26 March, 2020
Wannier90 School

Symmetry-adapted Wannier functions
lecture and tutorials

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If you have questions, please put them in chat !
Mute your audio and unmute it when necessary

Maximally localized Wannier functions

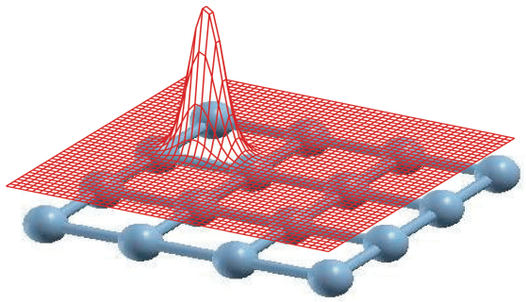
N. Marzari and D. Vanderbilt, Phys. Rev. B. 56 12847 (1997)
I. Souza et al., ibid. 65, 035109 (2001)

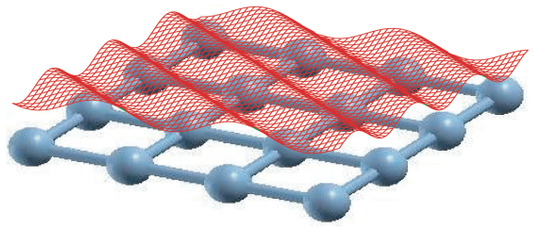
$$|w_{n\mathbf{R}}\rangle = a^{\dagger}_{n\mathbf{R}}|0\rangle$$

Wannier State

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

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 Ω

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

where,

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

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

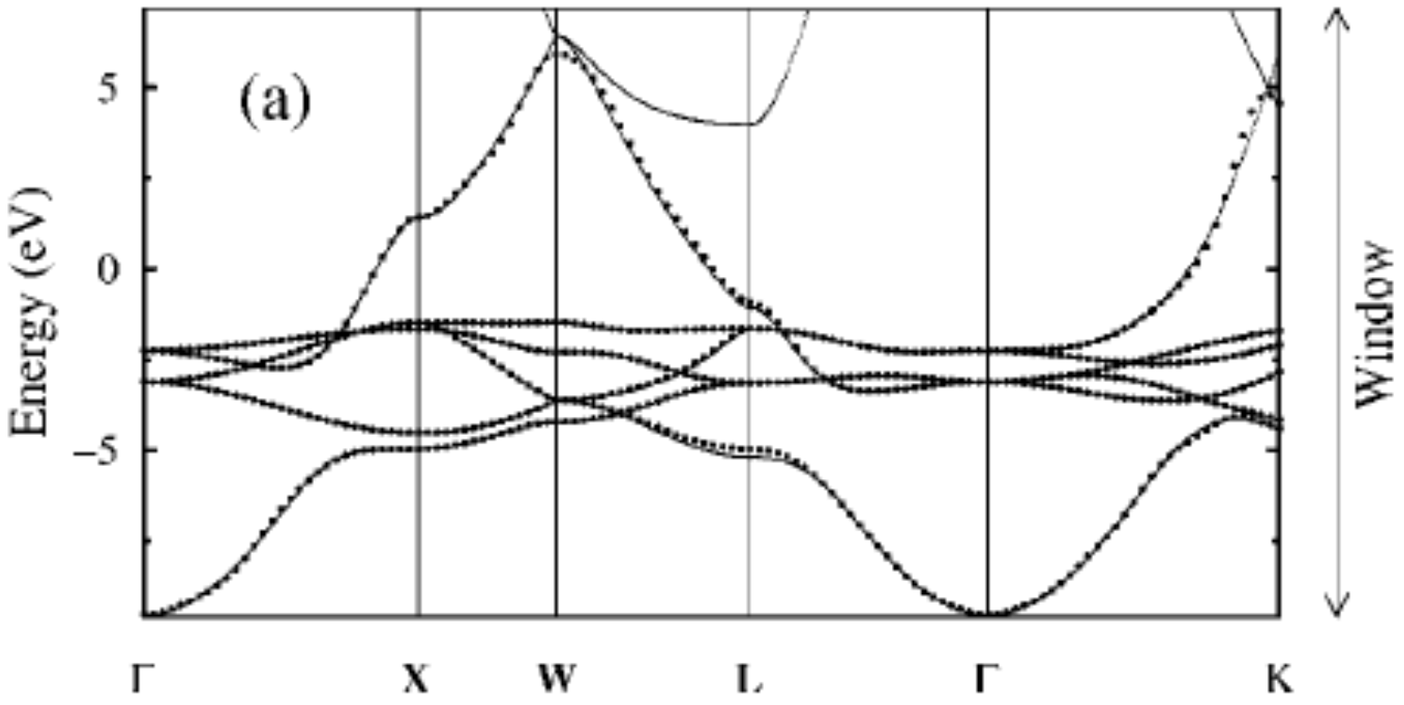
Symmetry breaking of “maxloc" Wannier functions : Copper

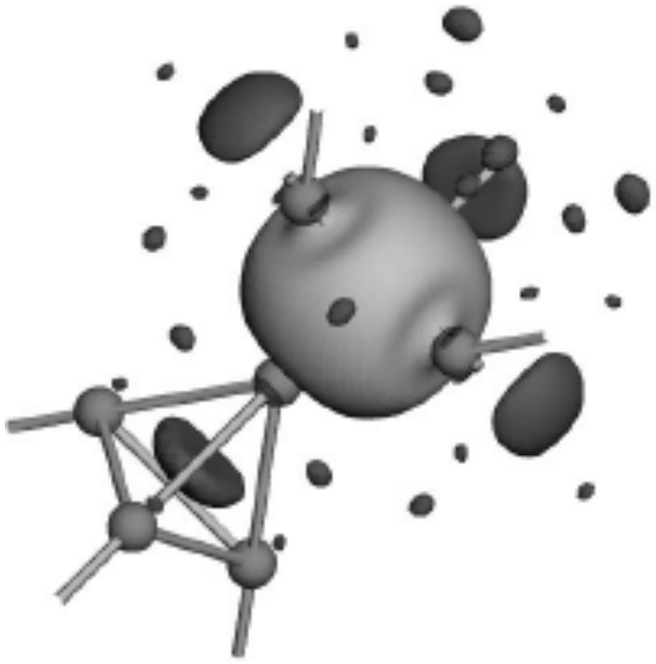
I. Souza et al., Phys. Rev. B 65 035109 (2001)

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)





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 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

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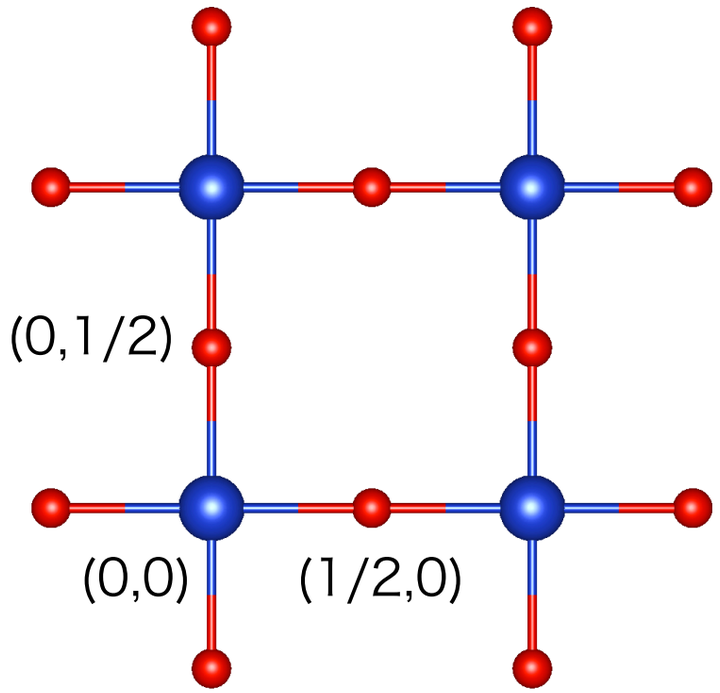
Site-symmetry group

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)

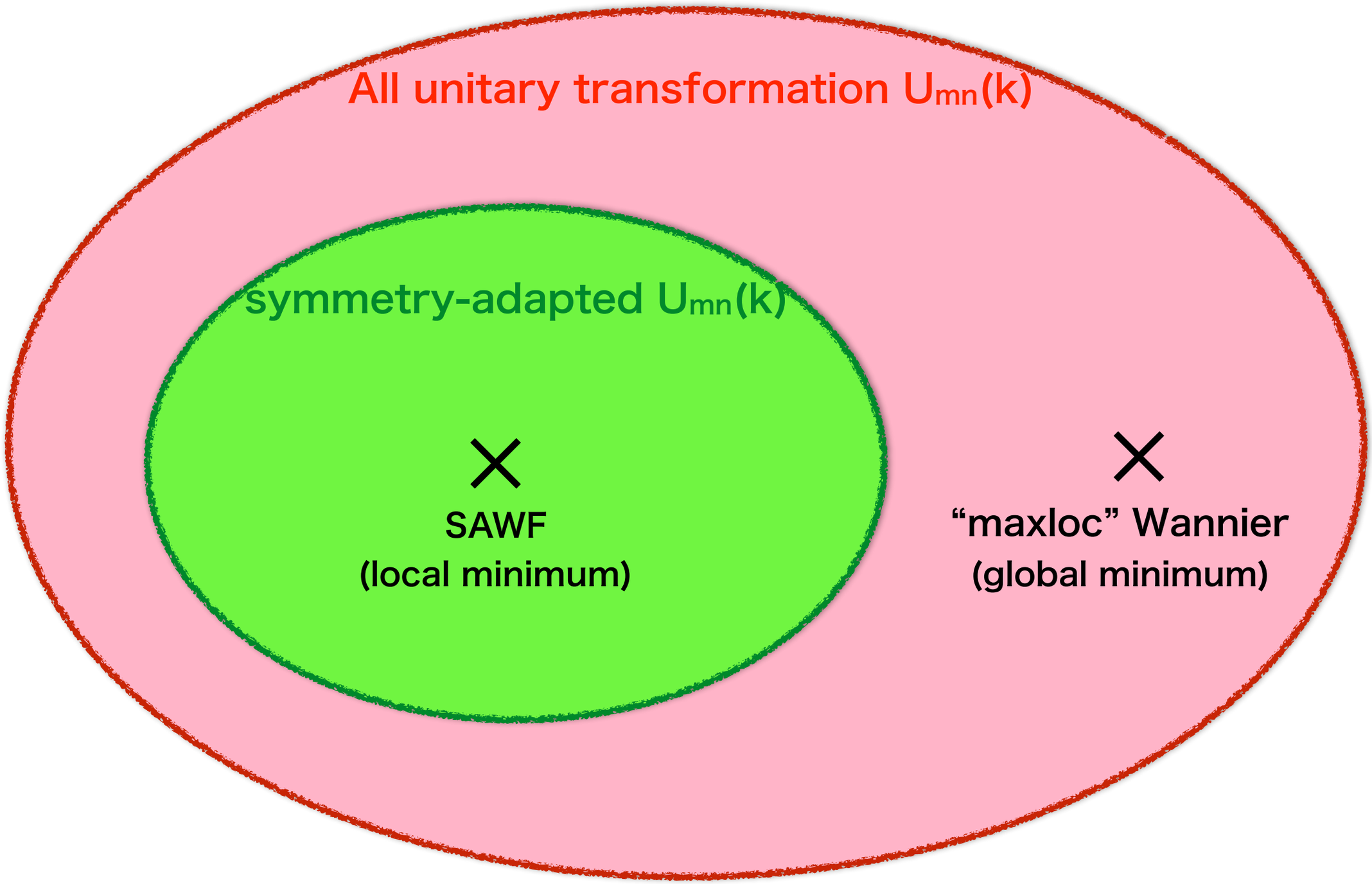
Multiplicity : 2

Multiplicity = (# full sym. ops.)/(# 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)

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

- Constraint on U(**k**) for **k** in irreducible BZ

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

matrices related to symmetry

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

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

- Unitary matrix for other **k** points

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

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**

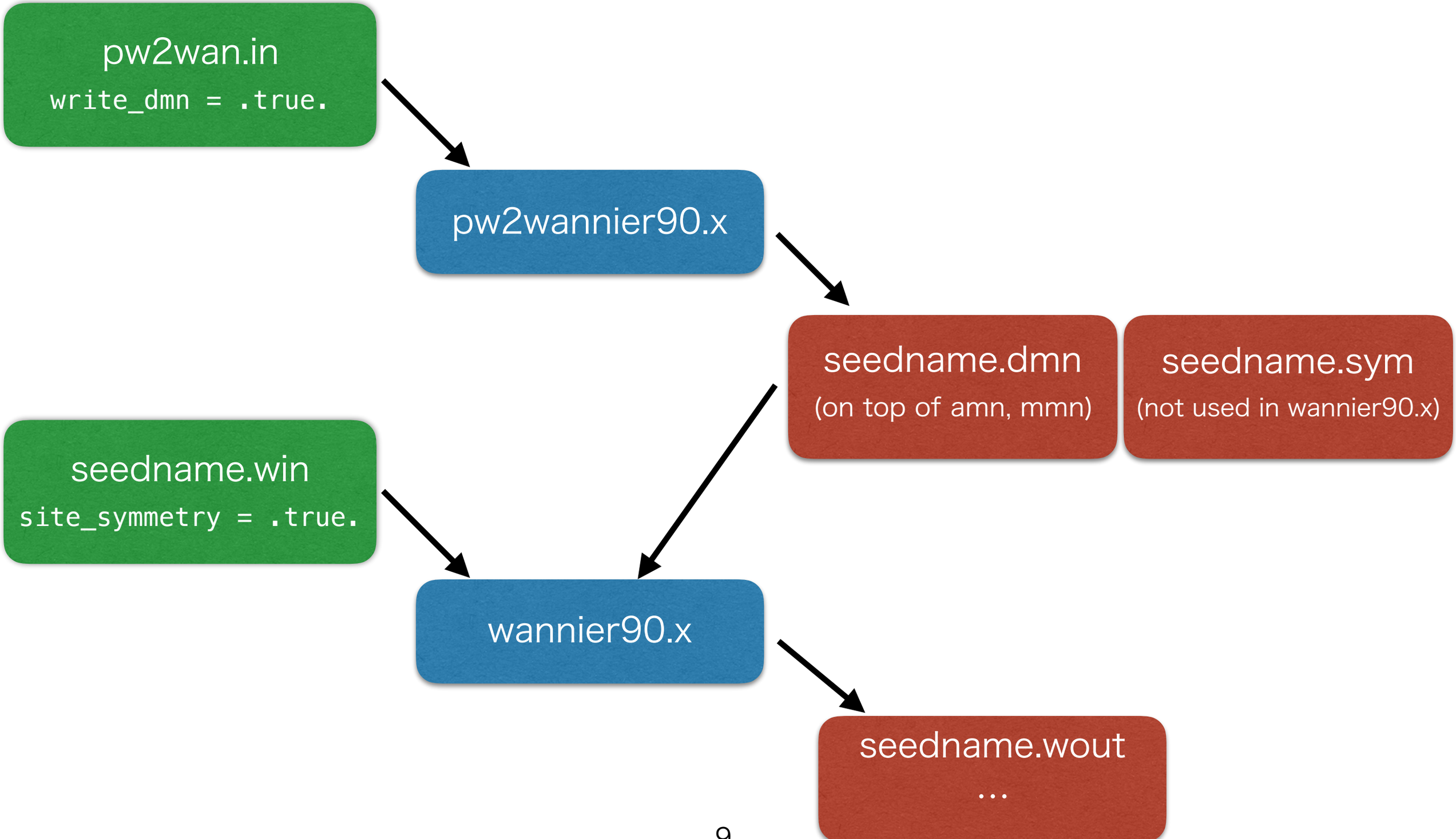
$$\hat{g}\psi^{\mathrm{KS}}_{\mathbf{k}\mu}(\mathbf{r}) = \sum_{\mu'} \tilde{d}_{\mu'\mu}(g,\mathbf{k})\psi^{\mathrm{KS}}_{R\mathbf{k}\mu'}(\mathbf{r})$$

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

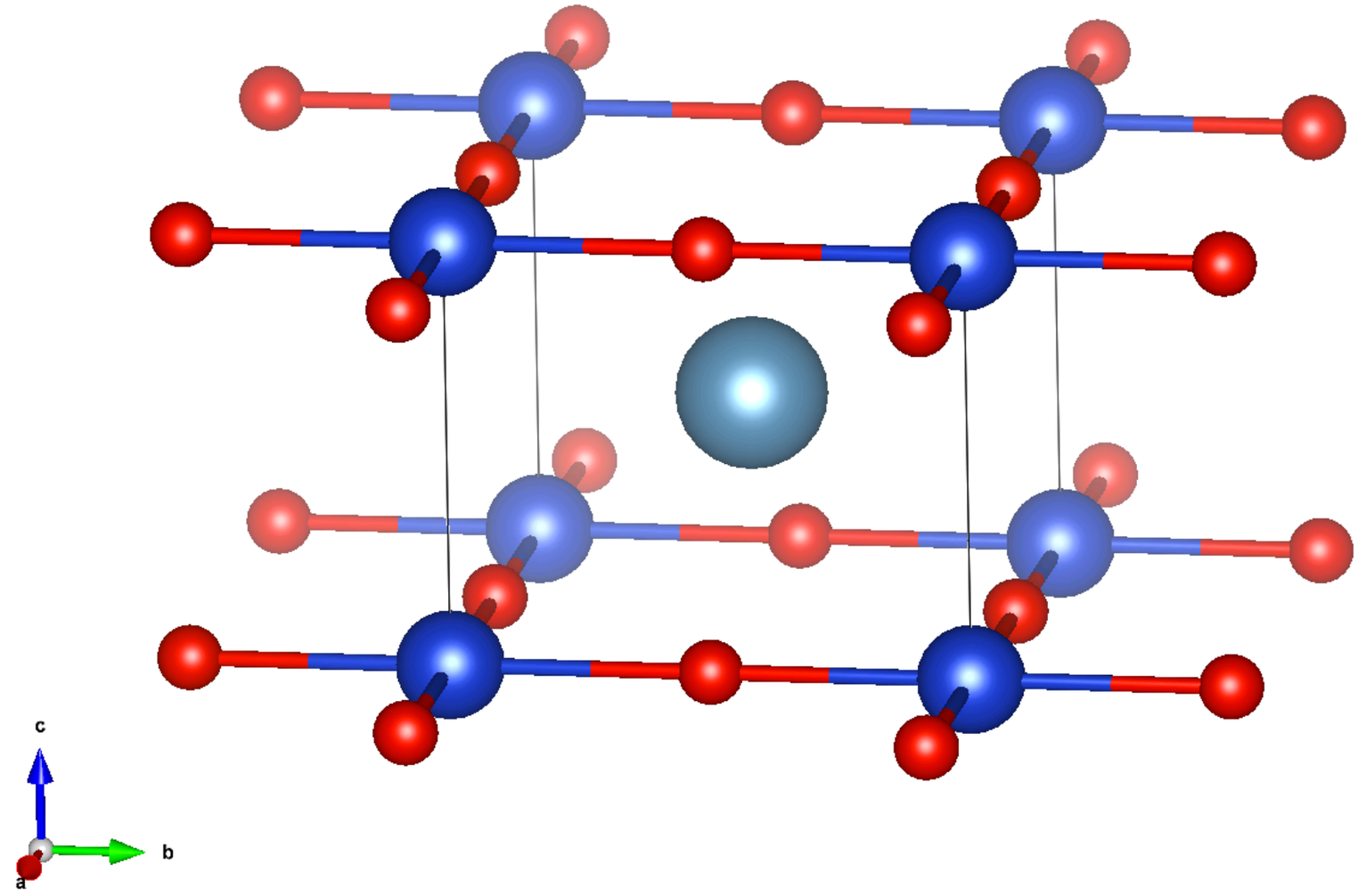
written in seedname.dmn file

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

input **executable** **output/input**



Example of D_{mn} : $CaCuO_2$ d-p model

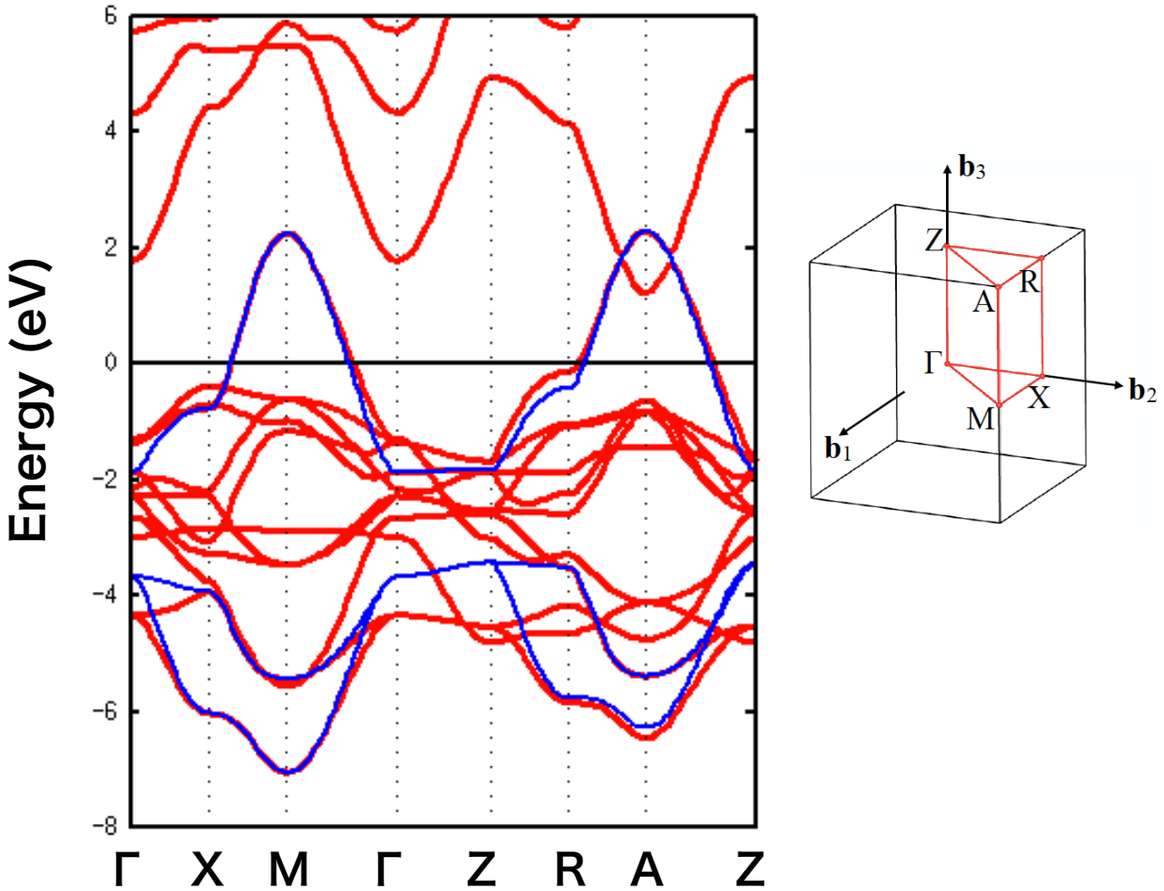


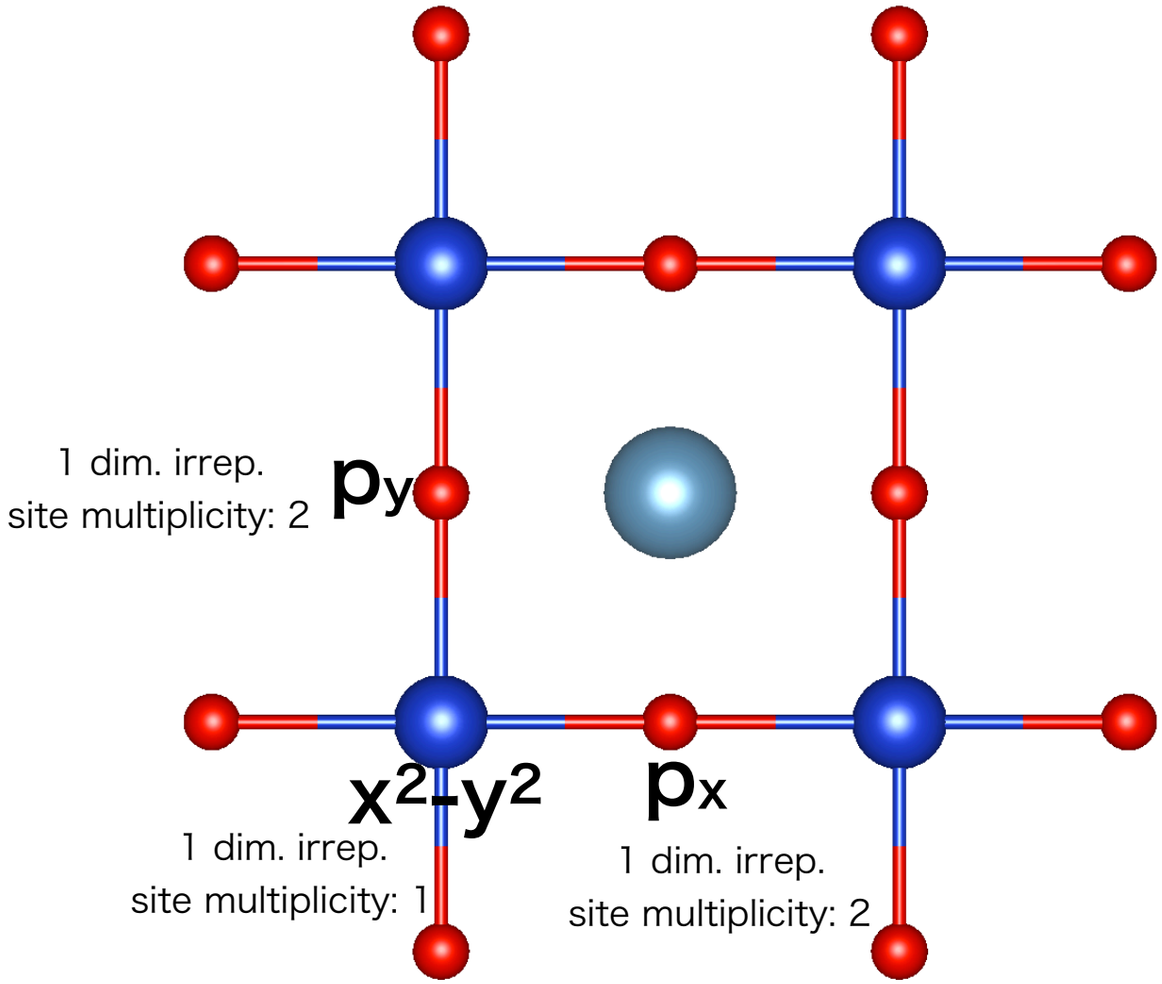
Ca layer

CuO_2 layer

- Famous family of high-Tc cuprates
- Quasi-2D (layered) material
- 16 symmetry operations (P4/mmm)

Example of D_{mn} : $CaCuO_2$ 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)

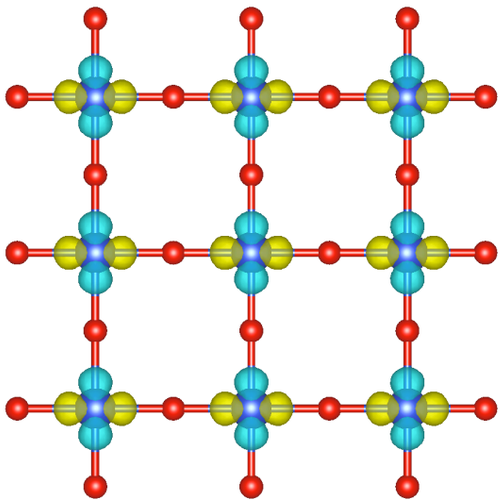
$$\hat{g}\psi^{\mathrm{KS}}_{\mathbf{k}\mu}(\mathbf{r}) = \sum_{\mu'} \tilde{d}_{\mu'\mu}(g,\mathbf{k})\psi^{\mathrm{KS}}_{R\mathbf{k}\mu'}(\mathbf{r})$$

Example of D_{mn} (90° rotation, Γ): $CaCuO_2$ d-p model

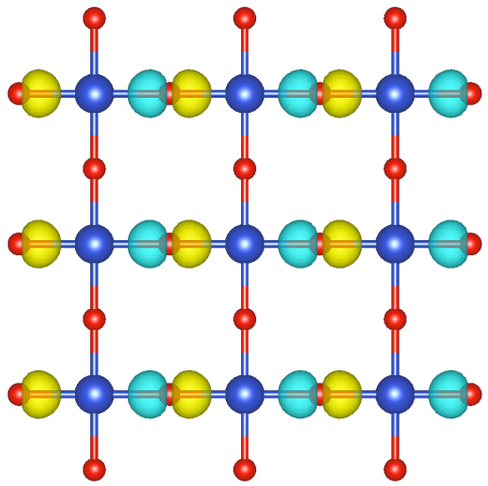
$$\hat{R}_{\pi/2}\Psi_{\Gamma n}(\mathbf{r}) = \sum_m D_{mn}\Psi_{\Gamma m}(\mathbf{r})$$

Wannier-gauge Bloch at Γ

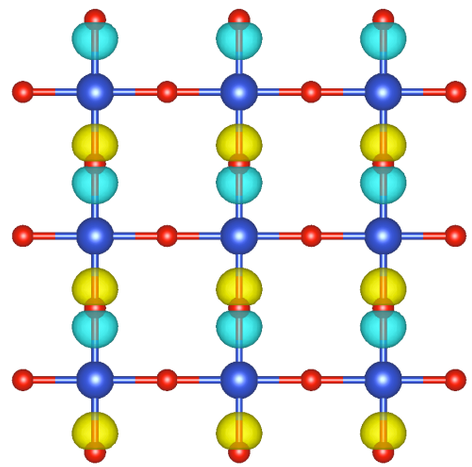
$\Psi_{\Gamma,x^2-y^2,(0,0,0)}$



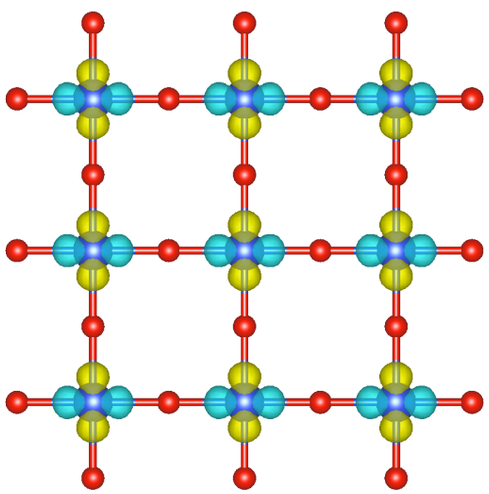
$\Psi_{\Gamma,p_x,(1/2,0,0)}$



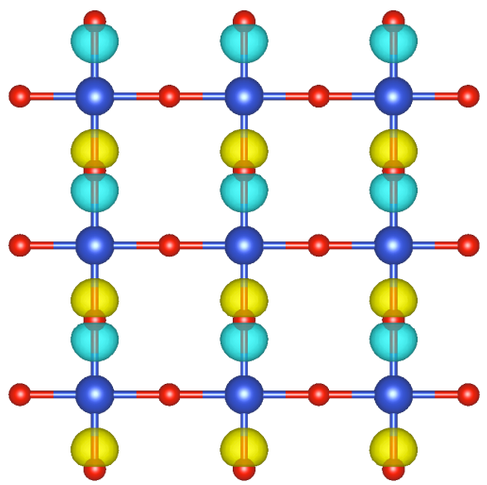
$\Psi_{\Gamma,p_y,(0,1/2,0)}$



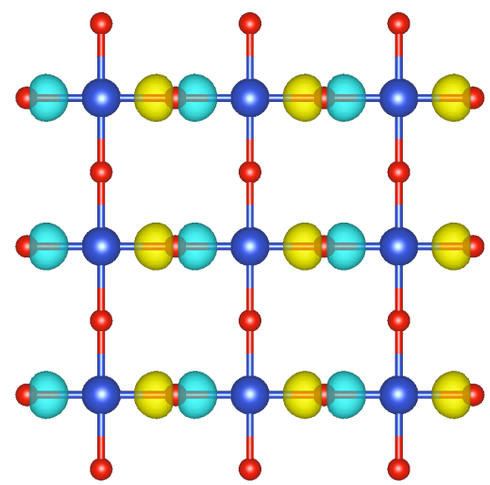
after 90° rotation



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



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



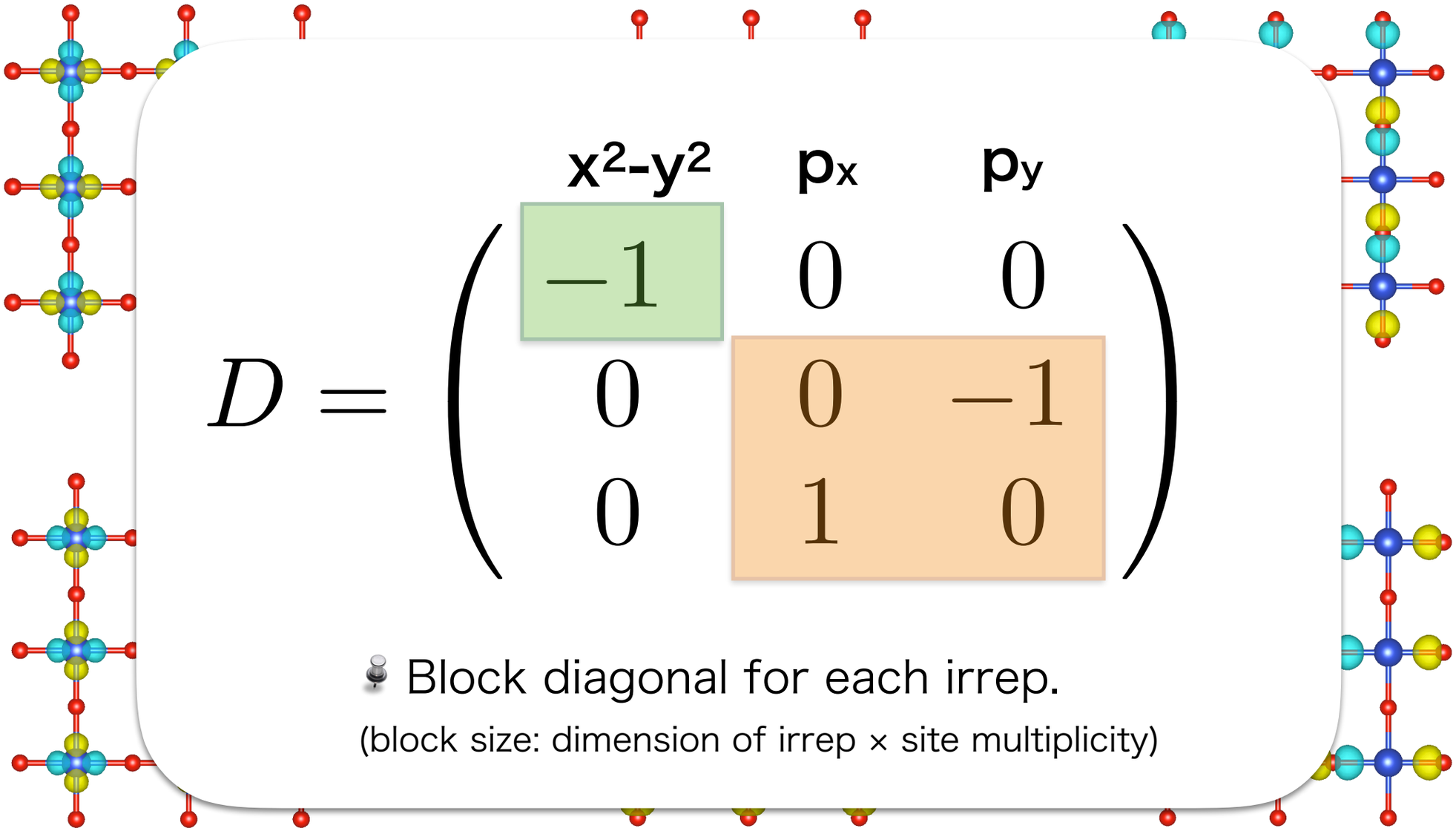
$\rightarrow (-1)\Psi_{\Gamma,p_x,(1/2,0,0)}$

Example of D_{mn} (90° rotation, Γ): $CaCuO_2$ d-p model

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

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

Wannier-gauge Bloch at Γ



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

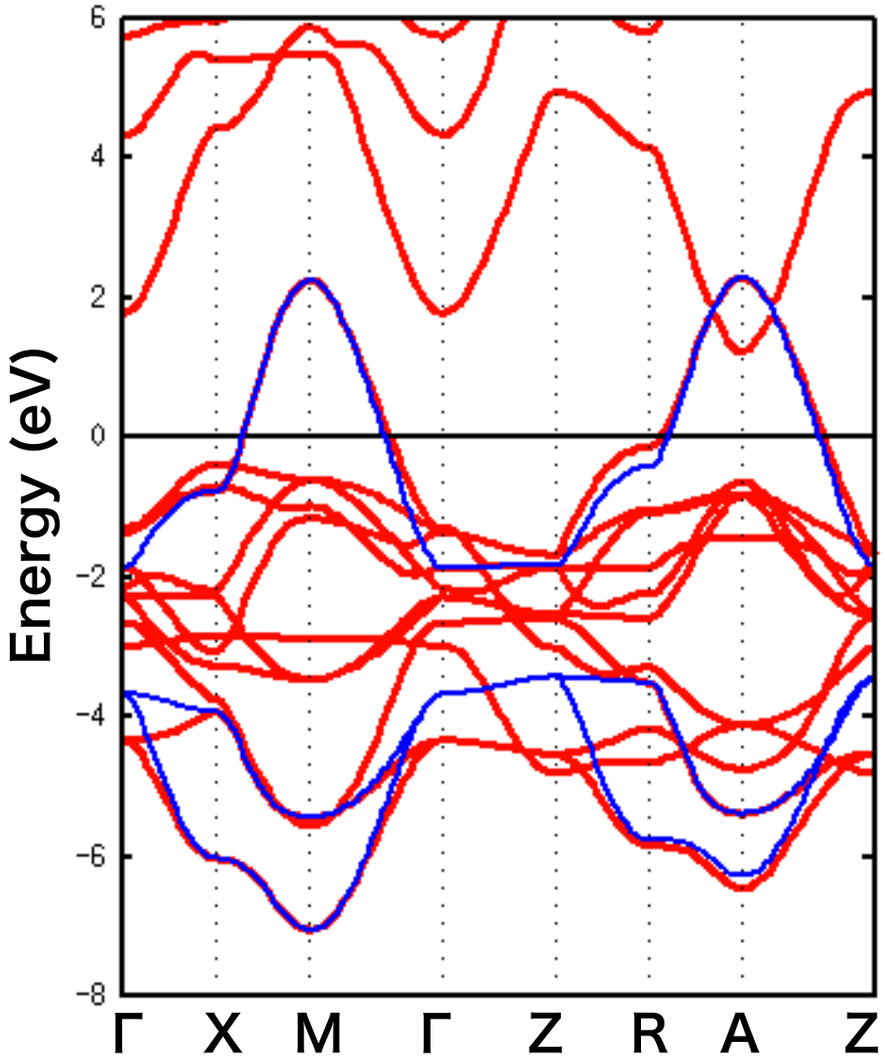
- Block diagonal for each irrep.

(block size: dimension of irrep × site multiplicity)

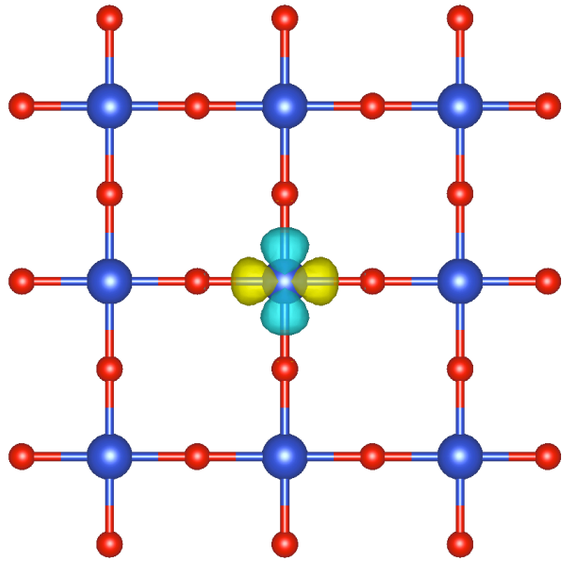
after 90° rotation

→ (-1)$\Psi_{\Gamma,x^2-y^2,(0,0,0)}$ → $\Psi_{\Gamma,p_y,(0,1/2,0)}$ → (-1)$\Psi_{\Gamma,p_x,(1/2,0,0)}$

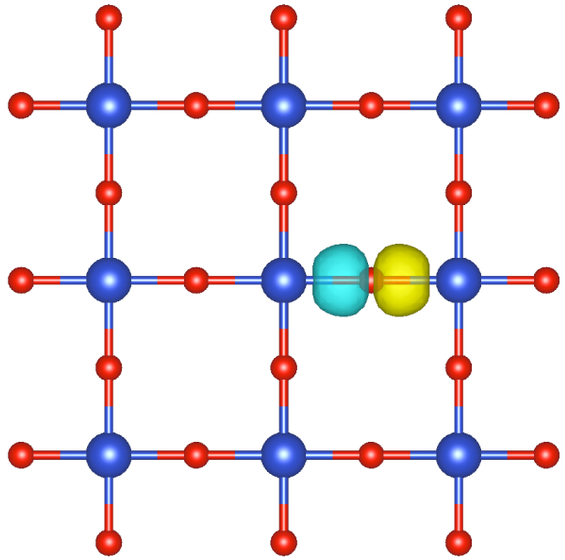
SAWFs : $CaCuO_2$ d-p model



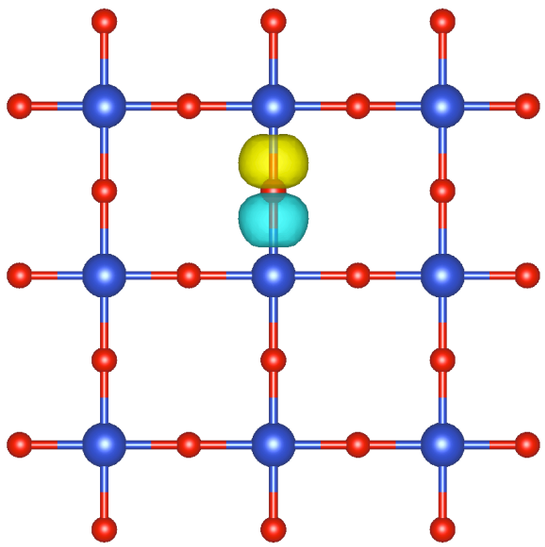
x^2-y^2



p_x



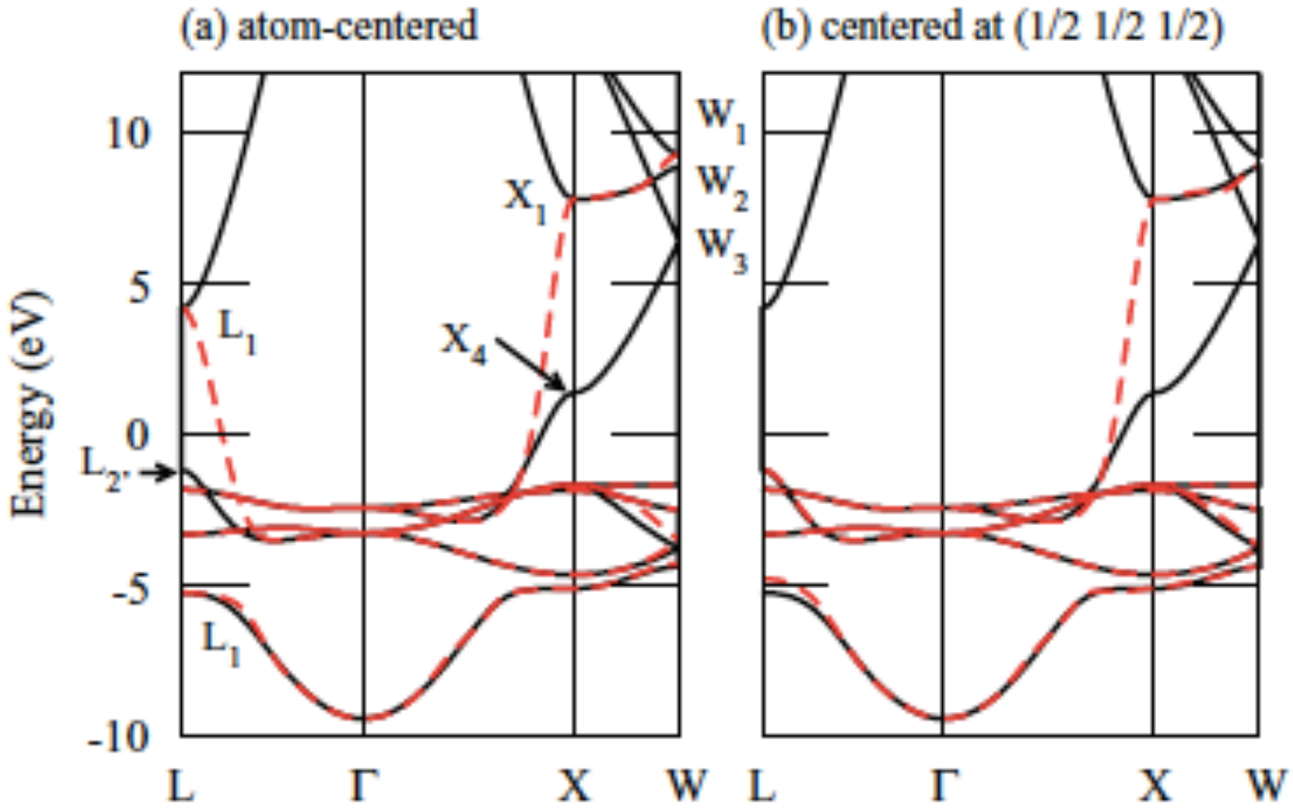
p_y

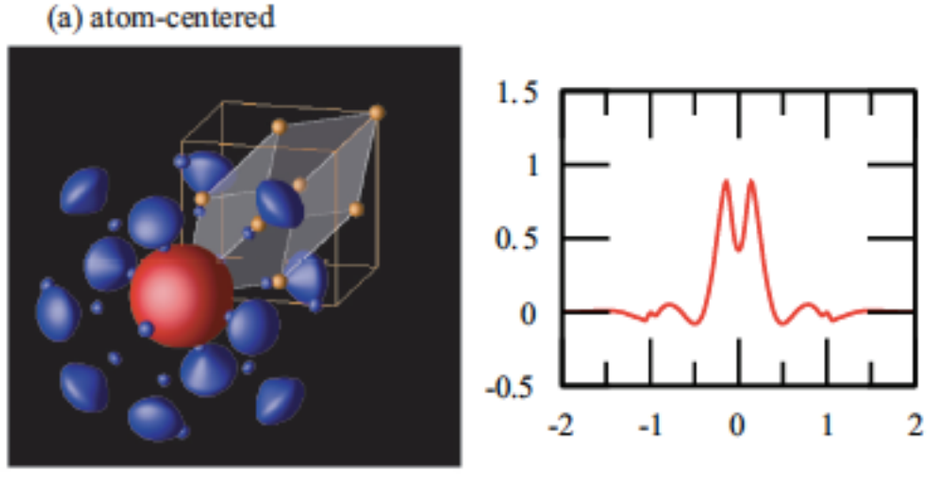


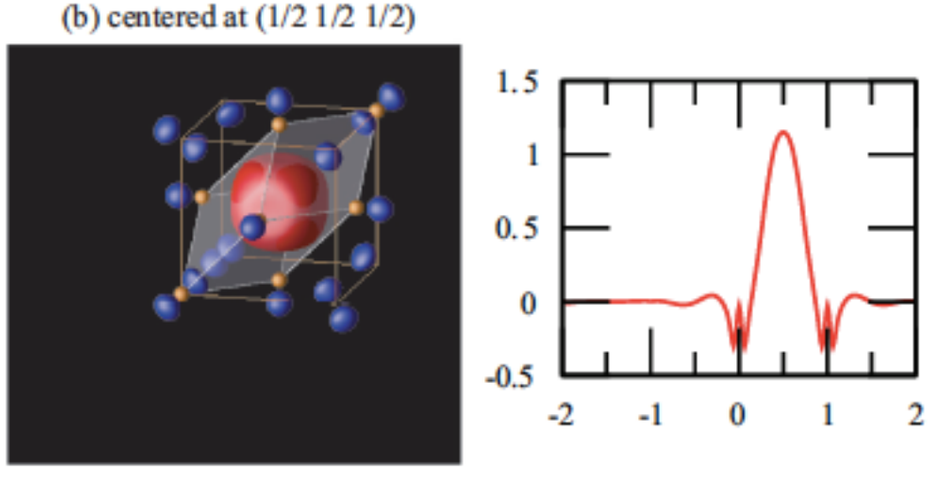
- In this case, SAWF = “maxloc” Wannier function

SAWFs : Copper

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

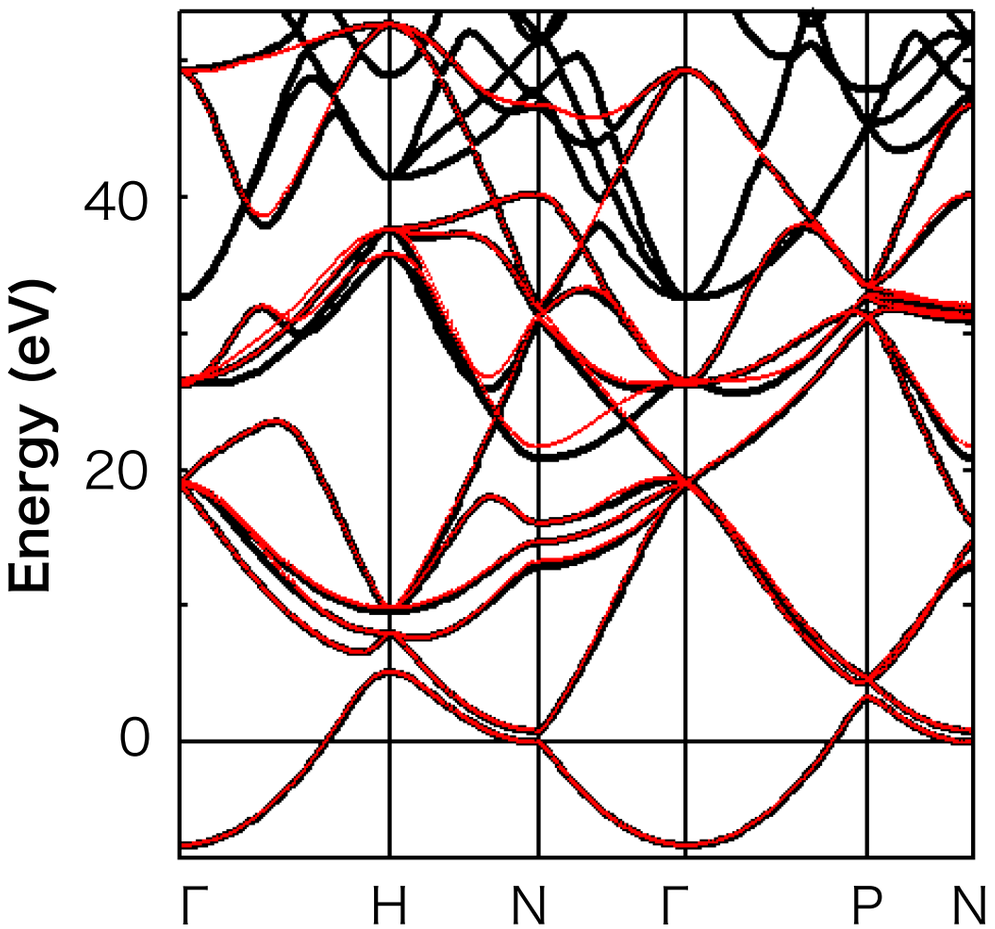




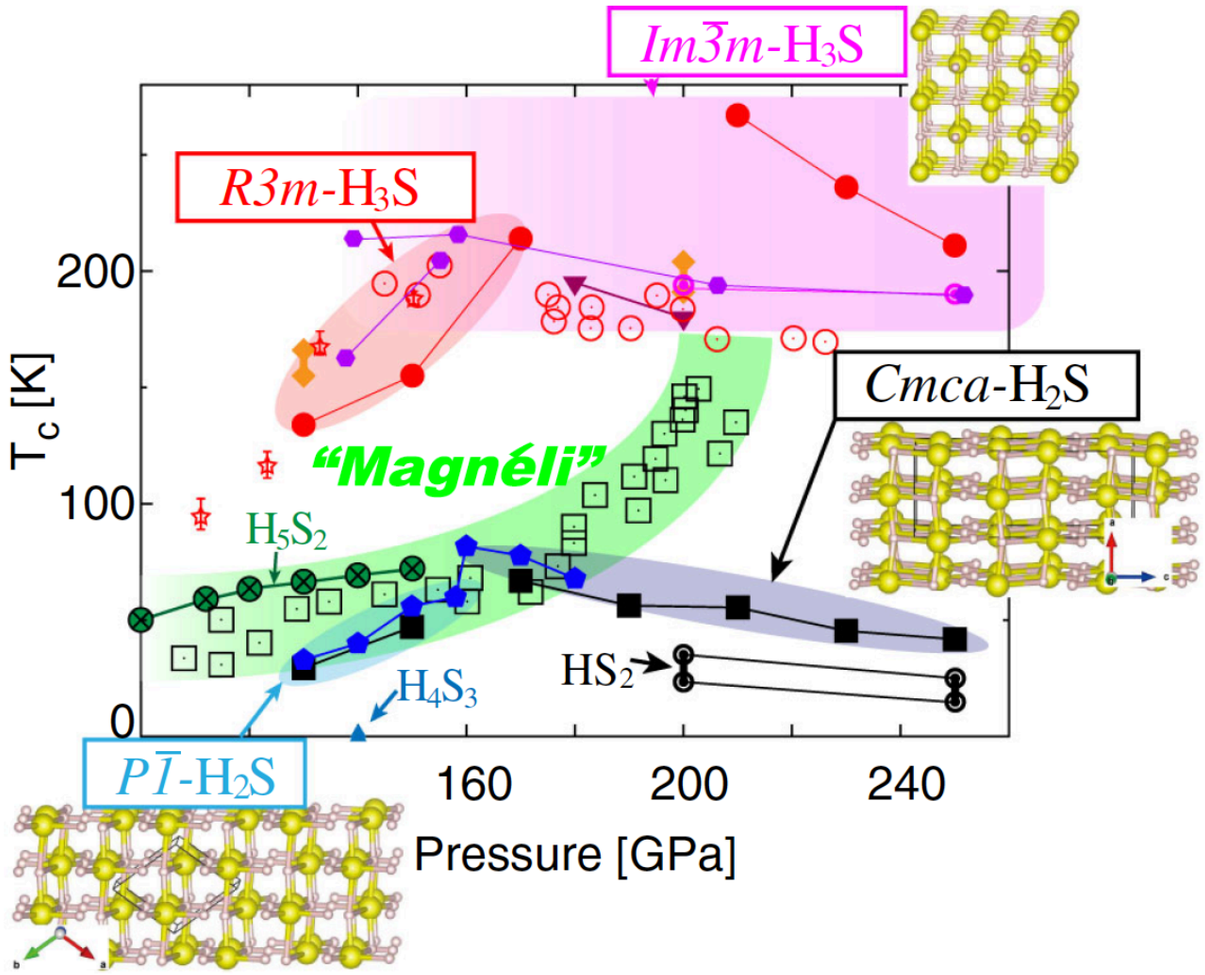


Applications to H_3S ①

Band structure of Im-3m H_3S

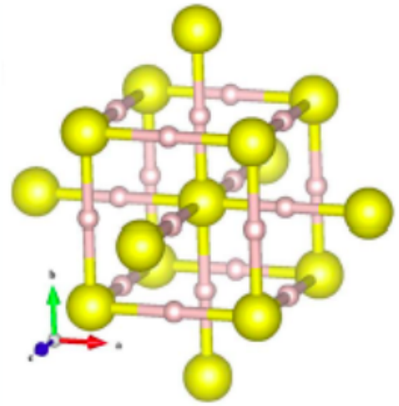


bcc, 48 sym. ops.



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

Applications to H_3S ②



Im3-m H_3S

Maximally localized Wannier functions

```
Final State
 WF centre and spread    1  (  0.396807, -0.313554,  0.345678 )     0.67398410
 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
 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
 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
 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
```

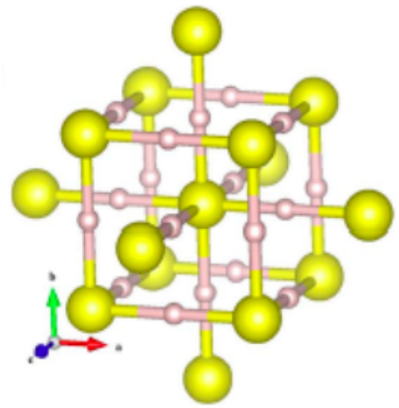
S s

S p

S d

H s

Applications to H_3S ③



Im3-m H_3S

Symmetry adapted Wannier functions

```
Final State
 WF centre and spread    1  (  0.000000,  0.000000,  0.000000 )      0.68140242
 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
 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
 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
 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
```

S s

S p

S d

H s

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
```

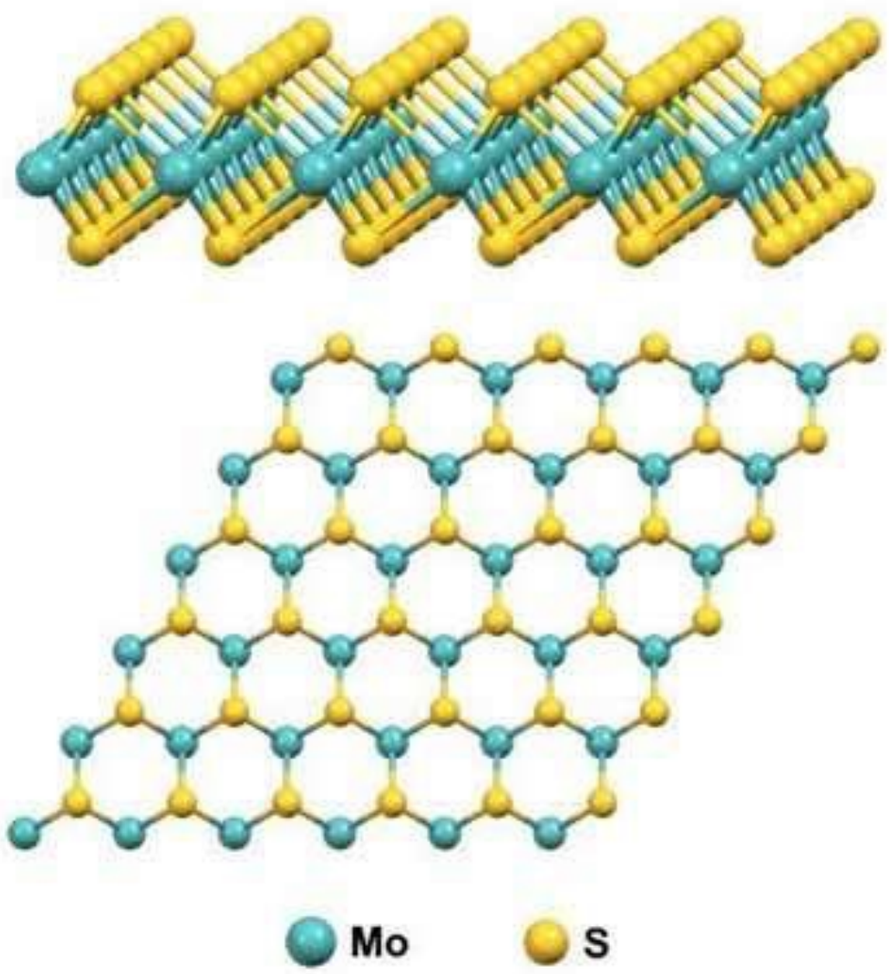
You can try SAWF

※ Please use version 3.1.0 !!!

Be careful …

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

Example: MoS_2 monolayer



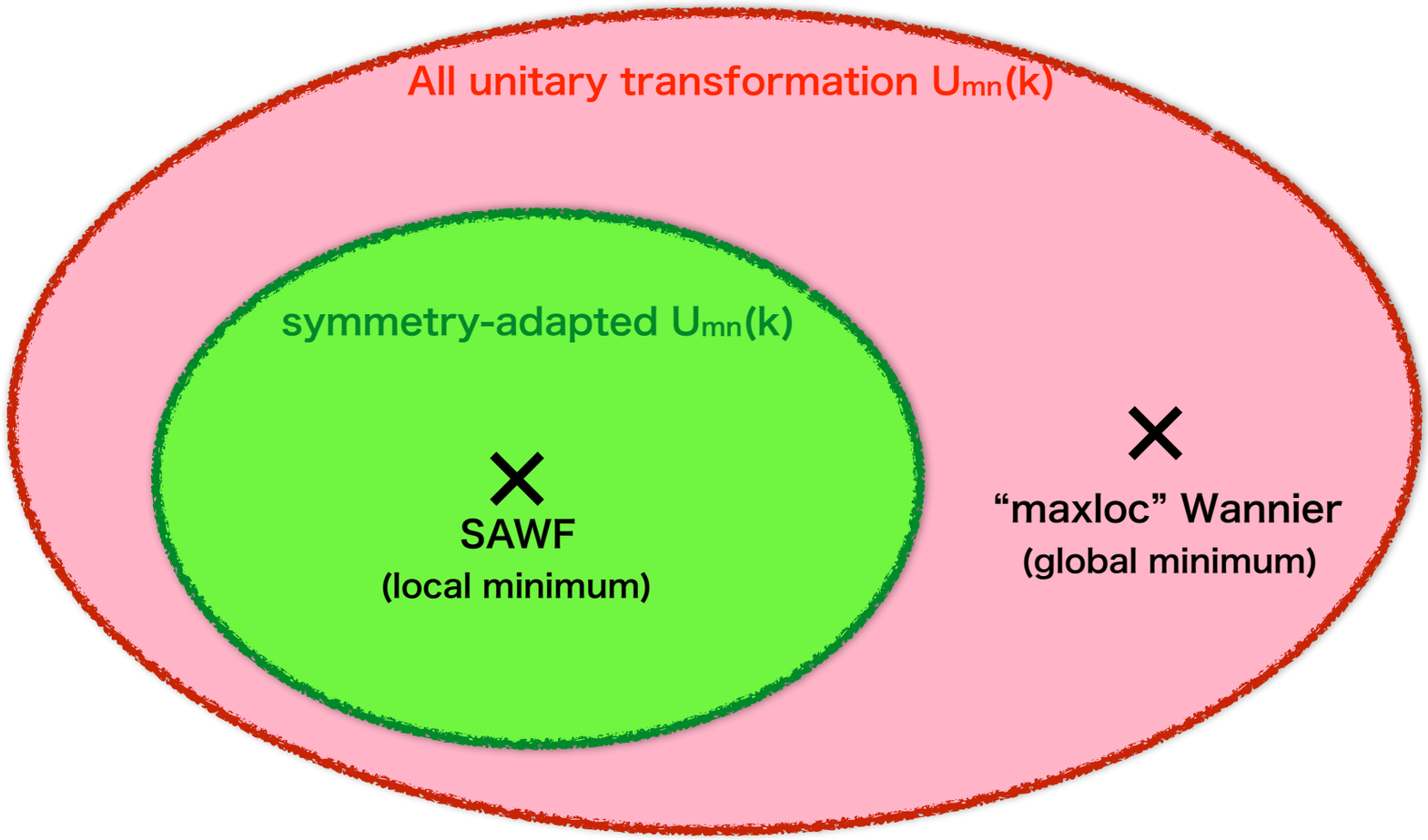
sulphur p orbitals cannot be exactly atom-centered

Summary and future perspective

Summary

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

→ obtain irreducible representations of site-symmetry group



Future perspective

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

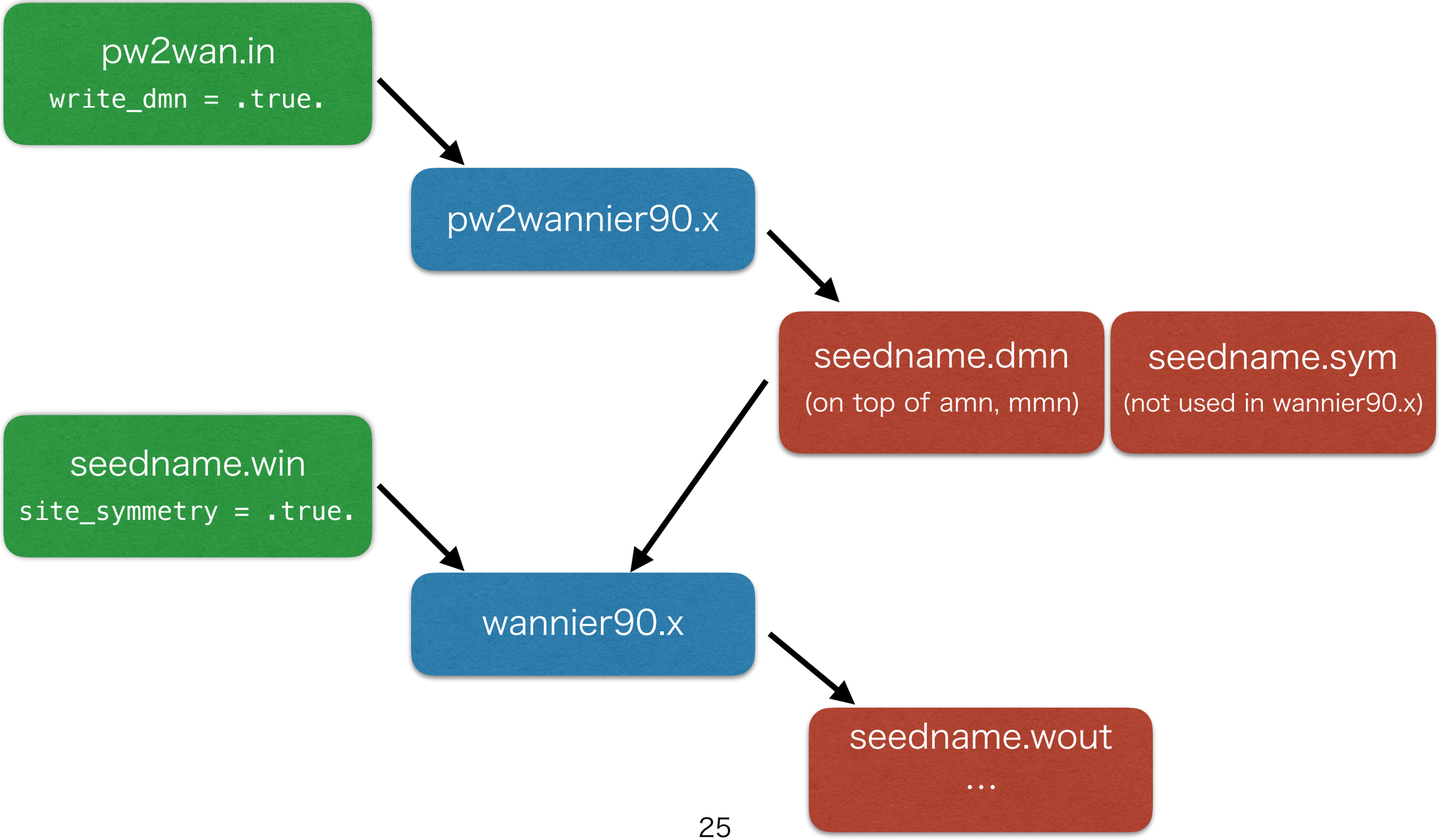
Tutorials

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 the instruction pdf file or README in each directory
- For “`GaAs`” and “`Cu`”, refer also to Wannier90 Tutorials and Tutorial Solutions

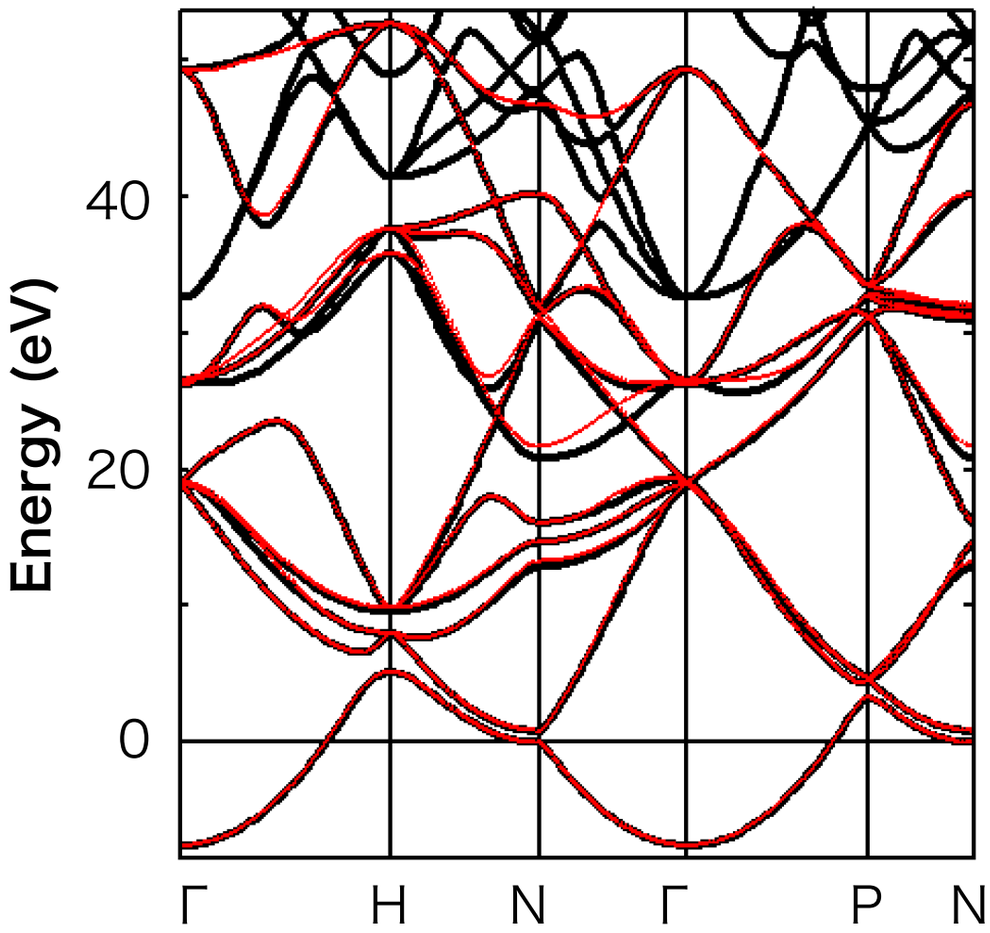
Flow of calculation (after nscf calculations and creating .nnkp file)

input **executable** **output/input**

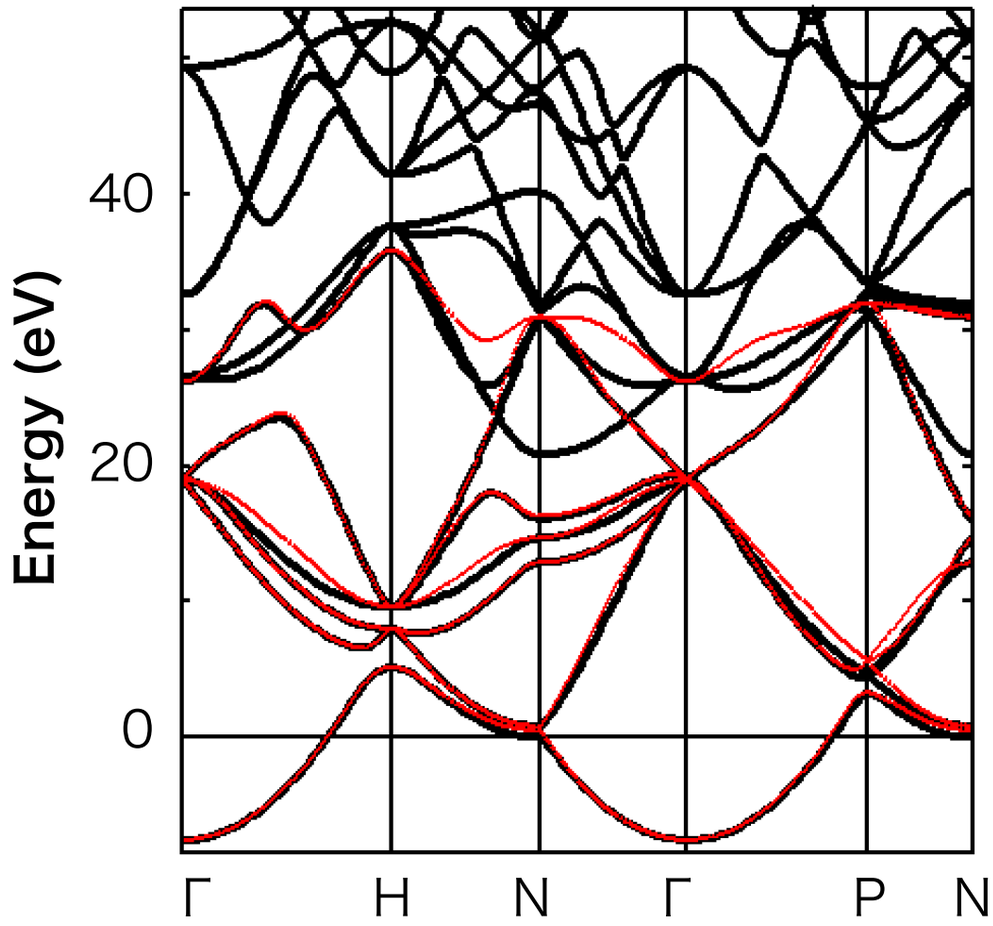


Reference: H_3S

12 band model



7 band model



Flow of calculation in Cu tutorial : advanced usage

(after nscf calculations and creating .nnkp file)

input **executable** **output/input**

pw2wan.in

```
write_dmn = .true.
read_sym = .true.
```

seedname.sym

(prepare it by ourselves)

pw2wannier90.x

seedname.win

```
site_symmetry = .true.
```

seedname.dmn

(on top of amn, mmn)

wannier90.x

seedname.wout

…