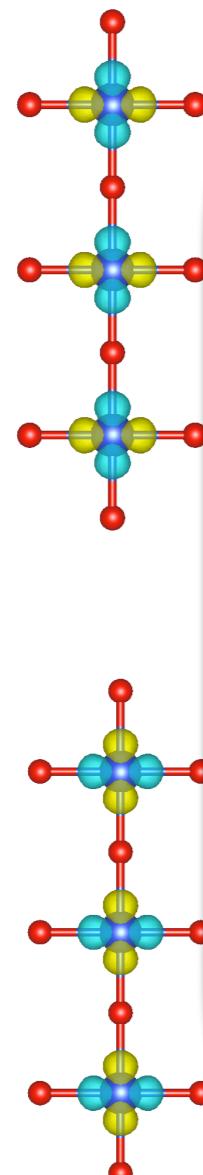
$$\rightarrow (-1) \Psi_{\Gamma, p_x, (1/2,0,0)}$$

# Example of $D_{mn}$ ( $90^\circ$ rotation, $\Gamma$ ): CaCuO<sub>2</sub> d-p model

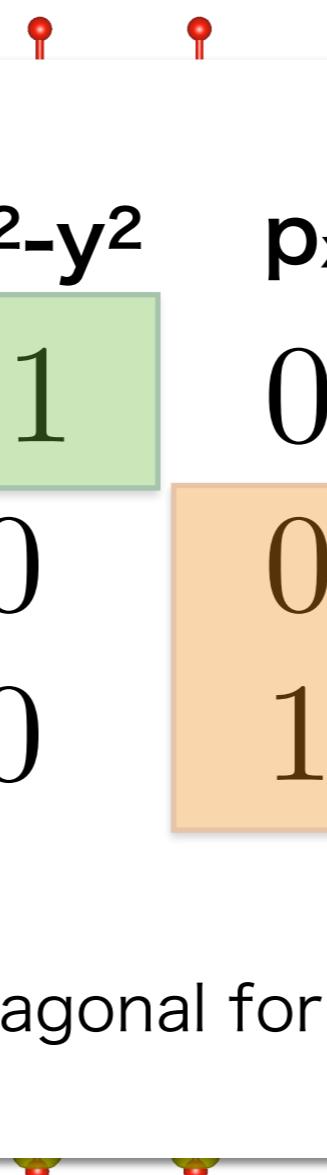
$$\hat{R}_{\pi/2} \Psi_{\Gamma n}(\mathbf{r}) = \sum_m D_{mn} \Psi_{\Gamma m}(\mathbf{r})$$

Wannier-gauge Bloch at  $\Gamma$   
after  $90^\circ$  rotation

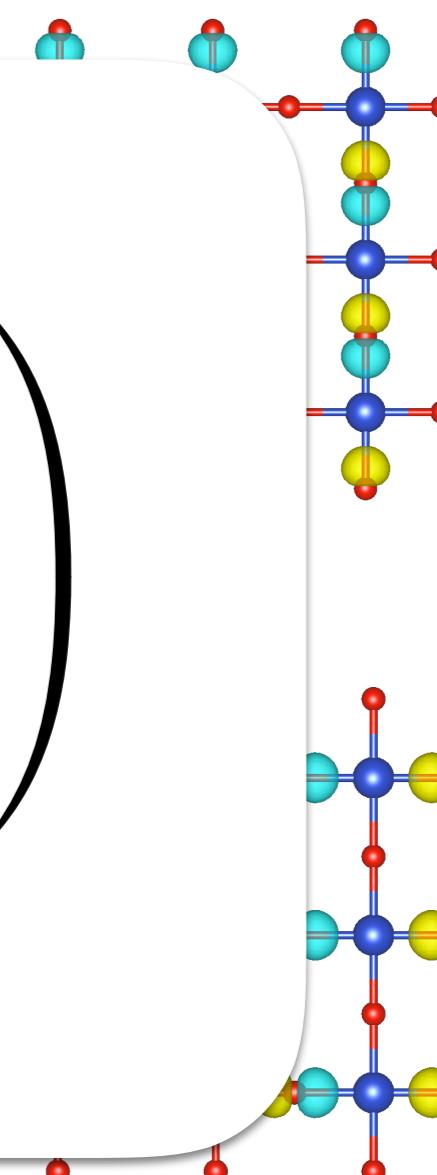
$\Psi_{\Gamma, x^2-y^2, (0,0,0)}$



$\Psi_{\Gamma, p_x, (1/2,0,0)}$



$\Psi_{\Gamma, p_y, (0,1/2,0)}$



$$D = \begin{pmatrix} x^2-y^2 & & \\ & p_x & p_y \\ -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

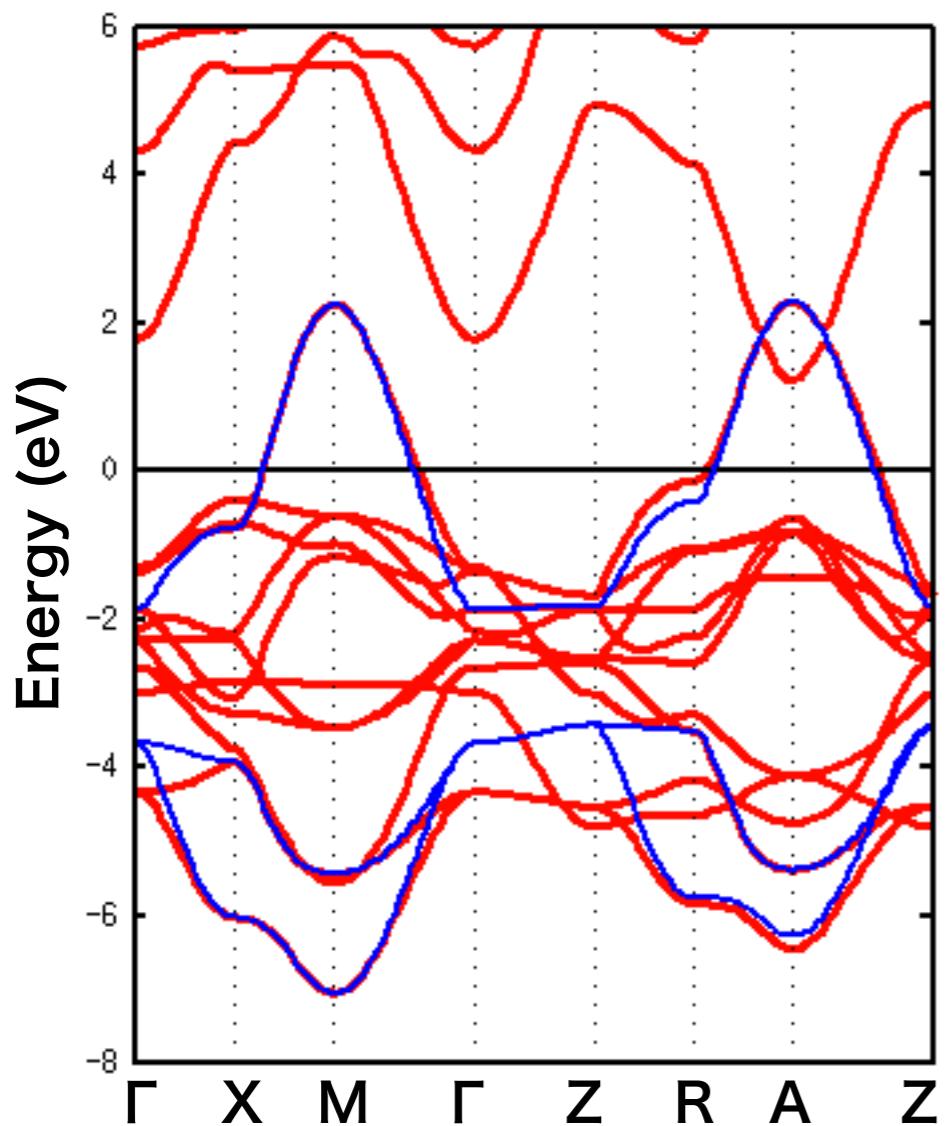
📌 Block diagonal for each irrep.

$\rightarrow (-1) \Psi_{\Gamma, x^2-y^2, (0,0,0)}$

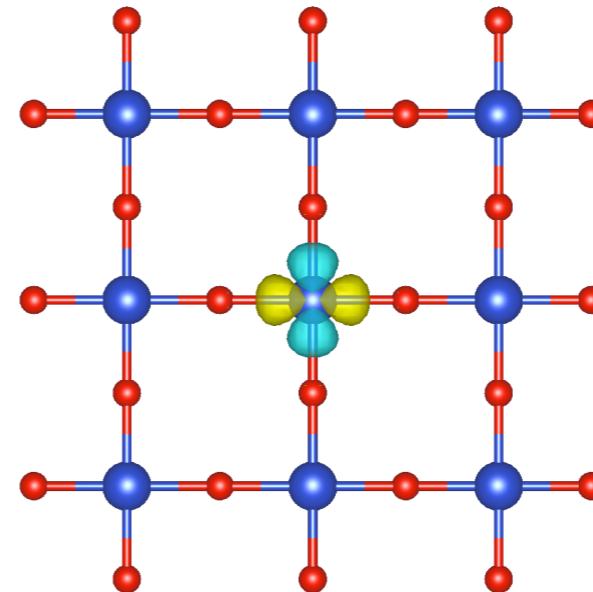
$\rightarrow \Psi_{\Gamma, p_y, (0,1/2,0)}$

$\rightarrow (-1) \Psi_{\Gamma, p_x, (1/2,0,0)}$

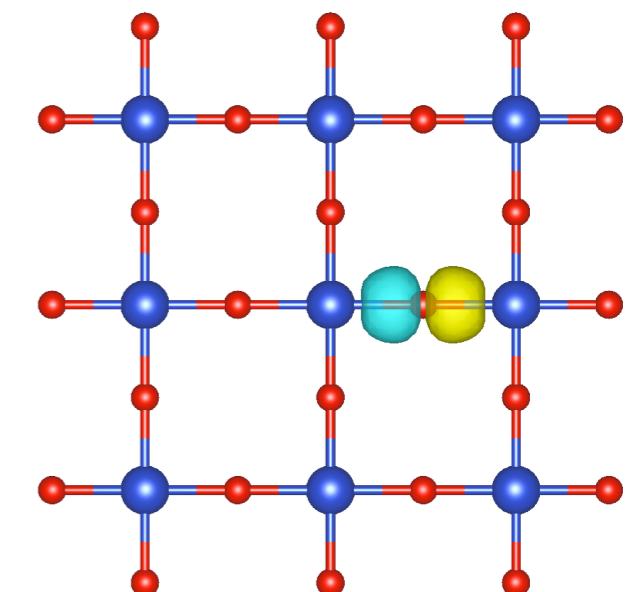
# SAWFs : CaCuO<sub>2</sub> d-p model



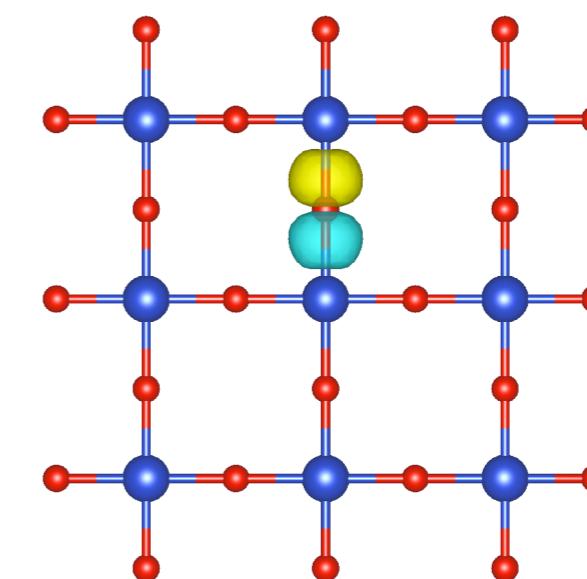
$x^2-y^2$



$p_x$



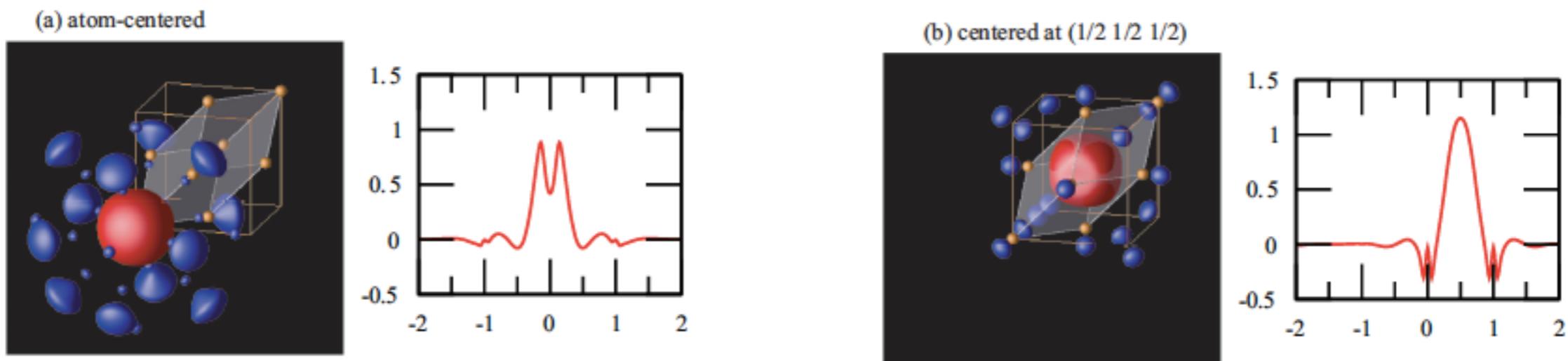
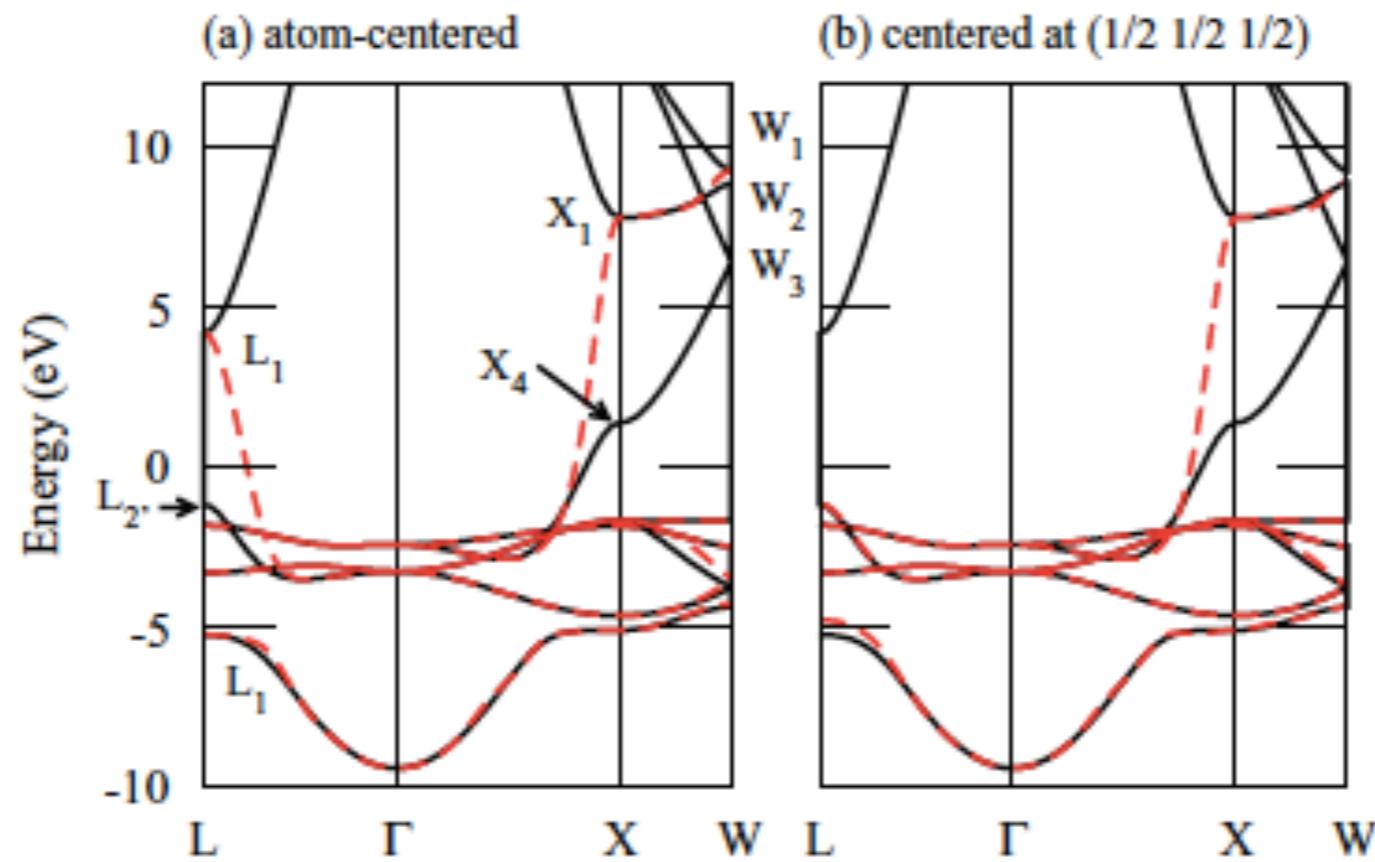
$p_y$



• In this case, SAWF = “maxloc” Wannier function

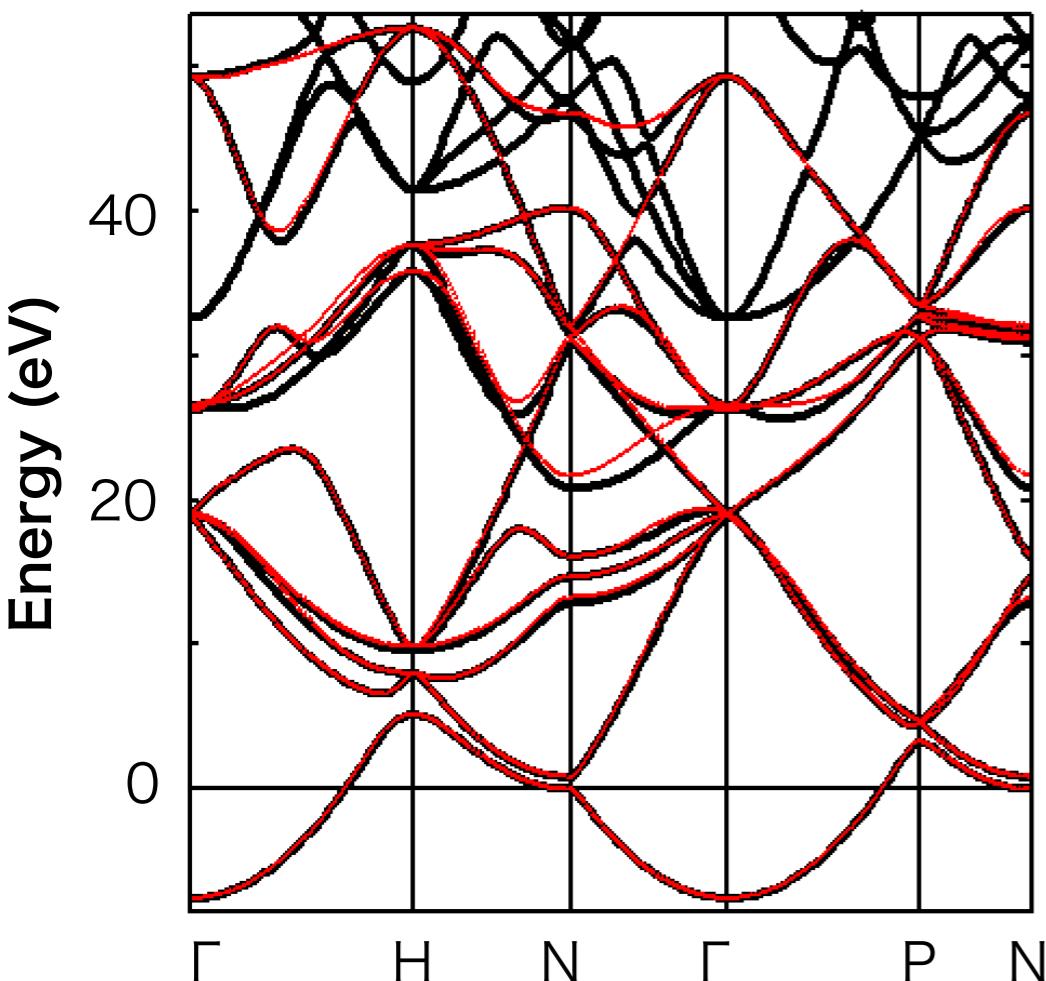
# SAWFs : Copper

Rei Sakuma, Phys. Rev. B **87** 235109 (2013)

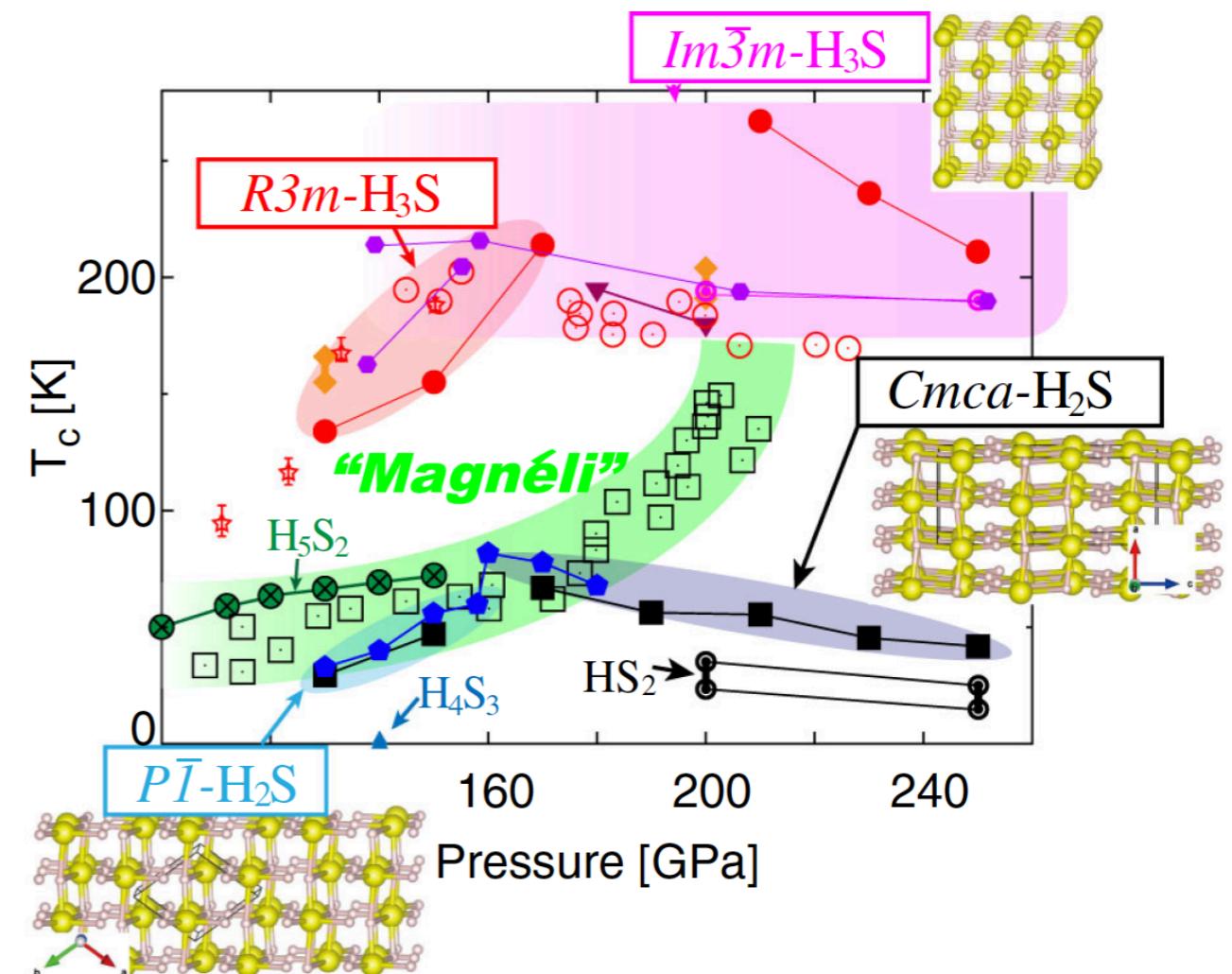


# Applications to H<sub>3</sub>S ①

Band structure of Im-3m H<sub>3</sub>S

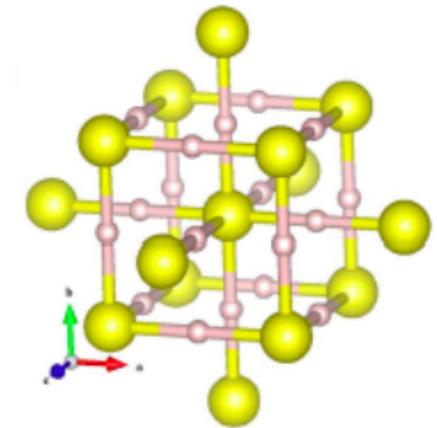


bcc, 48 sym. ops.



A. P. Drozdov et al., Nature 2015  
M. Einaga et al., Nat. Phys. 2016  
R. Akashi et al., PRL 2016

# Applications to H<sub>3</sub>S ②



Im3-m H<sub>3</sub>S

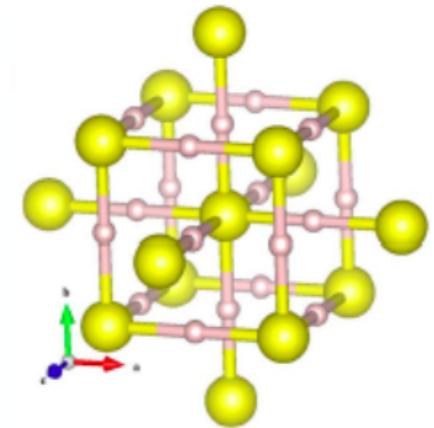
## Maximally localized Wannier functions

### Final State

WF centre and spread	1 ( 0.396807, -0.313554, 0.345678 )	0.67398410	S s
WF centre and spread	2 ( -0.406556, -0.136459, -0.412993 )	0.69230057	
WF centre and spread	3 ( -0.418930, -0.303754, 0.323009 )	0.67664806	S p
WF centre and spread	4 ( 0.421416, 0.396216, 0.113791 )	0.70067659	
WF centre and spread	5 ( -0.013744, 0.173331, 0.462649 )	0.83791701	
WF centre and spread	6 ( 0.423112, -0.149360, -0.392309 )	0.69147489	
WF centre and spread	7 ( 0.018786, 0.382413, -0.407176 )	0.75999389	S d
WF centre and spread	8 ( -0.003392, -0.455380, -0.115887 )	0.86674560	
WF centre and spread	9 ( -0.417388, 0.404753, 0.084644 )	0.70297783	H s
WF centre and spread	10 ( 1.484447, 0.000036, -0.000002 )	0.52171917	
WF centre and spread	11 ( -0.000005, 1.484334, -0.000360 )	0.51792603	
WF centre and spread	12 ( -0.000040, 0.000451, 1.484517 )	0.51871564	
Sum of centres and spreads	( 1.484511, 1.483026, 1.485561 )	8.16107938	

Spreads (Ang^2)	Omega I = 6.536108655
=====	
	Omega D = 0.001557835
	Omega OD = 1.623412888
Final Spread (Ang^2)	Omega Total = 8.161079378

# Applications to H<sub>3</sub>S ③



Im3-m H<sub>3</sub>S

## Symmetry adapted Wannier functions

### Final State

WF centre and spread	1 ( 0.000000, 0.000000, 0.000000 )	0.68140242	S s
WF centre and spread	2 ( 0.000000, 0.000000, 0.000000 )	0.85028025	
WF centre and spread	3 ( 0.000000, 0.000000, 0.000000 )	0.85028025	S p
WF centre and spread	4 ( 0.000000, 0.000000, 0.000000 )	0.85028025	
WF centre and spread	5 ( 0.000000, 0.000000, 0.000000 )	1.19162797	
WF centre and spread	6 ( 0.000000, 0.000000, 0.000000 )	1.26459287	
WF centre and spread	7 ( 0.000000, 0.000000, 0.000000 )	1.26459287	S d
WF centre and spread	8 ( 0.000000, 0.000000, 0.000000 )	1.19162833	
WF centre and spread	9 ( 0.000000, 0.000000, 0.000000 )	1.26459257	
WF centre and spread	10 ( 1.484435, 0.000000, 0.000000 )	0.50881447	
WF centre and spread	11 ( 0.000000, 1.484435, 0.000000 )	0.50881447	H s
WF centre and spread	12 ( 0.000000, 0.000000, 1.484435 )	0.50881445	
Sum of centres and spreads	( 1.484435, 1.484435, 1.484435 )	10.93572116	

Spreads (Ang^2)	Omega I	=	6.536108658
=====	Omega D	=	0.000000000
	Omega OD	=	4.399612423
Final Spread (Ang^2)	Omega Total	=	10.935721081

# Examples in Wannier90

example21: Gallium Arsenide – Symmetry-adapted Wannier functions

- atom\_centered\_As\_sp
- atom\_centered\_Ga\_p
- atom\_centered\_Ga\_s
- atom\_centered\_Ga\_sp
- bond\_centered

example22: Copper – Symmetry-adapted Wannier functions

- s\_at\_0.00
- s\_at\_0.25
- s\_at\_0.50

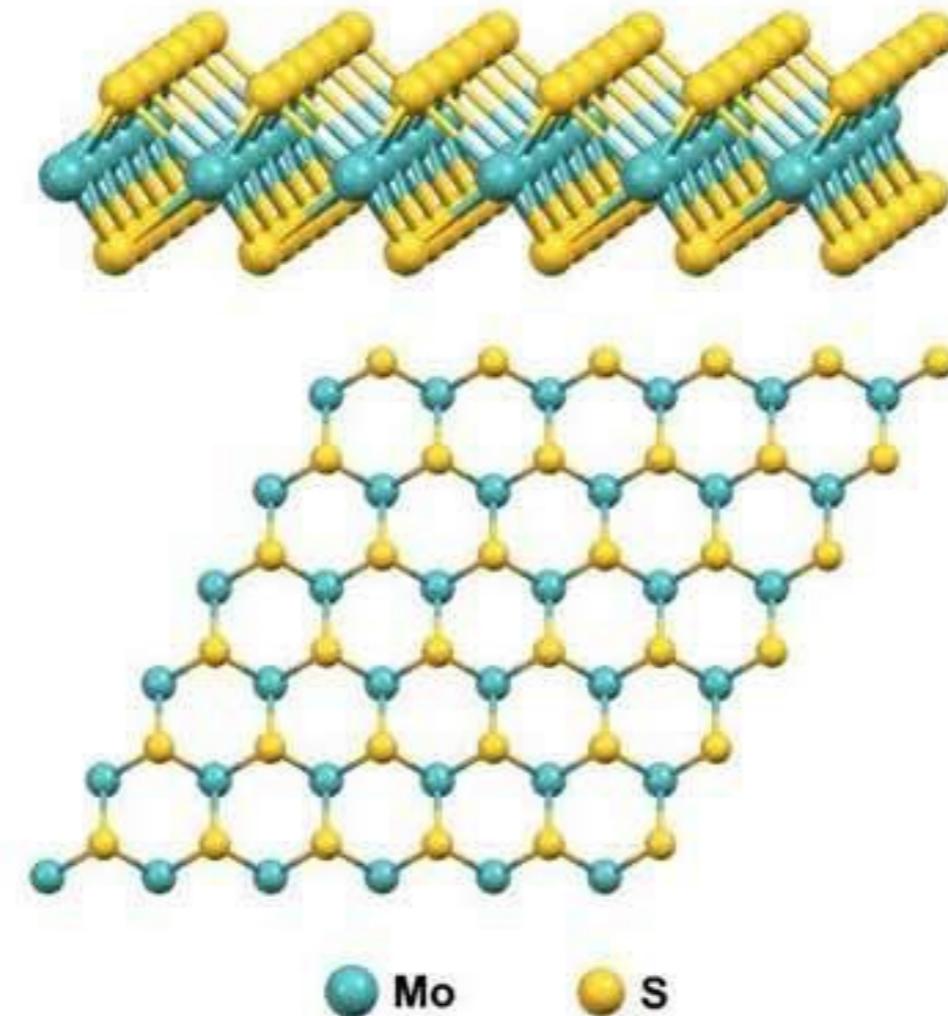
You can try SAWF

※ Please use version 3.1.0 !!!

Be careful ...

One cannot always get atom-centered Wannier orbitals  
with symmetry-adapted mode

Example: MoS<sub>2</sub> monolayer

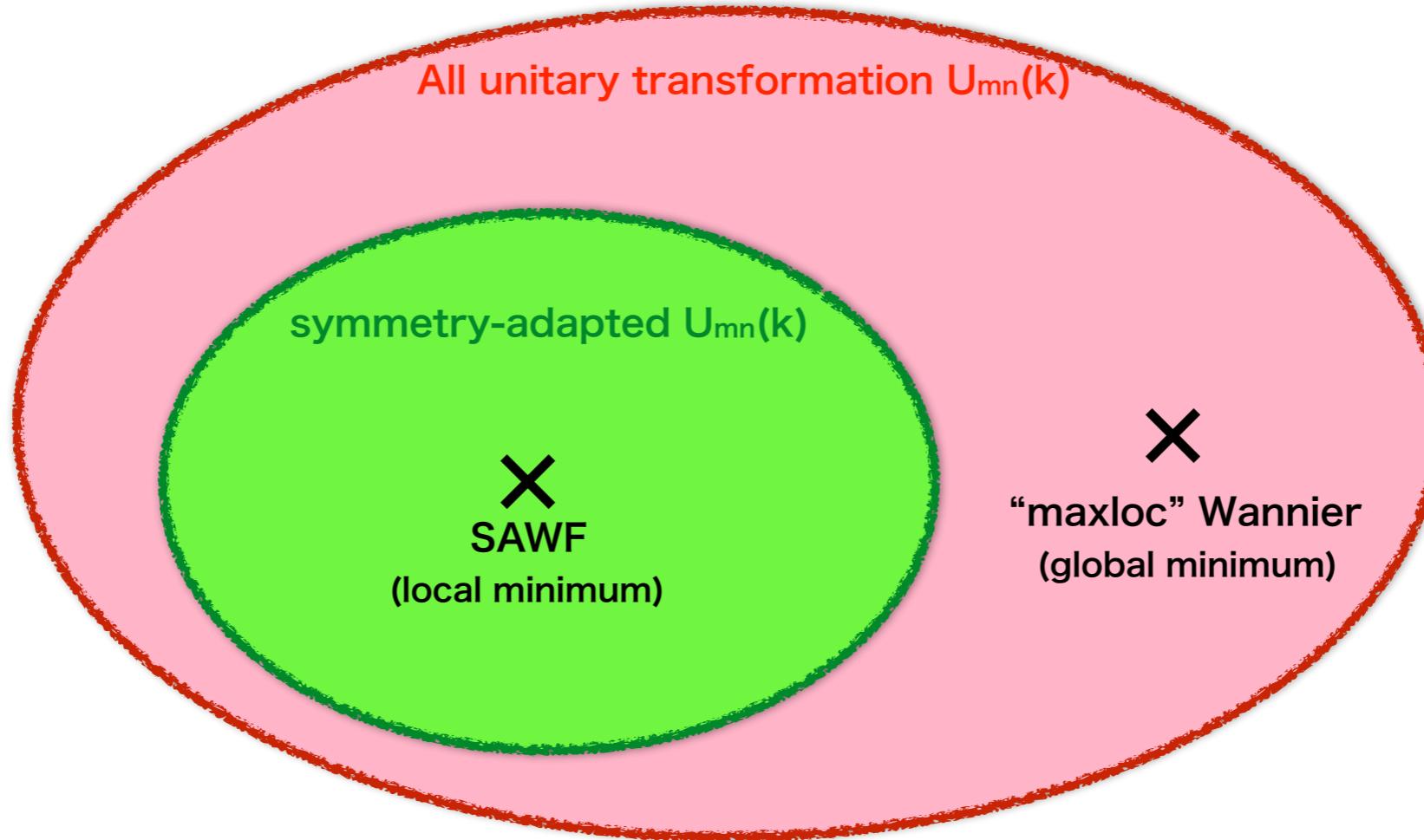


sulphur p orbitals cannot be atom-centered

# Summary and future perspective

## Summary

SAWF = “maxloc” procedure + **symmetry constraint**  
→ obtain irreducible representations of site-symmetry group



## Future perspective

- 📌 Frozen window (need to be symmetry-adapted)
- 📌 Extension to noncolliner case



# Tutorials

# Instructions

- Tutorials can be found in “Tutorials\_SAWF”
- Basic tutorial: “GaAs”
- (A little bit) advanced tutorials: “H3S” and “Cu”
- Work flow “GaAs” → “H3S” and “Cu”
- Follow README in each directory
- For “GaAs” and “Cu”, refer also to Wannier90 Tutorials and Tutorial Solutions

# Flow of calculation (after nscf calculations and creating .nnkp file)

**input**

**executable**

**output/input**

pw2wan.in  
write\_dmn = .true.

pw2wannier90.x

seedname.win  
site\_symmetry = .true.

wannier90.x

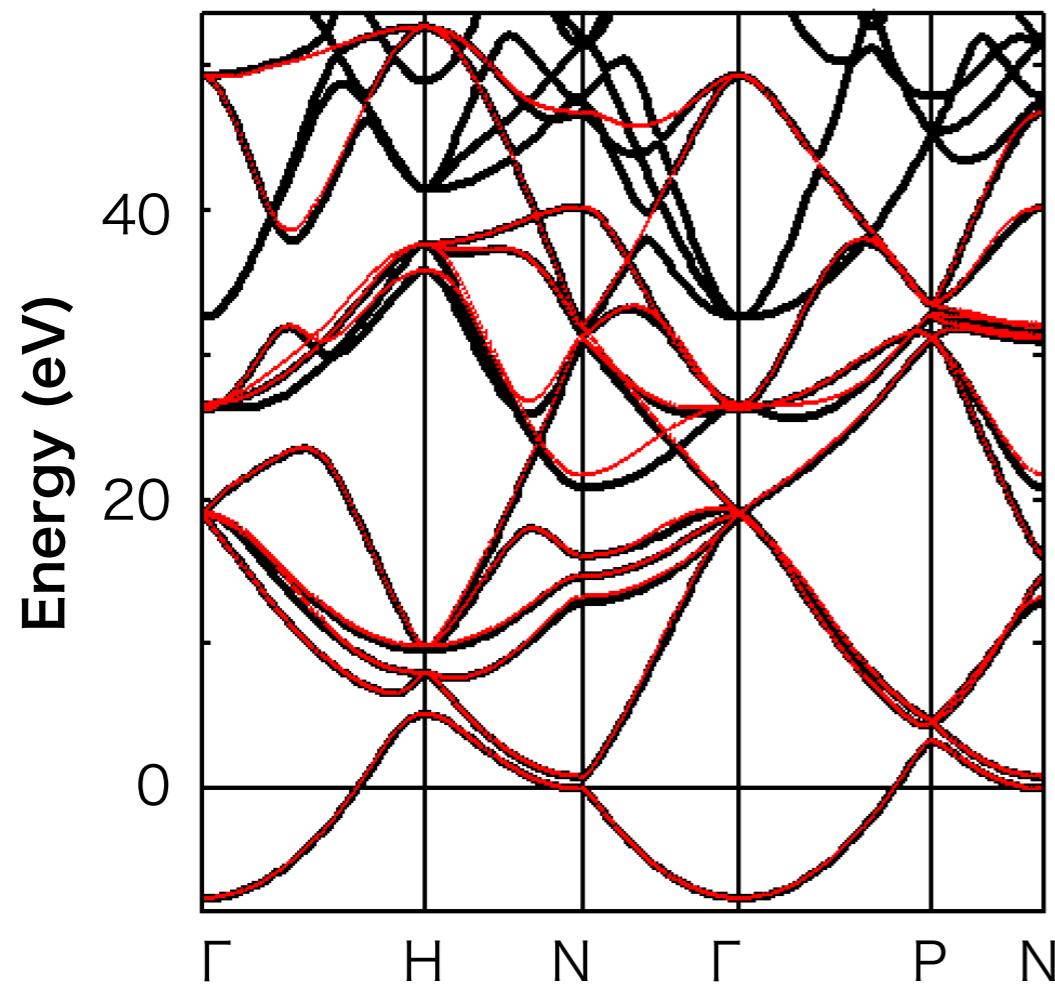
seedname.dmn  
(on top of amn, mmn)

seedname.sym  
(not used in wannier90.x)

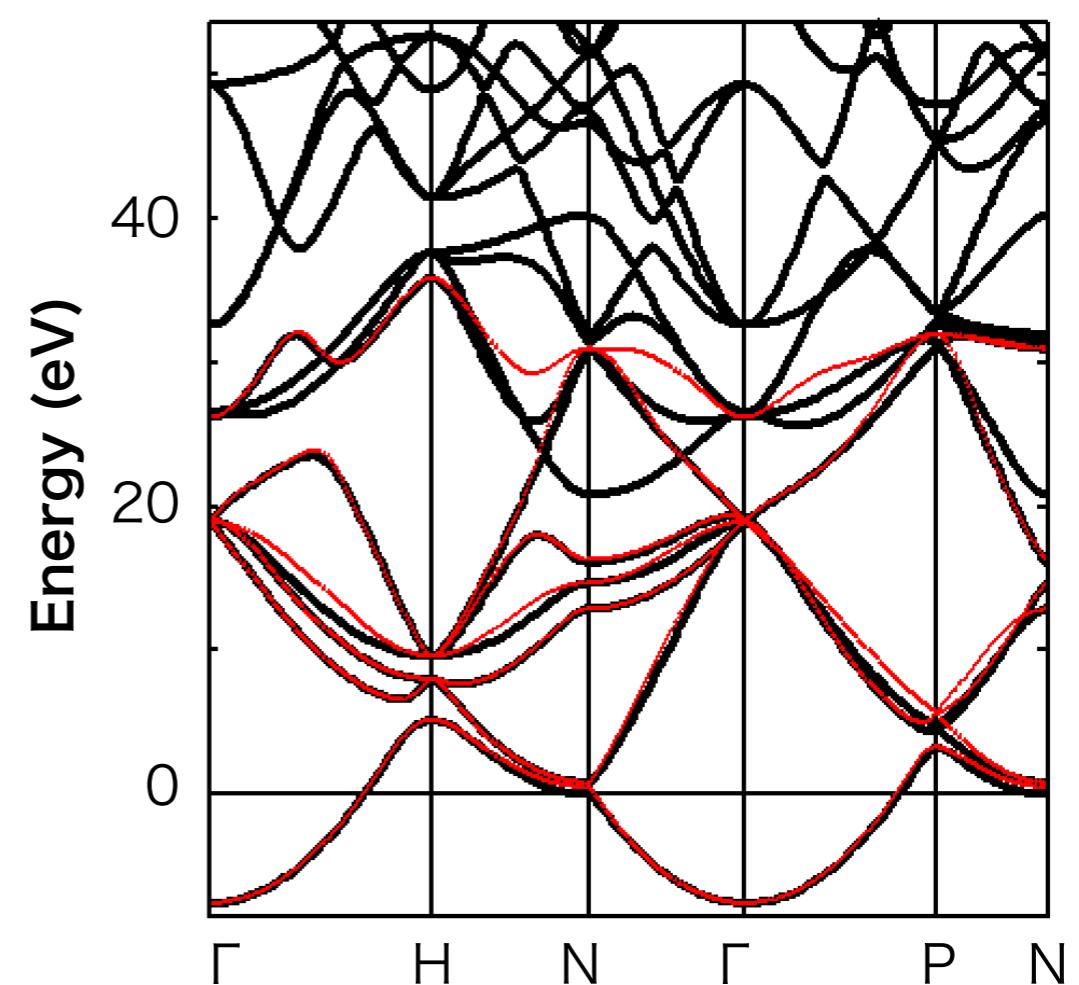
seedname.wout  
...

# Reference: H<sub>3</sub>S

12 band model



7 band model



# Flow of calculation in Cu tutorial : advanced usage

(after nscf calculations and creating .nnkp file)

