

May 20th, 2022  
Wannier 2022 Summer School

# Symmetry-adapted Wannier functions lecture and tutorials

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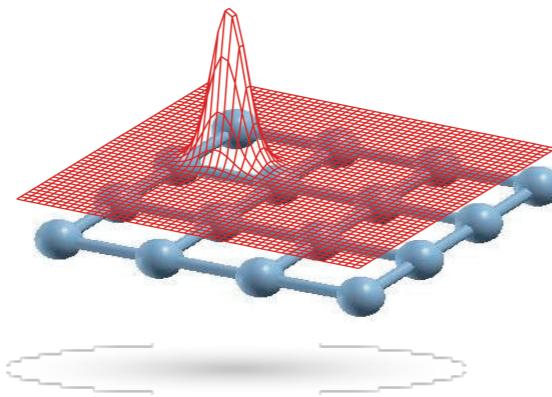
Collaborators (SAWF part): Yoshiro Nohara, Takashi Koretsune, and Ryotaro Arita

# Maximally localized Wannier functions

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

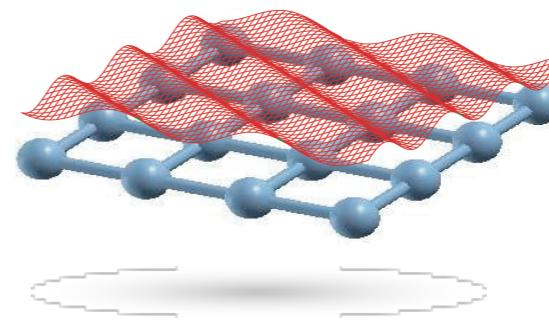
$$|w_{n\mathbf{R}}\rangle = a_{n\mathbf{R}}^\dagger |0\rangle$$

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 obtained by minimizing the spread functional  $\Omega$

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

where,

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

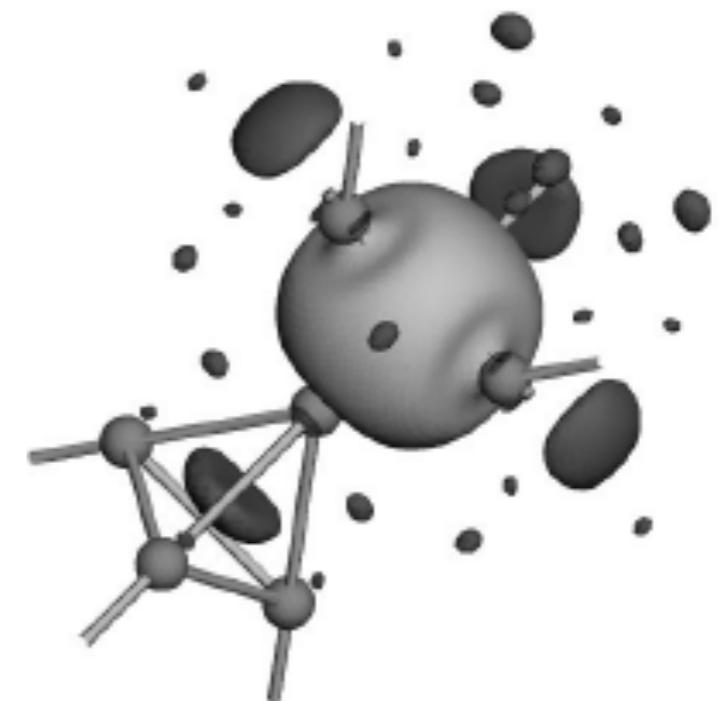
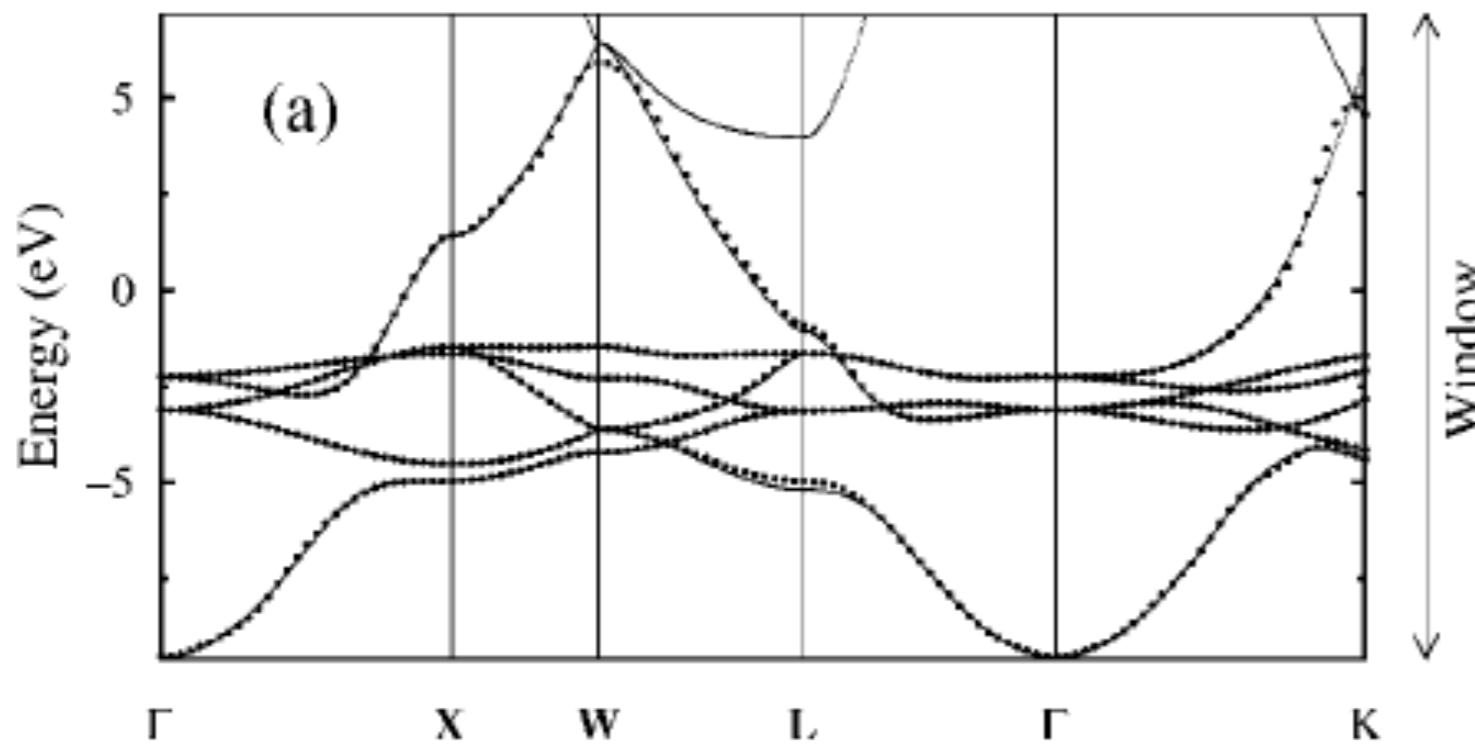
$$\langle r^2 \rangle_n = \langle w_{n\mathbf{0}} | r^2 | w_{n\mathbf{0}} \rangle$$

# 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)**





PHYSICAL REVIEW B 87, 235109 (2013)

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

R. Sakuma

*Division of Mathematical Physics, Lund University, Sölvegatan 14A, 223 62 Lund, Sweden*

(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)

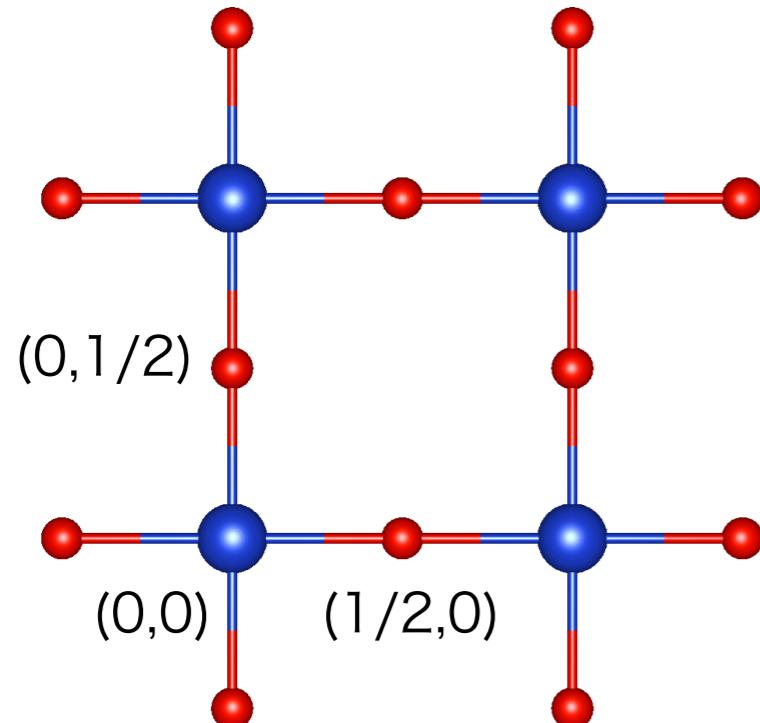
available in Wannier90 (from version 3)

# Site-symmetry group

A subgroup of full-symmetry group, whose elements leave the site-position unchanged

## Example: two-dimensional square lattice

Full symmetry group : 8 symmetry operations (sym. ops.)



### Wyckoff position $(0,0)$ :

Site-symmetry group : 8 sym. ops.  
Multiplicity : 1

### Wyckoff position $(1/2,0), (0,1/2)$ :

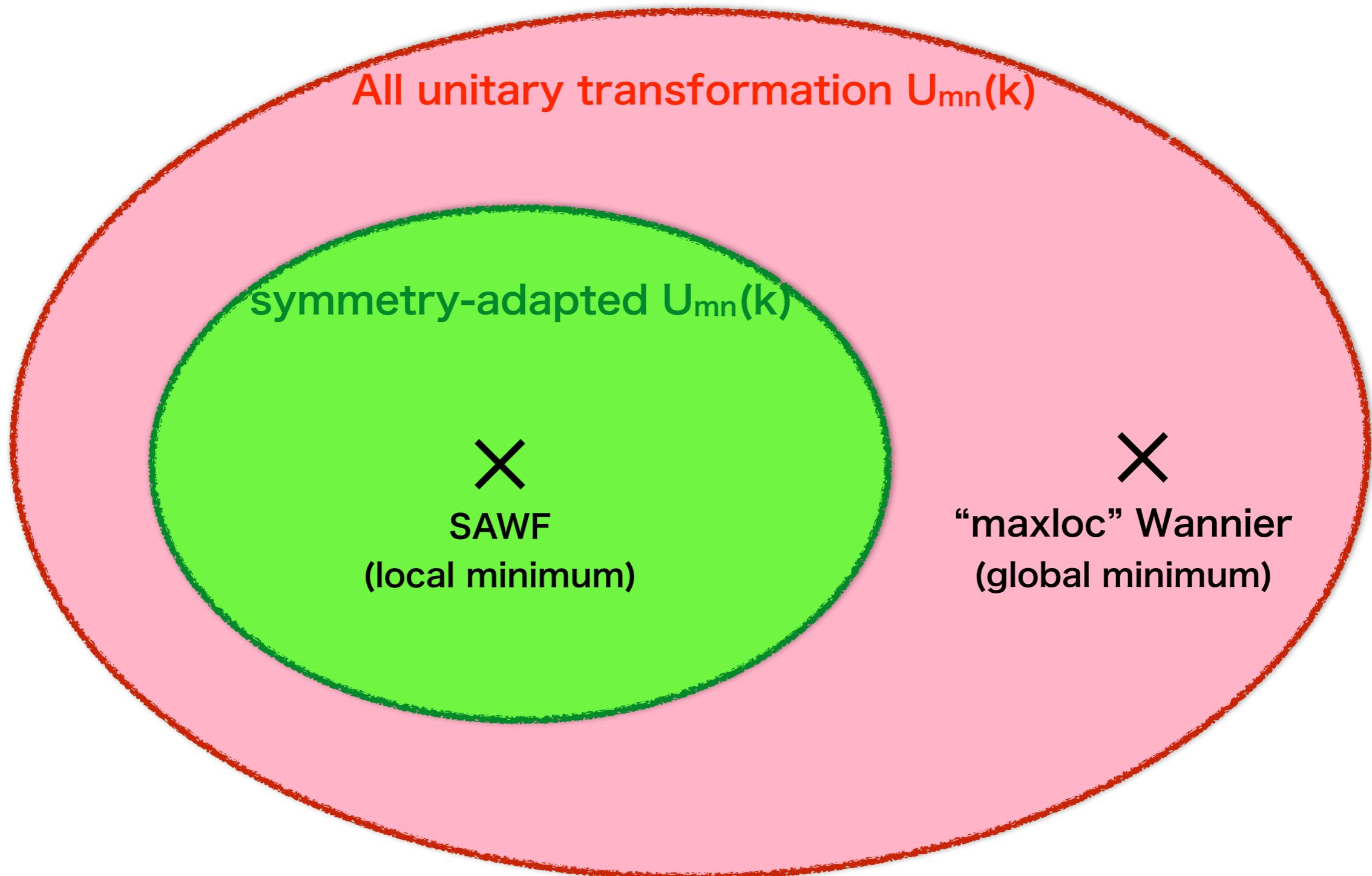
Site-symmetry group : 4 sym. ops. (without  $C_4$ )  
Multiplicity : 2

$$\text{Multiplicity} = (\# \text{ full sym. ops.}) / (\# \text{ sym. ops. in site-symmetry group})$$

# Concept of Symmetry-adapted Wannier functions (SAWF)

SAWF = “maxloc” procedure + **symmetry constraint**

→ obtain irreducible representations of site-symmetry group



# Symmetry-adapted Wannier functions

Rei 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

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

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

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

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

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

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

$D(g, \mathbf{k})$  num\_wannxnum\_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.

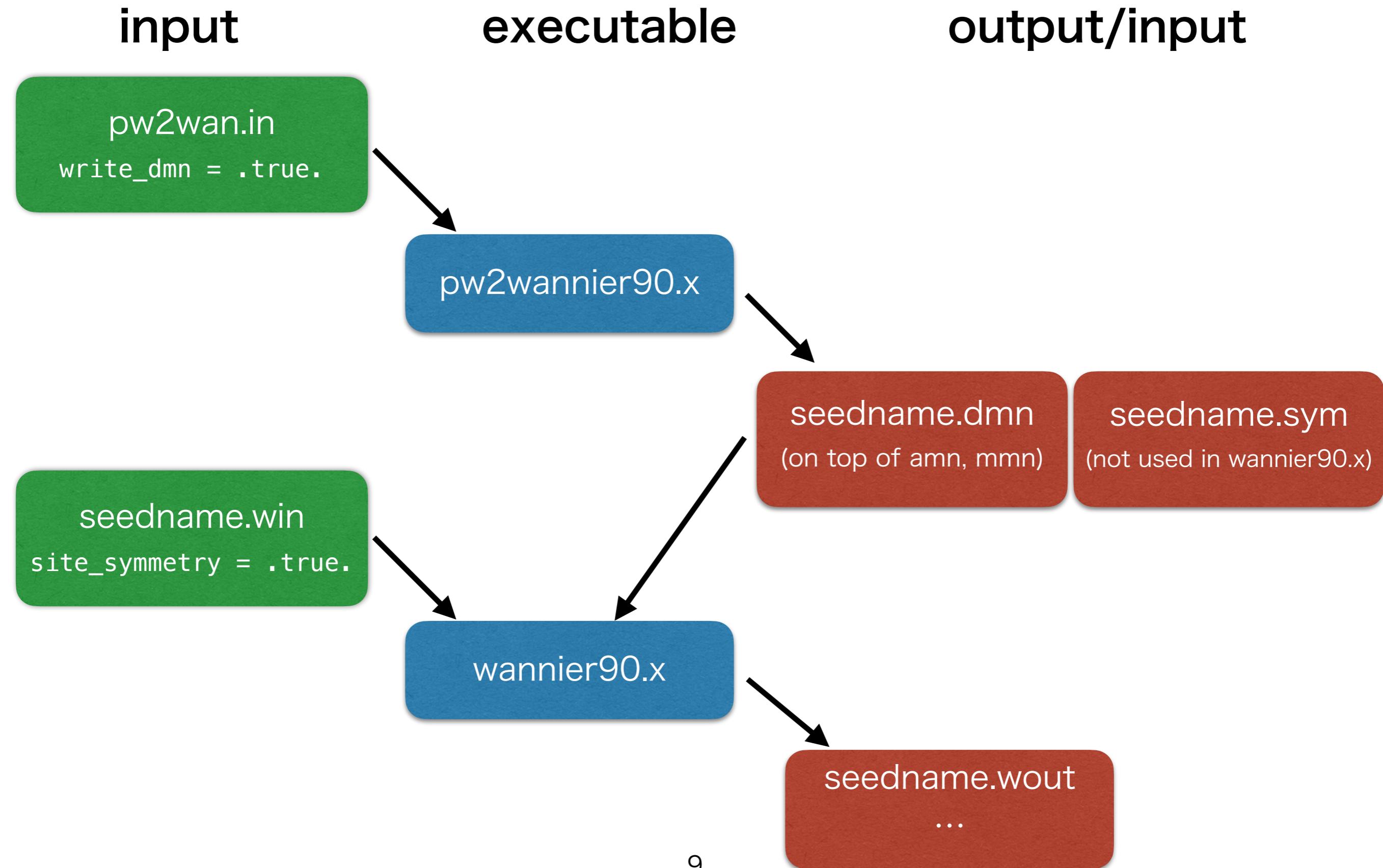
$\tilde{d}(g_{\mathbf{k}}, \mathbf{k})$  num\_bandsxnum\_bands matrix

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

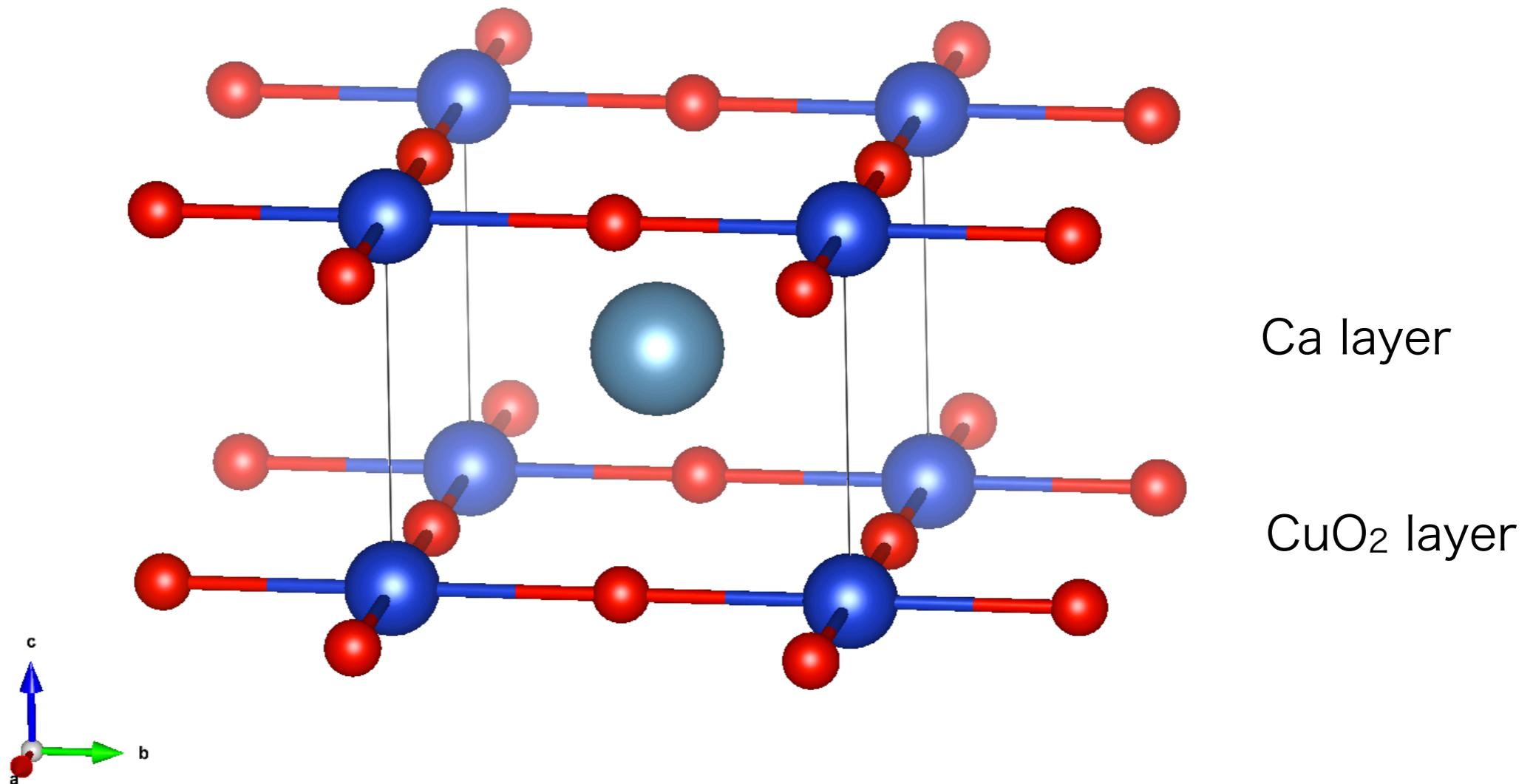
Transformation of Kohn-Sham Bloch functions by sym. ops.

written in **seedname.dmn** file

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

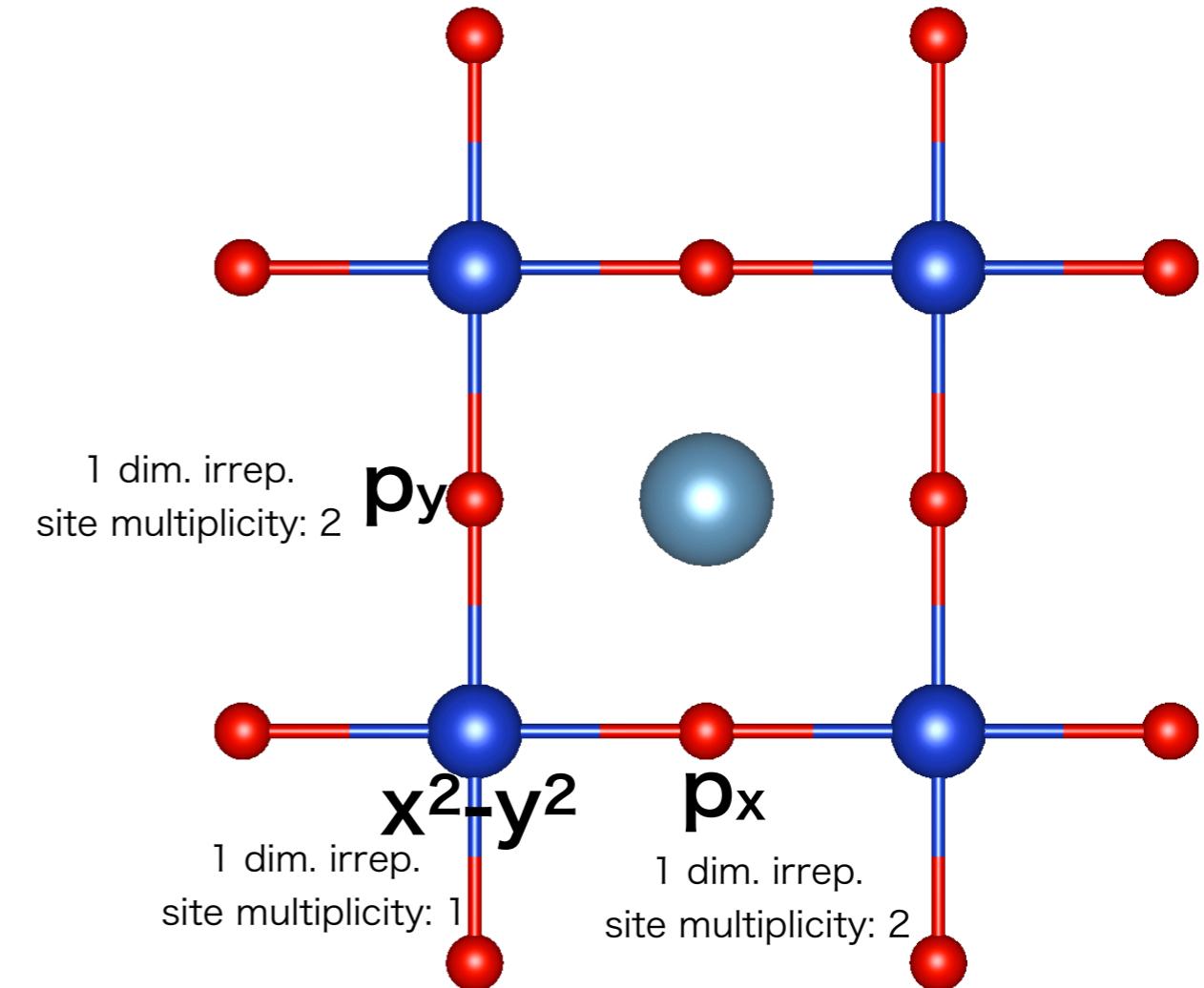
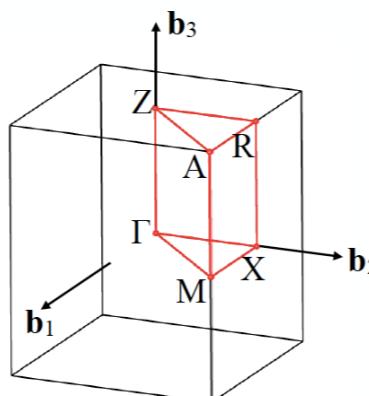
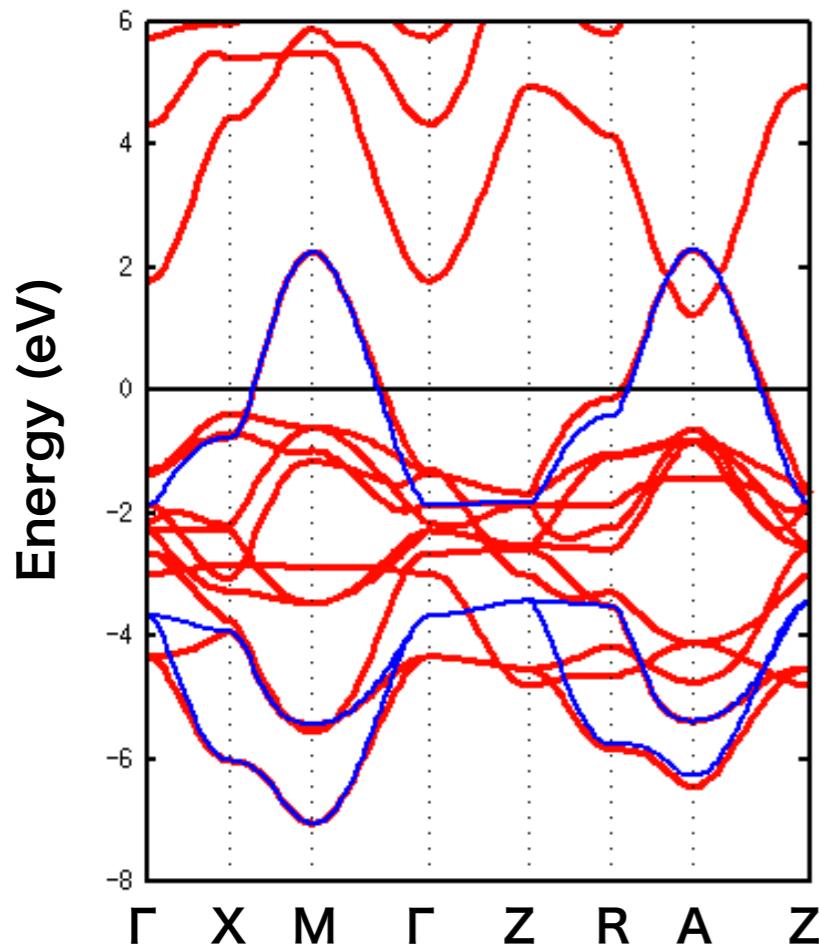


# Example of $D_{mn}$ : CaCuO<sub>2</sub> d-p model



- 📍 Famous family of high-Tc 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.

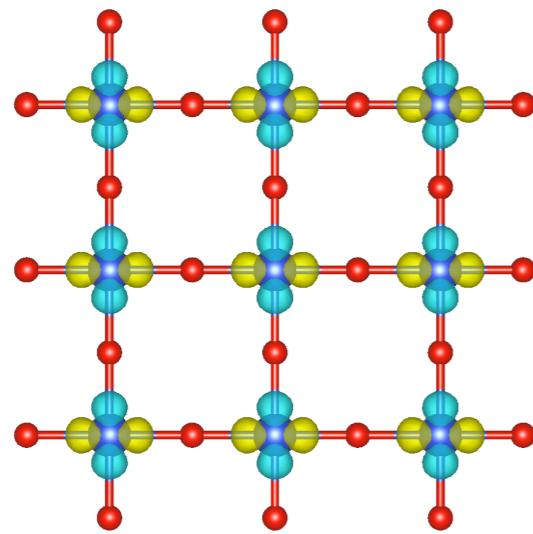
(We do not discuss  $\tilde{d}$  matrix because the global phase of KS wave function can be random)

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

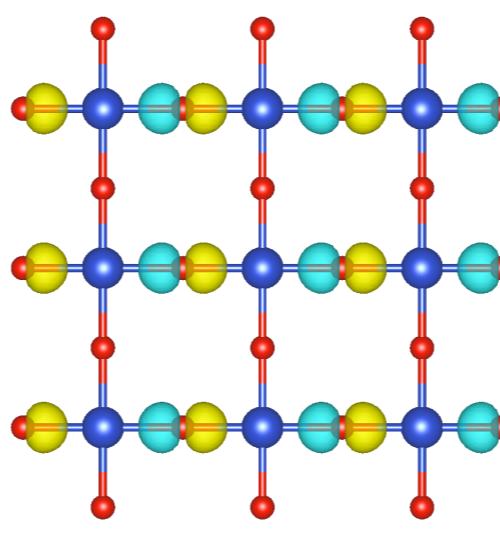
$$\hat{R}_{\pi/2} \Psi_{\Gamma n}(\mathbf{r}) = \sum_m D_{mn} \Psi_{\Gamma m}(\mathbf{r})$$

Wannier-gauge Bloch at  $\Gamma$

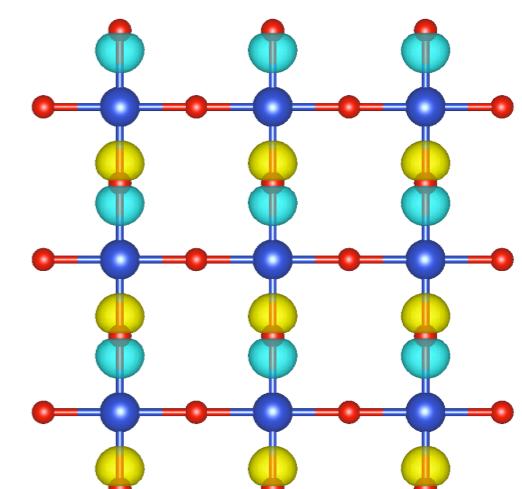
$$\Psi_{\Gamma, x^2-y^2, (0,0,0)}$$



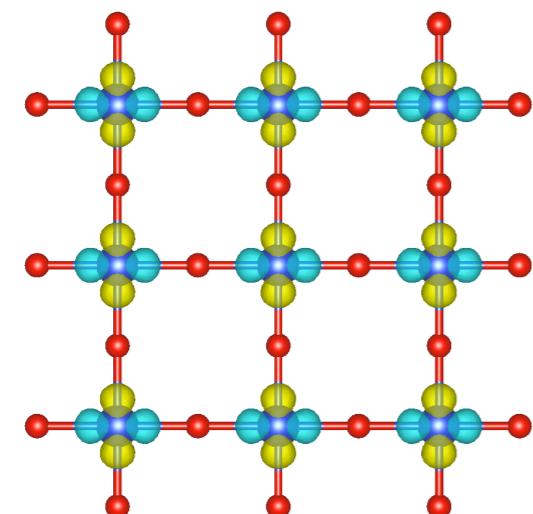
$$\Psi_{\Gamma, p_x, (1/2,0,0)}$$



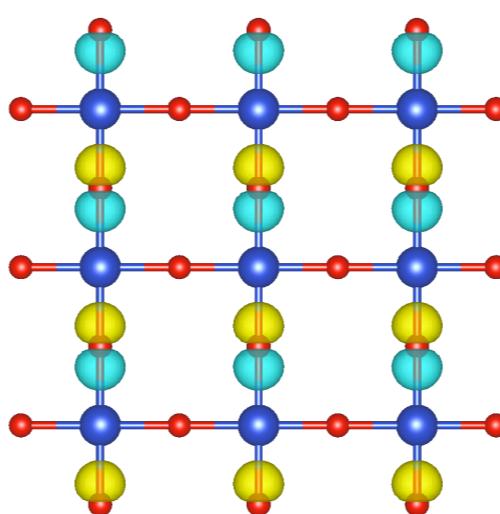
$$\Psi_{\Gamma, p_y, (0,1/2,0)}$$



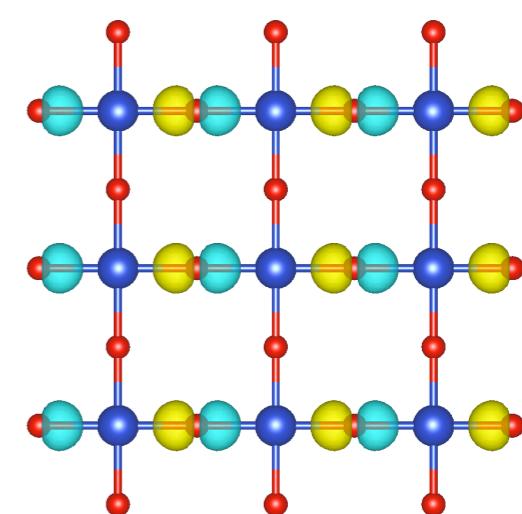
after  $90^\circ$  rotation



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



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

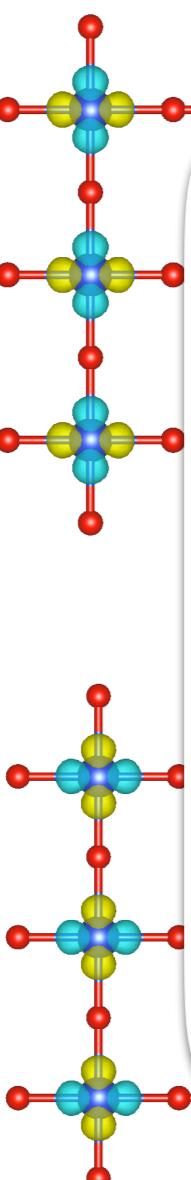


$$\rightarrow (-1) \Psi_{\Gamma, p_x, (1/2,0,0)}$$

# 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



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

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

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

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

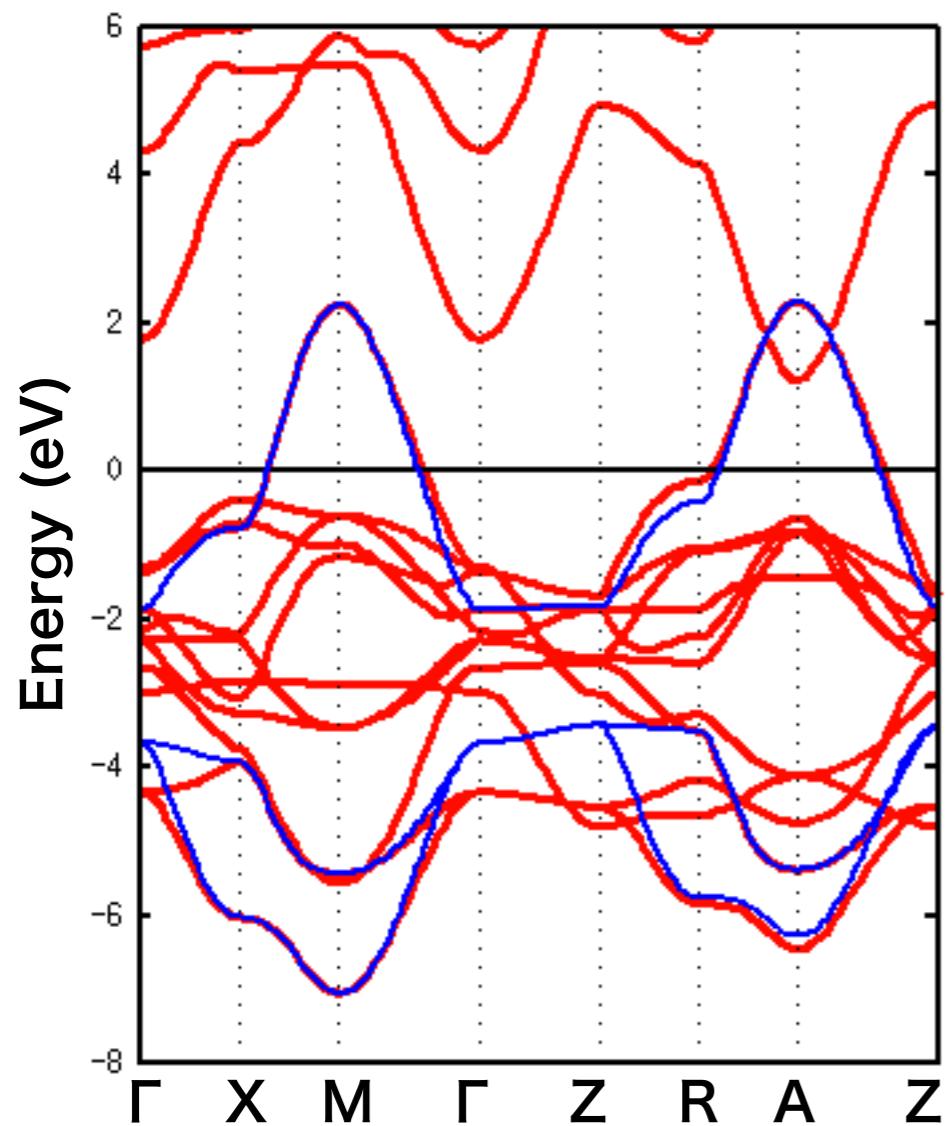
Block diagonal for each irrep.  
(block size: dimension of irrep  $\times$  site multiplicity)

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

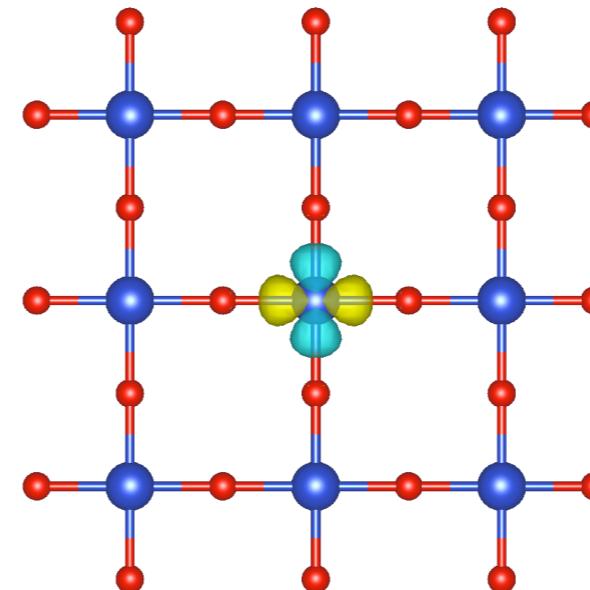
$\rightarrow \Psi_{\Gamma, p_y, (0,1/2,0)}$

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

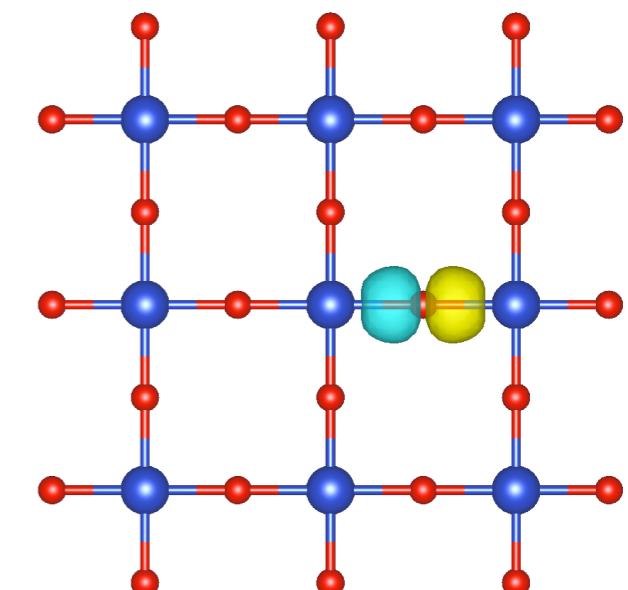
# SAWFs : CaCuO<sub>2</sub> d-p model



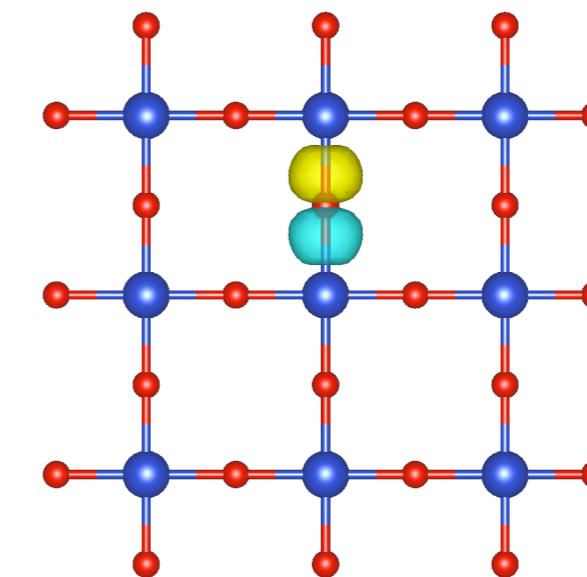
$x^2-y^2$



$p_x$



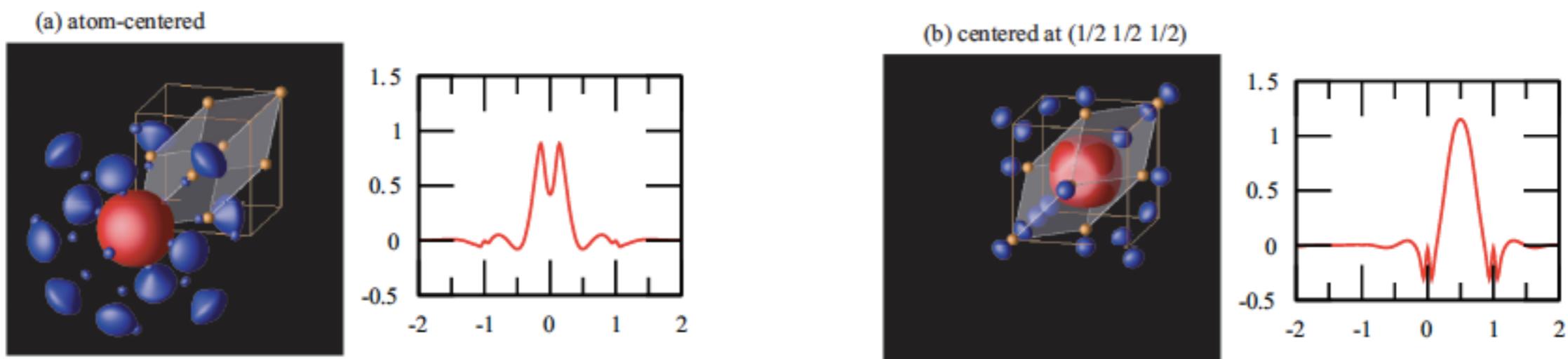
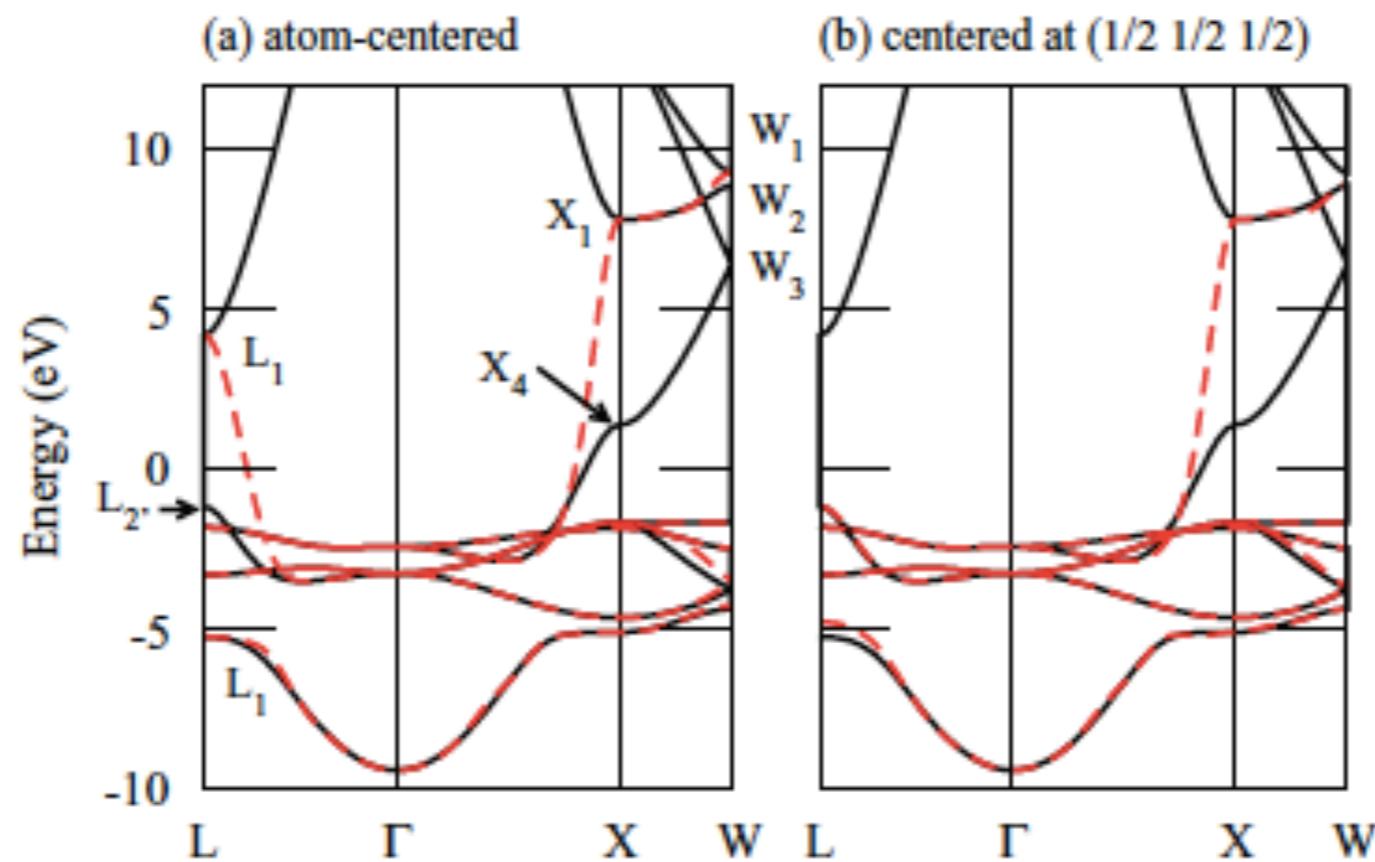
$p_y$



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

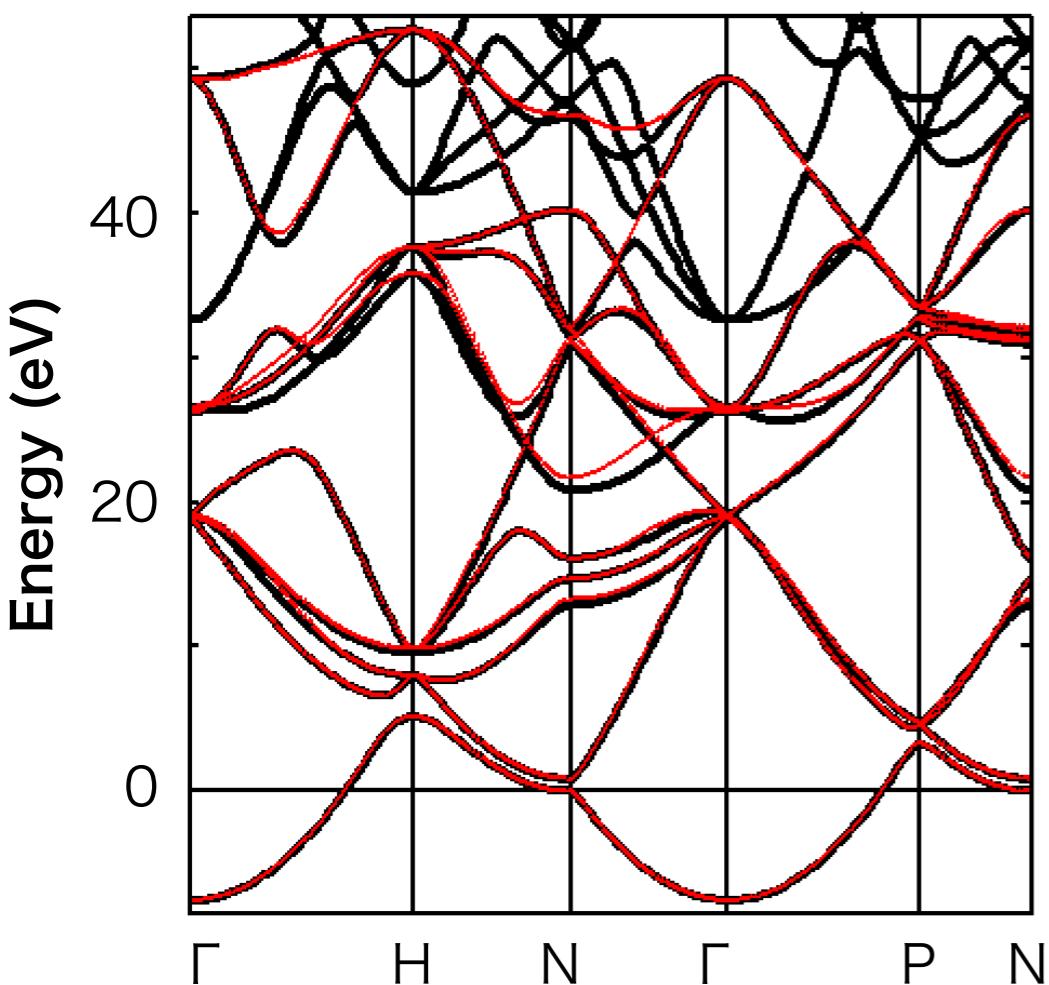
# SAWFs : Copper

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

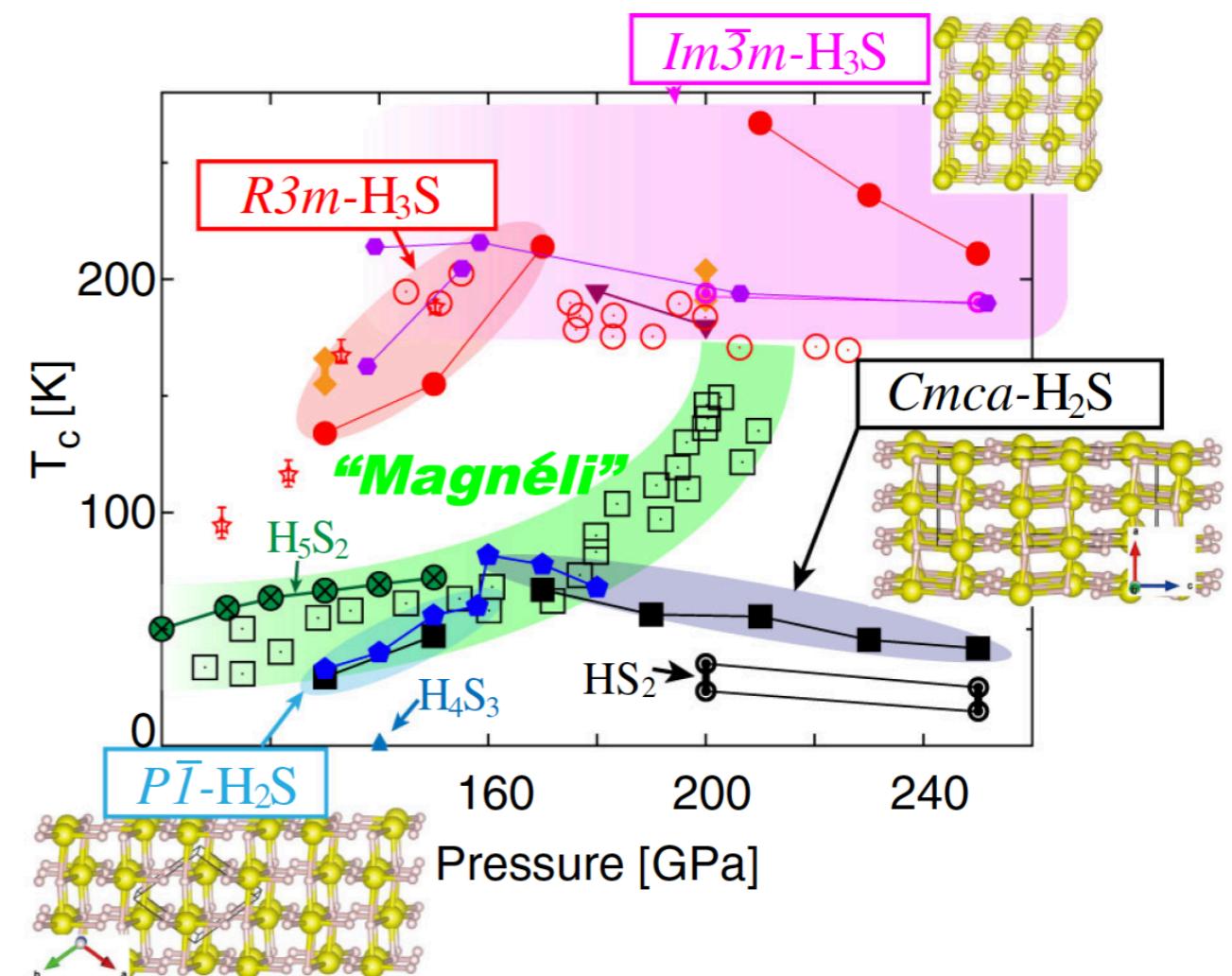


# Applications to H<sub>3</sub>S ①

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

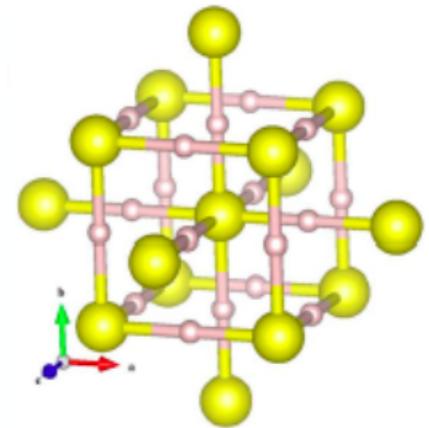


bcc, 48 sym. ops.



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

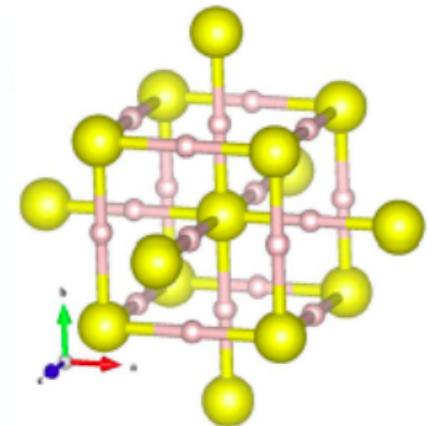
## Maximally localized Wannier functions

### 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

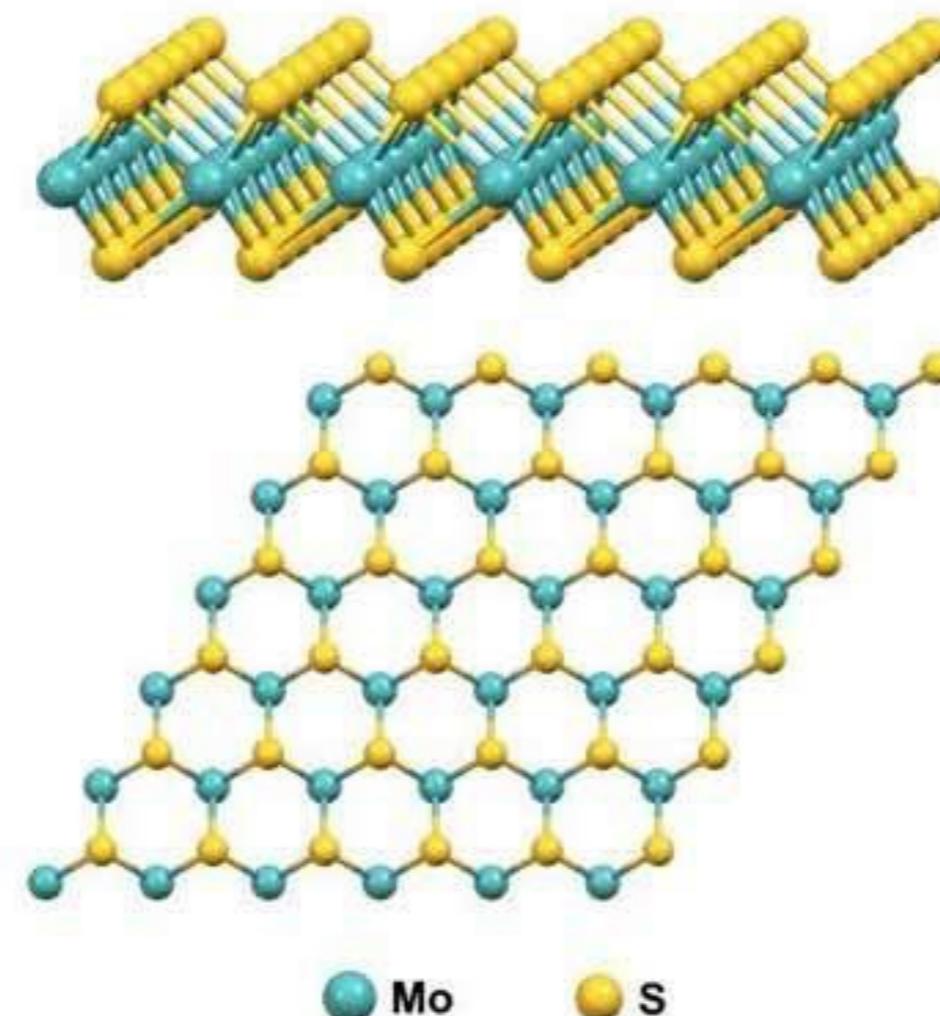
- s\_at\_0.00
- s\_at\_0.25
- s\_at\_0.50

Please try symmetry-adapted mode !

Be careful ...

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

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

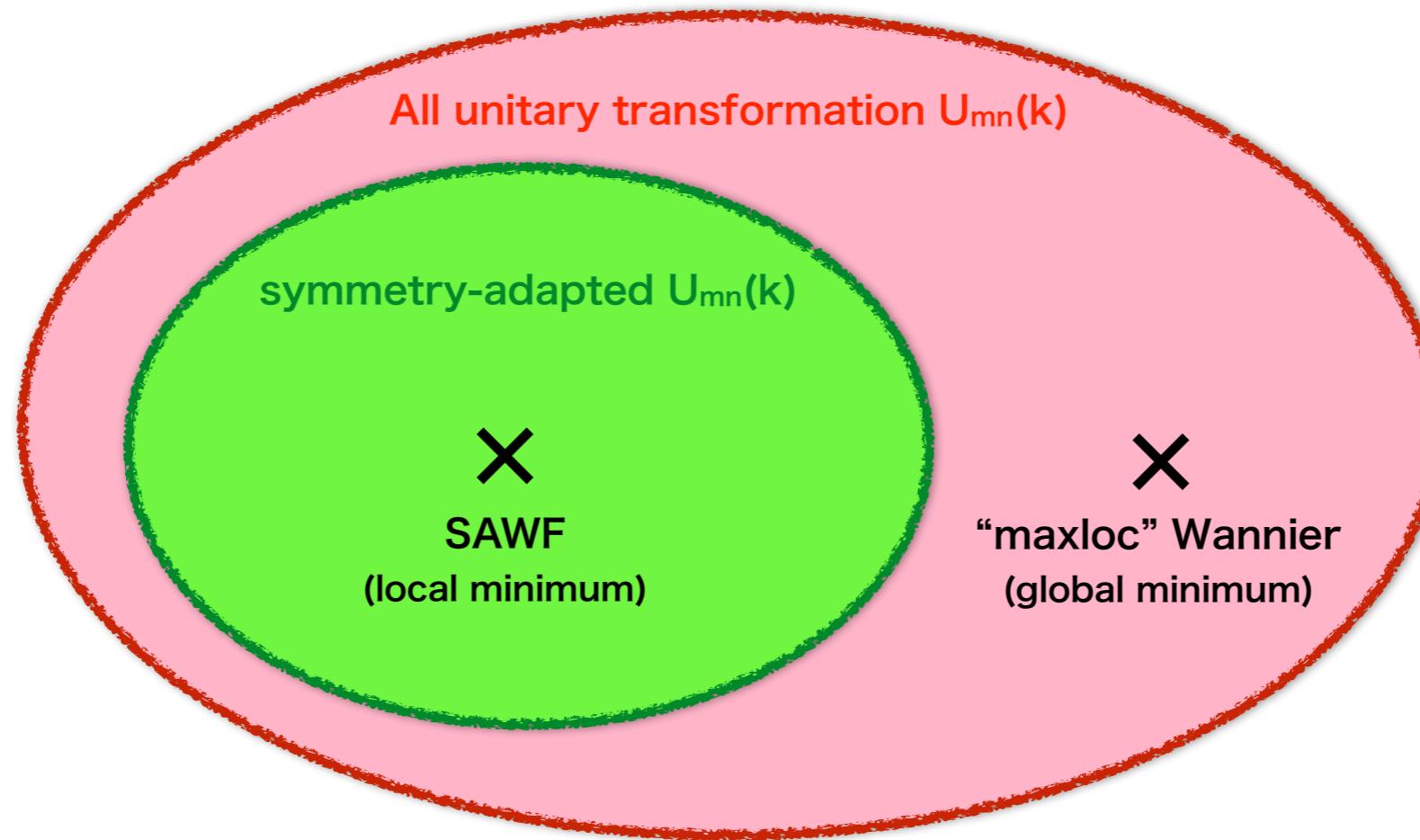


sulphur p orbitals cannot be exactly atom-centered

# Summary and future perspective

## Summary

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



## Future perspective

- 💡 Frozen window (need to be compatible with symmetry-adapted mode)  
→ developer's meeting (Takashi Koretsune)
- 💡 Extension to noncolliner case

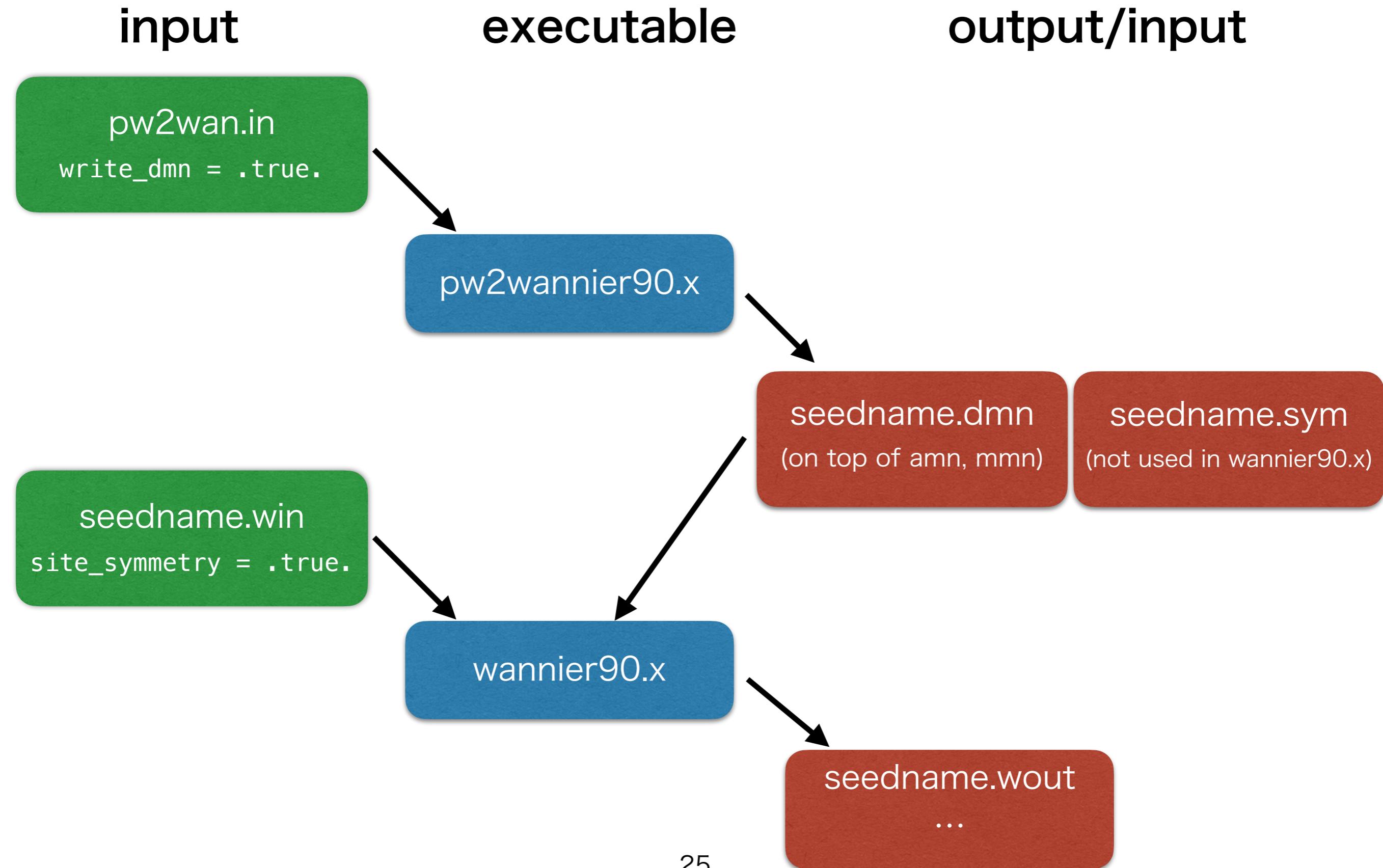


# Tutorials

# Instructions

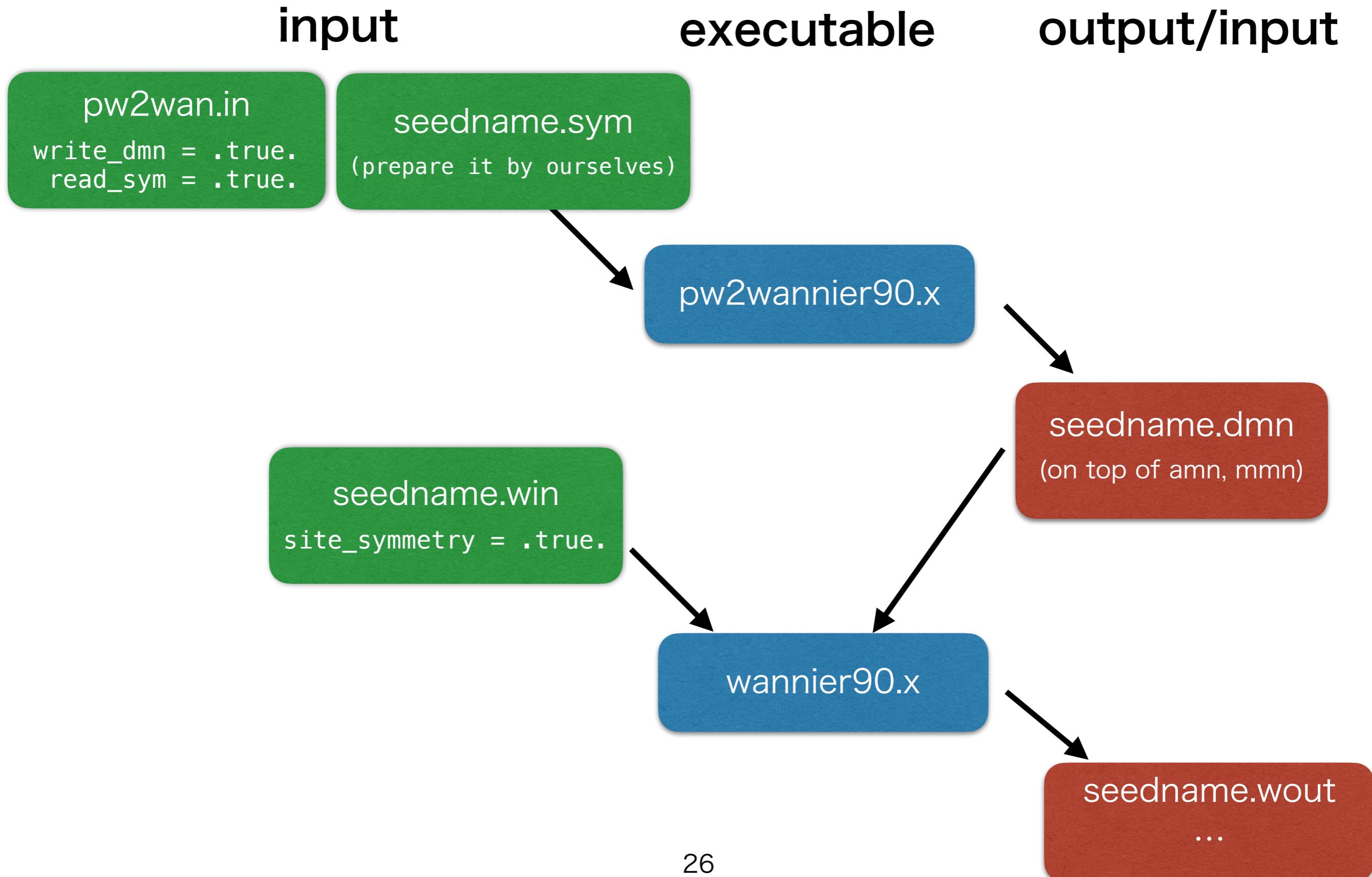
- Tutorials can be found in “Tutorials\_SAWF”
- Basic tutorial: “GaAs”
- (A little bit) advanced tutorials: “Cu” and “H3S”
- Work flow “GaAs” → “Cu” and “H3S”
- Follow the instruction pdf file or README in each directory
- For “GaAs” and “Cu”, refer also to Wannier90 Tutorials and Tutorial Solutions

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



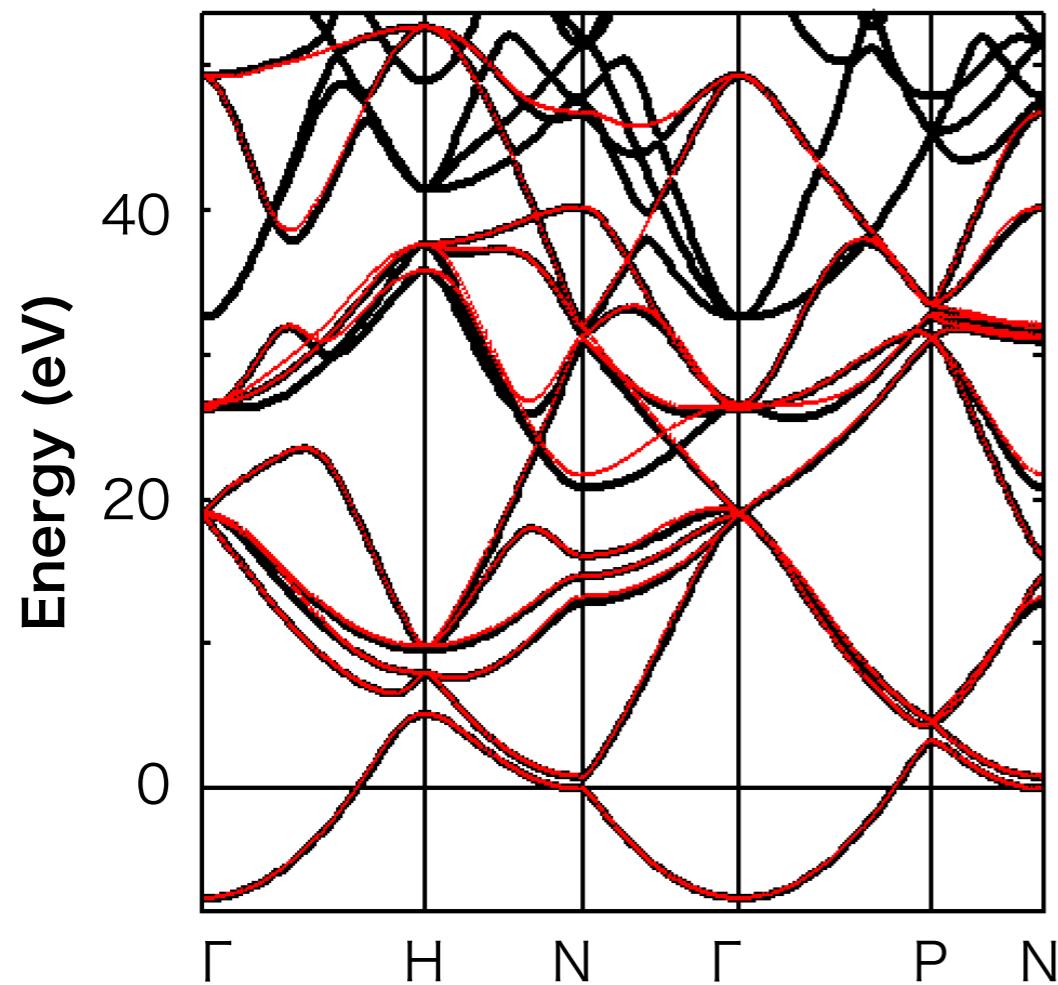
# Flow of calculation in Cu tutorial : advanced usage

(after nscf calculations and creating .nnkp file)



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

12 band model



7 band model

