issp CCMS Center of Computational Materials Science

東京大学 物性研究所

CCMSハンズオン: RESPACK講習会
（TIA“かけはし”連携講座）

中村 和磨 (九州工業大学大学院基礎科学研究系)

日時: 2019年3月1日(金) 13:30−17:00

東京大学柏の葉キャンパス駅前サテライト205号室

RESPACK

Welcome to homepage of RESPACK which is a free software of ab initio many-body perturbation codes including calculations for response function with random-phase approximation, Wannier function, and matrix-element evaluations of frequency-dependent screened direct and exchange interactions. Discussions and communications are always open and let us heap up this community together!

Download codes (20190226): RESPACK-20190226.tar.gz

Download codes (20171220): RESPACK-20171220.tar.gz

Download tutorial (20171220): TUTORIAL.pptx

Download codes (20171014): RESPACK-20171014.tar.gz

Download manual (20171014): MANUAL-20171014.pdf

- Kazuma NAKAMURA, Associate Professor, Dr. Kyushu Institute of Technology
- Yoshihide YOSHIMOTO, Associate Professor, Dr. The University of Tokyo
- Yoshiro NOHARA, Researcher, Dr
- Yusuke NOMURA, Research Associate, Dr. The University of Tokyo
- Terumasa TADANO, ICYS researcher, Dr. National Institute for Materials Science
- Mitsuaki KAWAMURA, Research Associate, Dr. The Institute for Solid State Physics
- Maxime CHARLEBOIS, Researcher, Dr. The University of Tokyo

2018年度ソフトウェア開発・高度化課題プログラム

第一原理有効模型導出プログラムRESPACKと模型解析プログラムHΦ/mVMCの融合による非経験的強相関電子構造解析ソフトウェアの整備

Development of first principles electronic-structure calculation software by combining effective-model derivation code (RESPACK) and model-analysis codes (HΦ/mVMC)

mVMC/HΦ

- Takahiro MISAWA, Project Researcher, Dr., issp-CCMS, The University of Tokyo
- Kazuyoshi YOSHIMI, Project reader, Dr., The Institute for Solid State Physics
- Yuichi MOTOYAMA, Researcher, Dr., The Institute for Solid State Physics
- Mitsuaki KAWAMURA, Research Associate, Dr. The Institute for Solid State Physics

RESPACK

- Kazuma NAKAMURA, Associate Professor, Dr., Kyushu Institute of Technology
- Yoshihide YOSHIMOTO, Associate Professor, Dr., The University of Tokyo
- Yusuke NOMURA, Research Associate, Dr., The University of Tokyo
- Terumasa TADANO, ICYS researcher, Dr., National Institute for Materials Science

Methods

1. Maximally localized Wannier function

Marzari-Vanderbilt, Phys. Rev. B 56, 12847 (1997).
Souza-Marzari-Vanderbilt, Phys. Rev. B 65, 035109 (2001).
KN-Arita-Yoshimoto-Tsuneyuki, Phys. Rev. B 74, 235113 (2006).

2. Dielectric function with random phase approximation

Hybertsen-Louie, Phys. Rev. B 35, 5585 (1987).
KN-Nohara-Yosimoto-Nomura, Phys. Rev. B 93, 085124 (2016).

3. Matrix-element evaluation of screened interaction

KN-Arita-Imada, J. Phys. Soc. jpn 77, 093711 (2008).
Miyake-Aryasetiawan, Phys. Rev. B 77, 085122 (2008).

4. GW spectral function

Hybertsen-Louie, Phys. Rev. B 34, 5390 (1986).
KN-Nohara-Yosimoto-Nomura, Phys. Rev. B 93, 085124 (2016).

Targets

- Metals
- Semiconductors
- Transition metal compounds
- Organic compounds, etc.

Physical quantities that can be calculated

- Maximally localized Wannier function (Wannier-interpolation band, real-space Wannier function, onsite-energy and transfer-integral parameters, etc)
- RPA response function (optical absorption spectrum, electron energy loss function, reflectance spectrum)
- Frequency-dependent electronic interaction parameters
- GW spectral function (almost finished)
- Extension to spinor format (developing)

License

- GNU GPL v3

Supported OS/environments

- Operate in UNIX environment
- Fortran 90 (intel Fortran, gfortran)
- MPI (OpenMPI, intelMPI), OpenMP
- LAPACK

Parallelization

- Parallel job support (MPI, OpenMP)
- Confirmation of operation in System B at ISSP, Univ. Tokyo

Related Applications

- as input data
  - xTAPP
  - Quantum ESPRESSO

    NOTE: the norm-conserving pseudopotential should be used
- drawing
  - VESTA (Wannier function)
  - FermiSurfer (Fermi surface).

Prospect

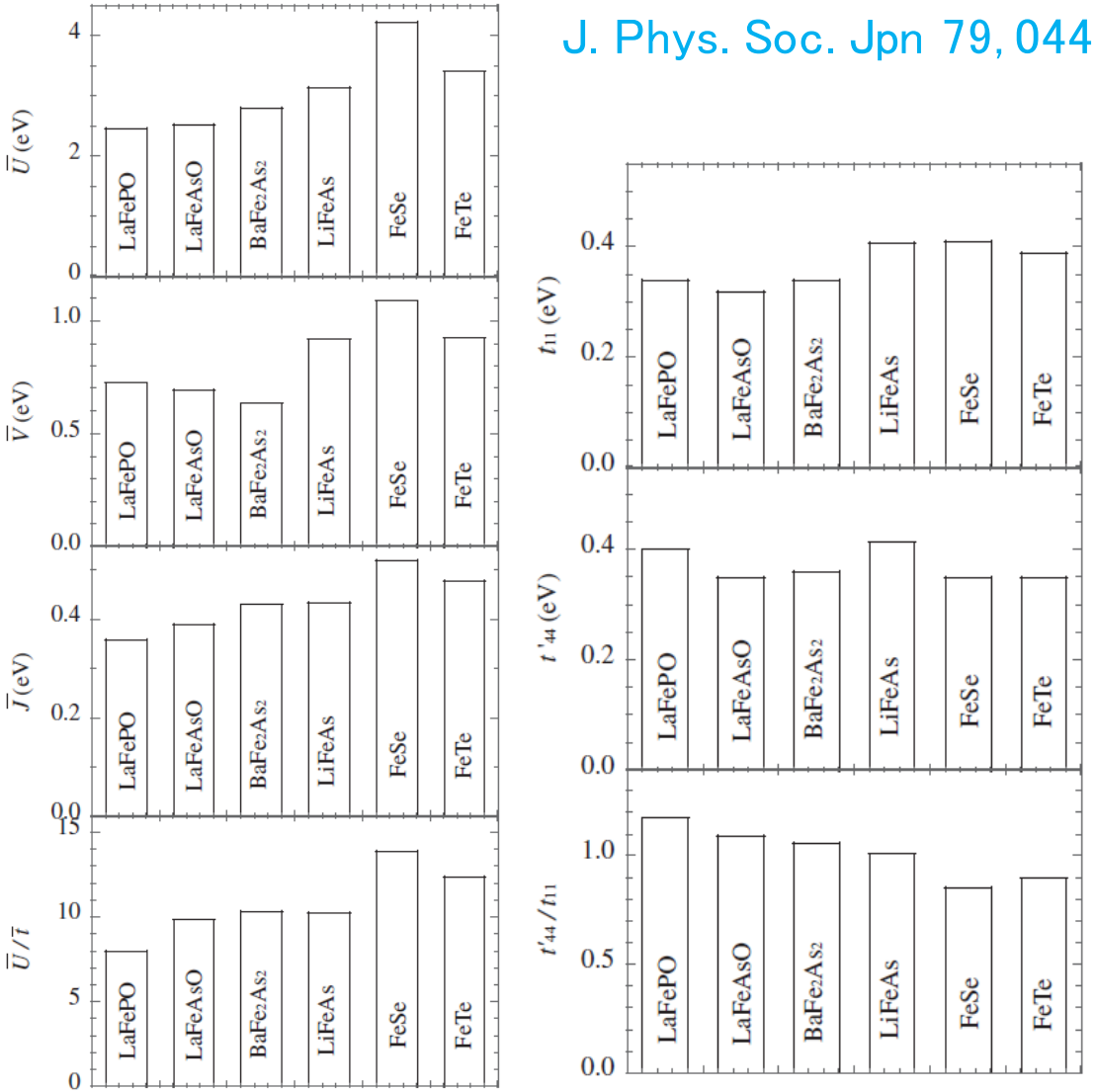
- Superconducting transition temperature evaluation
  (electron–phonon coupling, the Coulomb pseudopotential)

Application 1: Fe-based superconductor

Comparison of *Ab initio* Low-Energy Models for LaFePO, LaFeAsO, $BaFe_2As_2$, LiFeAs, FeSe, and FeTe: Electron Correlation and Covalency

Takashi MIYAKE[1,3,4*], Kazuma NAKAMURA[2,3,4], Ryotaro ARITA[2,3,4], and Masatoshi IMADA[2,3,4]

J. Phys. Soc. Jpn 79, 044705 (2010)



Application 2: doped C_{60}

Phys. Rev. B 85, 155452 (2012)

Ab initio derivation of electronic low-energy models for C_{60} and aromatic compounds

Yusuke Nomura,[1] Kazuma Nakamura,[1,2] and Ryotaro Arita[1,2,3]

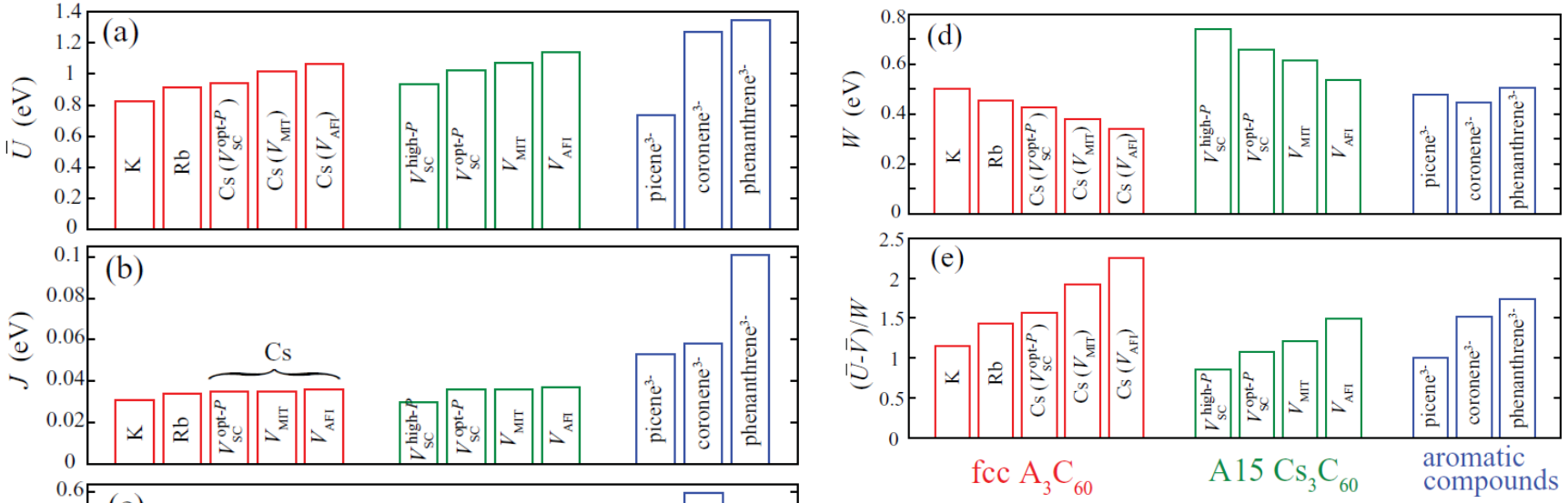


FIG. 6. (Color online) Material dependence of (a) the average of the on-site effective Coulomb repulsion $\bar{U}$, (b) the on-site effective exchange interaction J, (c) the average of the off-site effective Coulomb repulsion between neighboring sites $\bar{V}$, (d) the bandwidth of the target band W, and (e) the correlation strength $(\bar{U}-\bar{V})/W$, which are derived within the cRPA method.

Bottleneck

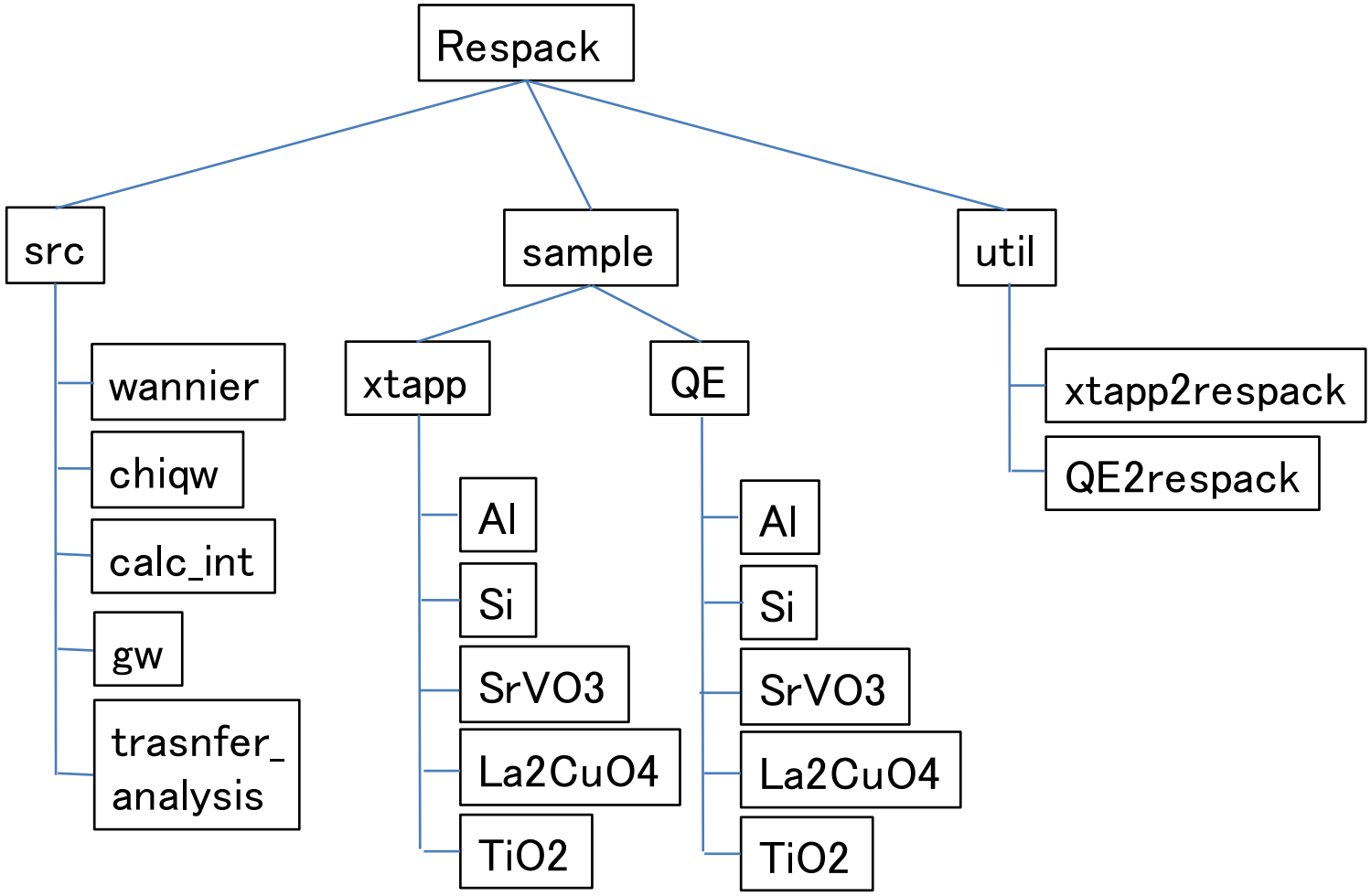
- Band calculation: Making input for crystal structure
- RESPACK: Making input for initial guess of Wannier function

```
# file map data
 &filemap
 basename = 'Al',
 number_PP_file = 1/
 ps-Al ps-Al.ichr

# symmetry data
 &SYMMETRY
 SYMMETRY_FORMAT =
'reciprocal',
 NUMBER_SYM_OP = 48,
 denom_trans =  1/
  1  0  0  0  1  0  0  0  1  0  0  0

# atom data
 3 13
 1  0.000  0.000  0.000

# k-points data
&smpl_kpt
dos_mode =
'METHFESSEL_PAXTON',
bz_mesh = 12,
bz_number_tile = 1/
 6 6 6
 2 2 2
```

```
# main data
&tappinput
lattice_factor = 7.60
LATTICE_LIST = 0.5, 0.5, 0.0,
               0.0, 0.5, 0.5,
               0.5, 0.0, 0.5,
cutoff_wave_function = 6.0,
number_element = 1,
number_atom = 1,
number_band = 50,
store_wfn = 1,
initial_lpt=0,
control_uptime = 3600,
SCF_CONVERGE = 1.0E-015,
xc_type = 'PBE',
STORE_VXC = 1,
elec_kbt=0.01/

# struct_opt data
&struct_opt
number_cycle = 0/

# str_opt_constr data
 1
 0
```

```
&param_chiqw
/
&param_wannier
N_wannier=9,
Lower_energy_window=-10.0d0,
Upper_energy_window= 36.0d0,
N_initial_guess=9/
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
&param_interpolation
N_sym_points=5/       !The total number of symmetry points
0.50d0 0.50d0 0.50d0 !L
0.00d0 0.00d0 0.00d0 !G
0.50d0 0.00d0 0.50d0 !X
0.50d0 0.25d0 0.75d0 !W
0.50d0 0.50d0 0.50d0 !L
&param_visualization
FLG_VIS_WANNIER = 1/
&param_calc_int
/
```

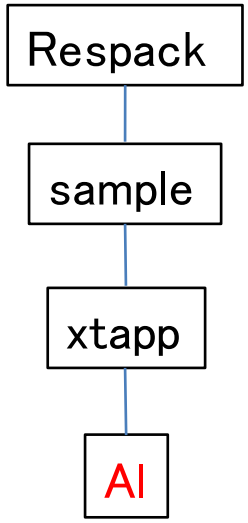
Directory structure (only principal parts)



Job script in MateriApps LIVE!

> cat Al.sh

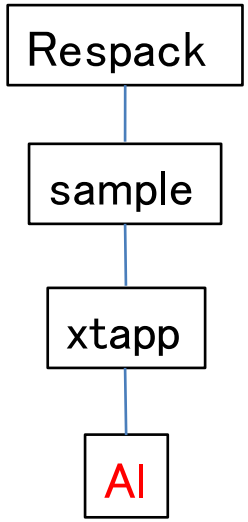
```
#!/bin/sh

set -x
#xtapp band calculation
rm -f fort.* Al.lpt Al.rho Al.str Al.wfn *.log
rm -f fort.10 ; ln -s Al.cg fort.10
mpirun -np 1 inipot > log.Al-inipot
mpirun -np 1 cgmrpt > log.Al-cgmrpt
rm -f fort.10 ; ln -s Al.vb fort.10
mpirun -np 1 inipot > log.Al-inipot-vb
mpirun -np 1 vbpef > log.Al-vbpef
vbpef2gp-lsda Al.band

#interface: from xTAPP to respack
./xtapp2respack.sh -b ./wfn2respack -s ./strconv Al

#respack
mpirun -np 1 calc_wannier < input.in > log.Al-wannier
mpirun -np 1 calc_chiqw < input.in > log.Al-chiqw
mpirun -np 1 calc_w3d < input.in > log.Al-calc_w3d
mpirun -np 1 calc_j3d < input.in > log.Al-calc_j3d
```



Input.in RESPACK

> cat input.in

```
&param_chiqw
/
&param_wannier
N_wannier=9,                        !Total number of considerd band in wannier calc
Lower_energy_window=-10.0d0, !LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window= 36.0d0,  !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=9/                  !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
&param_interpolation
N_sym_points=5/       !The total number of symmetry points
0.50d0 0.50d0 0.50d0 !L
0.00d0 0.00d0 0.00d0 !G
0.50d0 0.00d0 0.50d0 !X
0.50d0 0.25d0 0.75d0 !W
0.50d0 0.50d0 0.50d0 !L
&param_visualization
FLG_VIS_WANNIER = 1/
&param_calc_int
/
```



edit Al.cg and Al.vb

☐ Al.cg (Al.vb)

```
…
# k-points data
&smpl_kpt
dos_mode =
‘METHFESSEL_PAXTON’,
bz_mesh = 12,
bz_number_tile = 1/
  6  6  6
  2  2  2
…
```

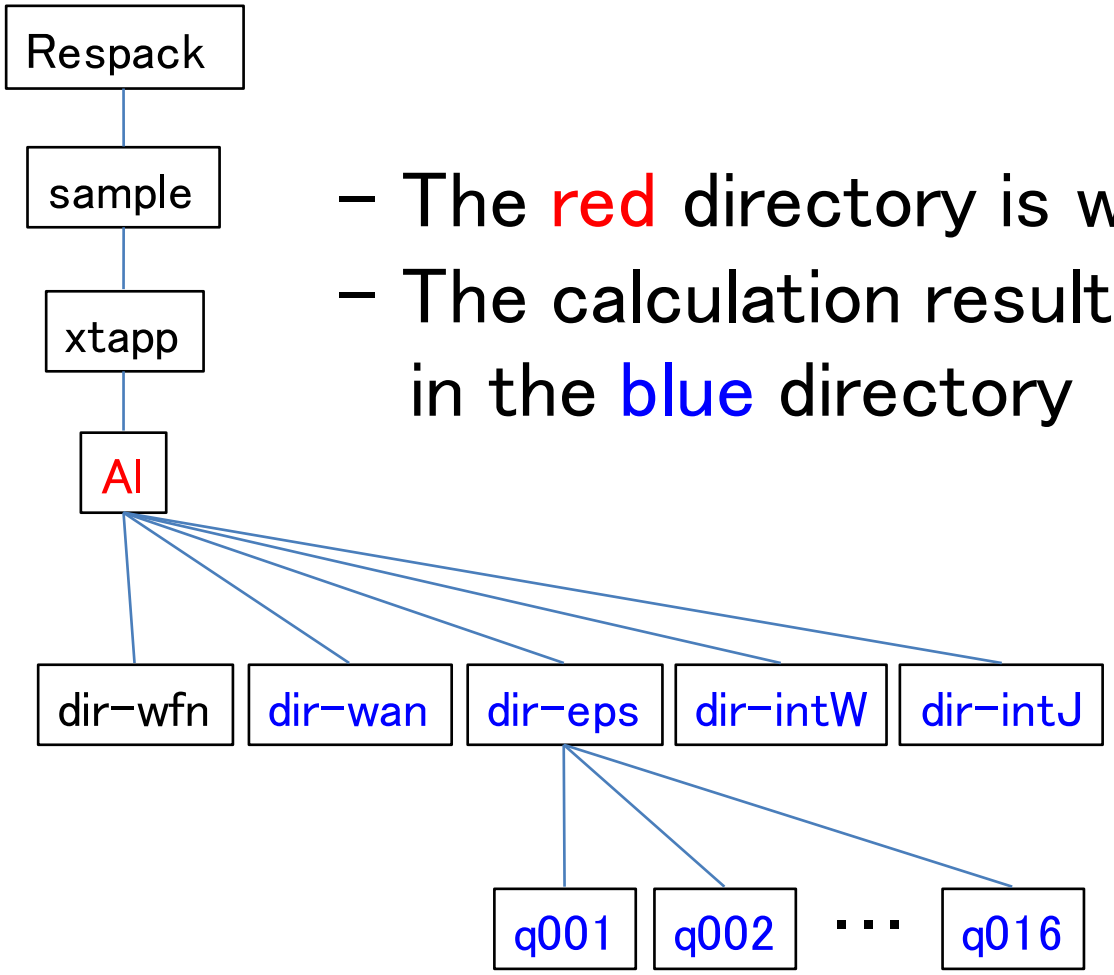
6x6x6 k points calc.

```
…
# k-points data
&smpl_kpt
dos_mode =
METHFESSEL_PAXTON,
bz_mesh = 8,
bz_number_tile = 1/
  4  4  4
  2  2  2
…
```

4x4x4 k points calc.

Execute in MateriApps LIVE!

```
./Al.sh &
```



- The red directory is working one
- The calculation results are output in the blue directory

Convergence check in wannier

1. Spillage functional minimization

```
> grep I_SCF  log.Al-wannier

 I_SCF=    1   DEL_OMEGA_I=      31.5534368140  OMEGA_I      31.5534368140
 I_SCF=    2   DEL_OMEGA_I=       0.0313174321  OMEGA_I      31.5221193819
 I_SCF=    3   DEL_OMEGA_I=       0.0294324421  OMEGA_I      31.4926869398
 I_SCF=    4   DEL_OMEGA_I=       0.0275955977  OMEGA_I      31.4650913421
 I_SCF=    5   DEL_OMEGA_I=       0.0258233155  OMEGA_I      31.4392680266
 I_SCF=    6   DEL_OMEGA_I=       0.0241261669  OMEGA_I      31.4151418597
 I_SCF=    7   DEL_OMEGA_I=       0.0225104451  OMEGA_I      31.3926314146
 I_SCF=    8   DEL_OMEGA_I=       0.0209793256  OMEGA_I      31.3716520890
 I_SCF=    9   DEL_OMEGA_I=       0.0195337283  OMEGA_I      31.3521183607
                                        ...
 I_SCF=   70   DEL_OMEGA_I=       0.0001840208  OMEGA_I      31.1054543359
 I_SCF=   71   DEL_OMEGA_I=       0.0001706829  OMEGA_I      31.1052836529
 I_SCF=   72   DEL_OMEGA_I=       0.0001583292  OMEGA_I      31.1051253238
 I_SCF=   73   DEL_OMEGA_I=       0.0001468860  OMEGA_I      31.1049784378
 I_SCF=   74   DEL_OMEGA_I=       0.0001362853  OMEGA_I      31.1048421525
 I_SCF=   75   DEL_OMEGA_I=       0.0001264644  OMEGA_I      31.1047156881
 I_SCF=   76   DEL_OMEGA_I=       0.0001173648  OMEGA_I      31.1045983232
 I_SCF=   77   DEL_OMEGA_I=       0.0001089330  OMEGA_I      31.1044893902
 I_SCF=   78   DEL_OMEGA_I=       0.0001011190  OMEGA_I      31.1043882712
 I_SCF=   79   DEL_OMEGA_I=       0.0000938770  OMEGA_I      31.1042943942
```

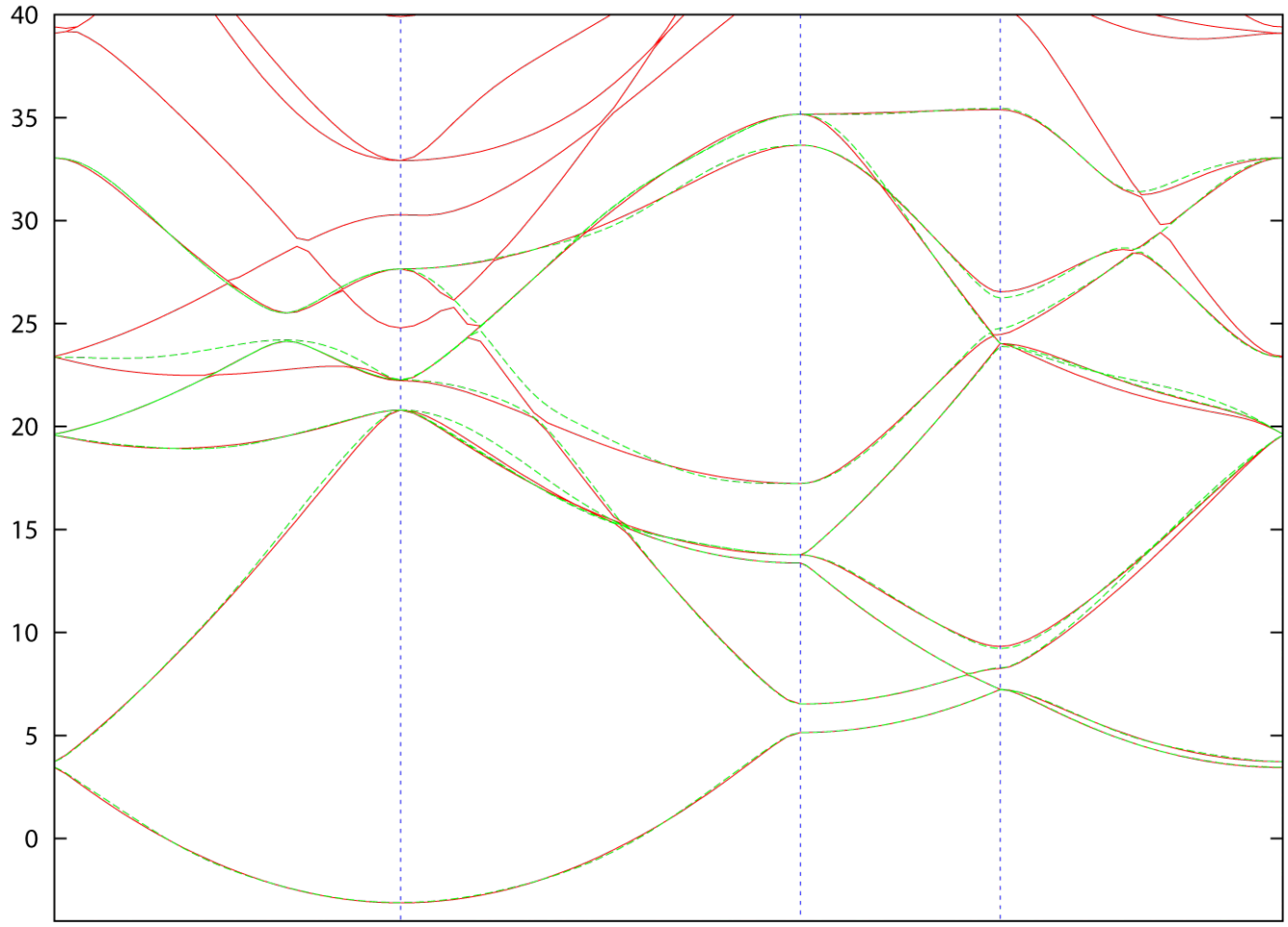
Convergence check in wannier

2. Spread functional minimization

```
> grep I_STEP  log.Al-wannier

I_STEP SPREAD DEL_SPREAD:     1     60.3111523152     60.3111523152
I_STEP SPREAD DEL_SPREAD:     2     59.6268066188      0.6843456964
I_STEP SPREAD DEL_SPREAD:     3     59.4793841760      0.1474224428
I_STEP SPREAD DEL_SPREAD:     4     59.4113317387      0.0680524373
I_STEP SPREAD DEL_SPREAD:     5     59.3707982003      0.0405335384
I_STEP SPREAD DEL_SPREAD:     6     59.3451416542      0.0256565460
I_STEP SPREAD DEL_SPREAD:     7     59.3283561616      0.0167854927
I_STEP SPREAD DEL_SPREAD:     8     59.3172959946      0.0110601669
I_STEP SPREAD DEL_SPREAD:     9     59.3099463779      0.0073496167
I_STEP SPREAD DEL_SPREAD:    10     59.3050531688      0.0048932091
I_STEP SPREAD DEL_SPREAD:    11     59.3017783648      0.0032748040
I_STEP SPREAD DEL_SPREAD:    12     59.2995842965      0.0021940683
I_STEP SPREAD DEL_SPREAD:    13     59.2981086110      0.0014756855
I_STEP SPREAD DEL_SPREAD:    14     59.2971155254      0.0009930856
I_STEP SPREAD DEL_SPREAD:    15     59.2964450744      0.0006704510
I_STEP SPREAD DEL_SPREAD:    16     59.2959923565      0.0004527179
I_STEP SPREAD DEL_SPREAD:    17     59.2956856224      0.0003067342
I_STEP SPREAD DEL_SPREAD:    18     59.2954777580      0.0002078644
I_STEP SPREAD DEL_SPREAD:    19     59.2953362511      0.0001415069
I_STEP SPREAD DEL_SPREAD:    20     59.2952398255      0.0000964256
```

OUTPUT in wannier: interpolated band

```
>gnuplot
gnuplot >plot [ ][-4:40] ‘bandfig.dat’ , ‘dir-wan/dat.iband’ , ‘bandfig.kpt’
```



OUTPUT in wannier: transfer integral

Transfer integral $\langle w_{i\mathbf{0}} | h_{KS} | w_{j\mathbf{R}} \rangle$

> less log.Al-wannier

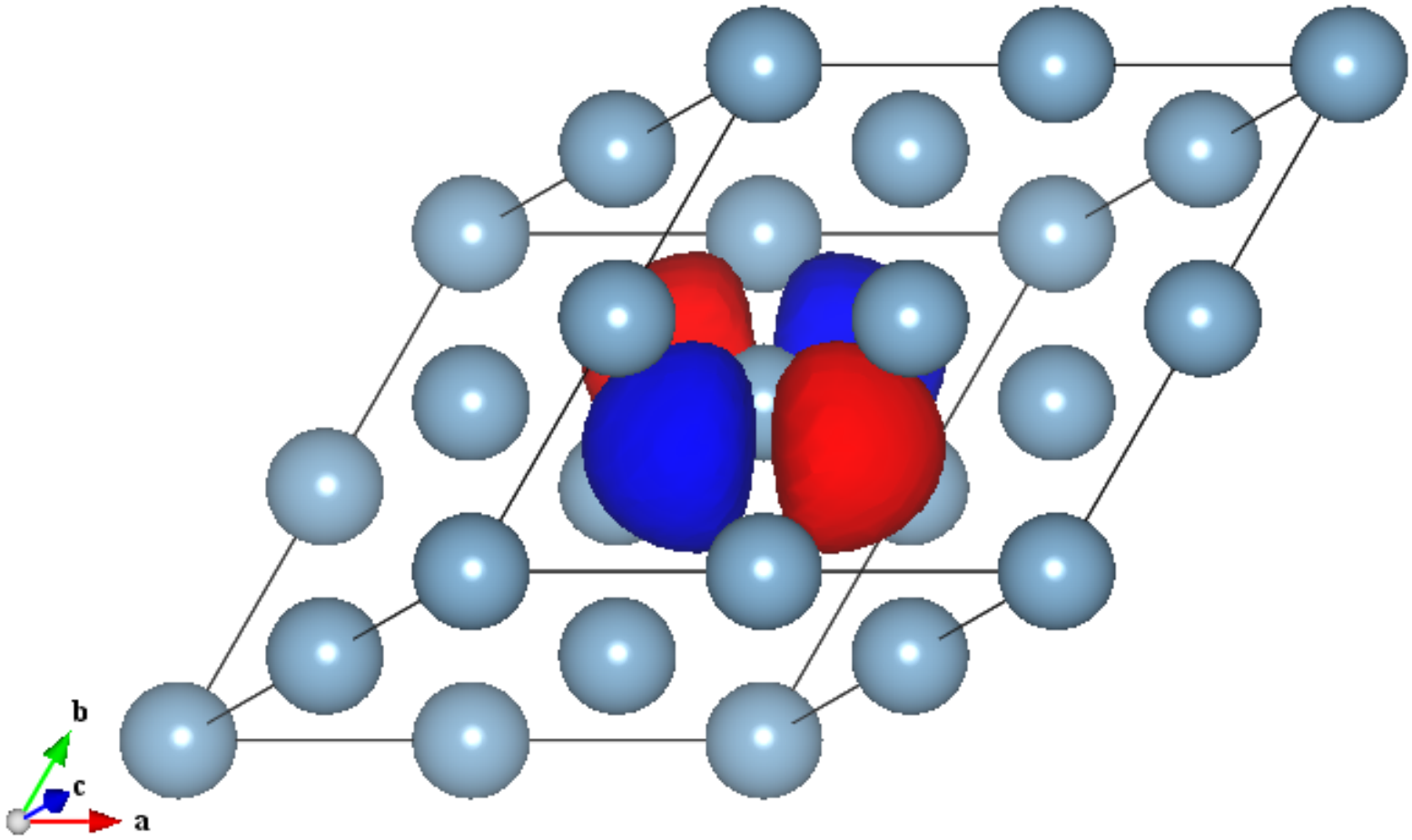
in eV

```
     0          0          0
  7.35914211   0.00000000   0.00000000  -0.00000000   0.00000000   0.00000000   0.04394082   0.00000000   0.00000000
  0.00000000  14.58743193  -0.00000000  -0.00000000   0.00000000  -0.00000000   0.00000000   0.00000000  -0.00000000
  0.00000000  -0.00000000  14.58743193   0.00000000   0.00000000  -0.00000000  -0.00000000   0.00000000  -0.00000000
 -0.00000000  -0.00000000   0.00000000  14.57653548  -0.00000000   0.00000000  -0.00000000  -0.00000000  -0.00000000
  0.00000000   0.00000000   0.00000000  -0.00000000  24.40958409   0.00000000  -0.00000000   0.00000000   0.00000000
  0.00000000  -0.00000000  -0.00000000   0.00000000   0.00000000  24.41260139  -0.00000000   0.00000000  -0.00000000
  0.04394082   0.00000000  -0.00000000  -0.00000000  -0.00000000  -0.00000000  22.91590733  -0.00000000   0.00000000
  0.00000000   0.00000000   0.00000000  -0.00000000   0.00000000   0.00000000  -0.00000000  24.41260139   0.00000000
  0.00000000  -0.00000000  -0.00000000  -0.00000000   0.00000000  -0.00000000   0.00000000   0.00000000  22.88144184

     0          0          1
 -0.79130283   0.97757492   0.00000000   0.97583990  -0.00000000  -0.00000000  -0.36648694  -1.17118700  -0.65185254
 -0.97757492   1.03680651   0.00000000   1.40359169  -0.00000000  -0.00000000  -0.91007695  -1.53870887  -0.60532305
  0.00000000  -0.00000000  -0.16813282  -0.00000000   0.28256323   0.28649970   0.00000000   0.00000000  -0.00000000
 -0.97583990   1.40359169   0.00000000   1.03814129   0.00000000   0.00000000  -0.05409258  -1.53803103  -1.09812055
  0.00000000  -0.00000000  -0.28256323  -0.00000000   0.56865377   0.59795880   0.00000000   0.00000000  -0.00000000
 -0.00000000   0.00000000  -0.28649970   0.00000000   0.59795880   0.56880611   0.00000000   0.00000000   0.00000000
 -0.36648694   0.91007695   0.00000000   0.05409258  -0.00000000   0.00000000   0.88281592  -0.60628805  -1.11961341
 -1.17118700   1.53870887  -0.00000000   1.53803103   0.00000000   0.00000000  -0.60628805  -2.22519781  -1.05277983
 -0.65185254   0.60532305   0.00000000   1.09812055  -0.00000000  -0.00000000  -1.11961341  -1.05277983  -0.41417899
```

OUTPUT in wannier: realspace Wannier

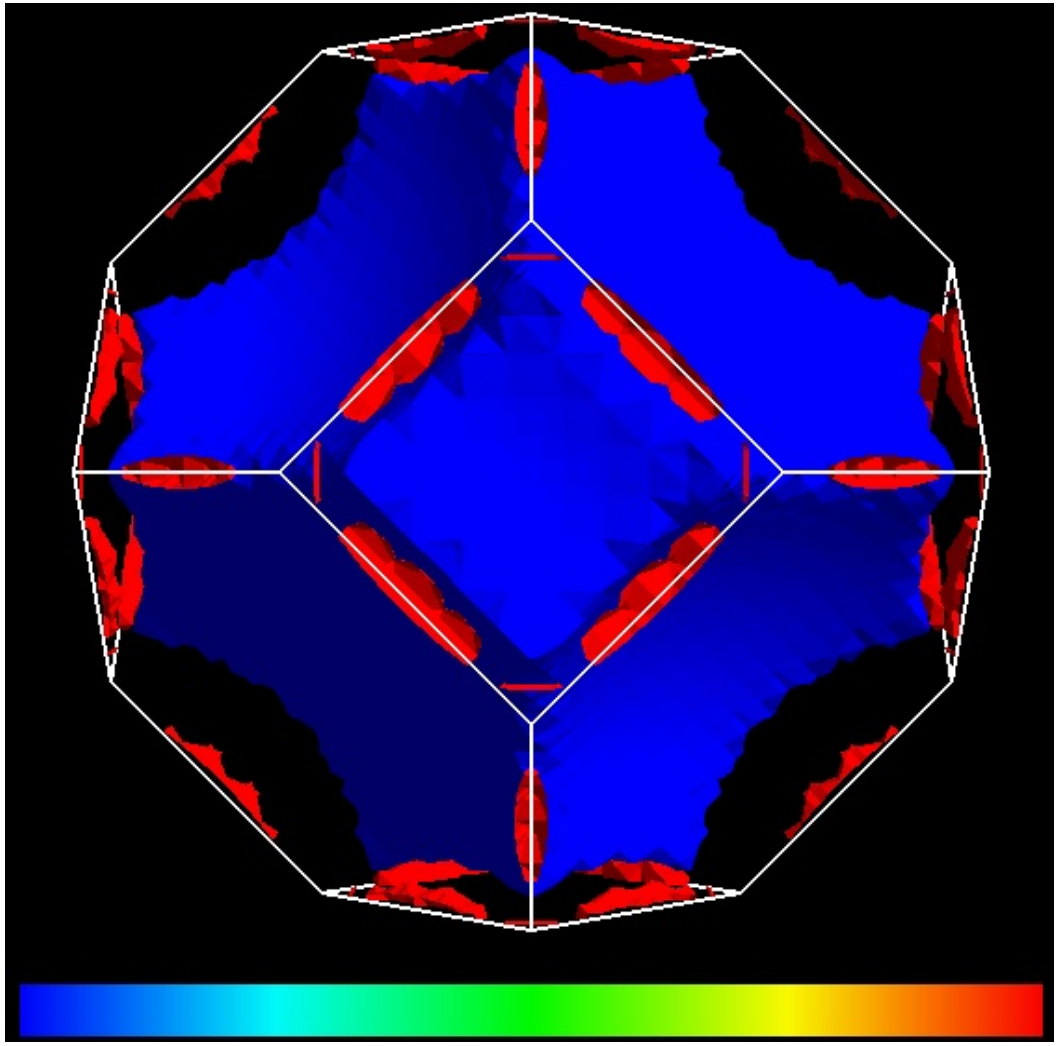
> cd dir-wan/
> vesta &

- File -> open -> dat.supercell-002x002x002.cif
- Edit -> Edit Data -> Volumetric data -> Import -> dat.wan-realspace-009.grd



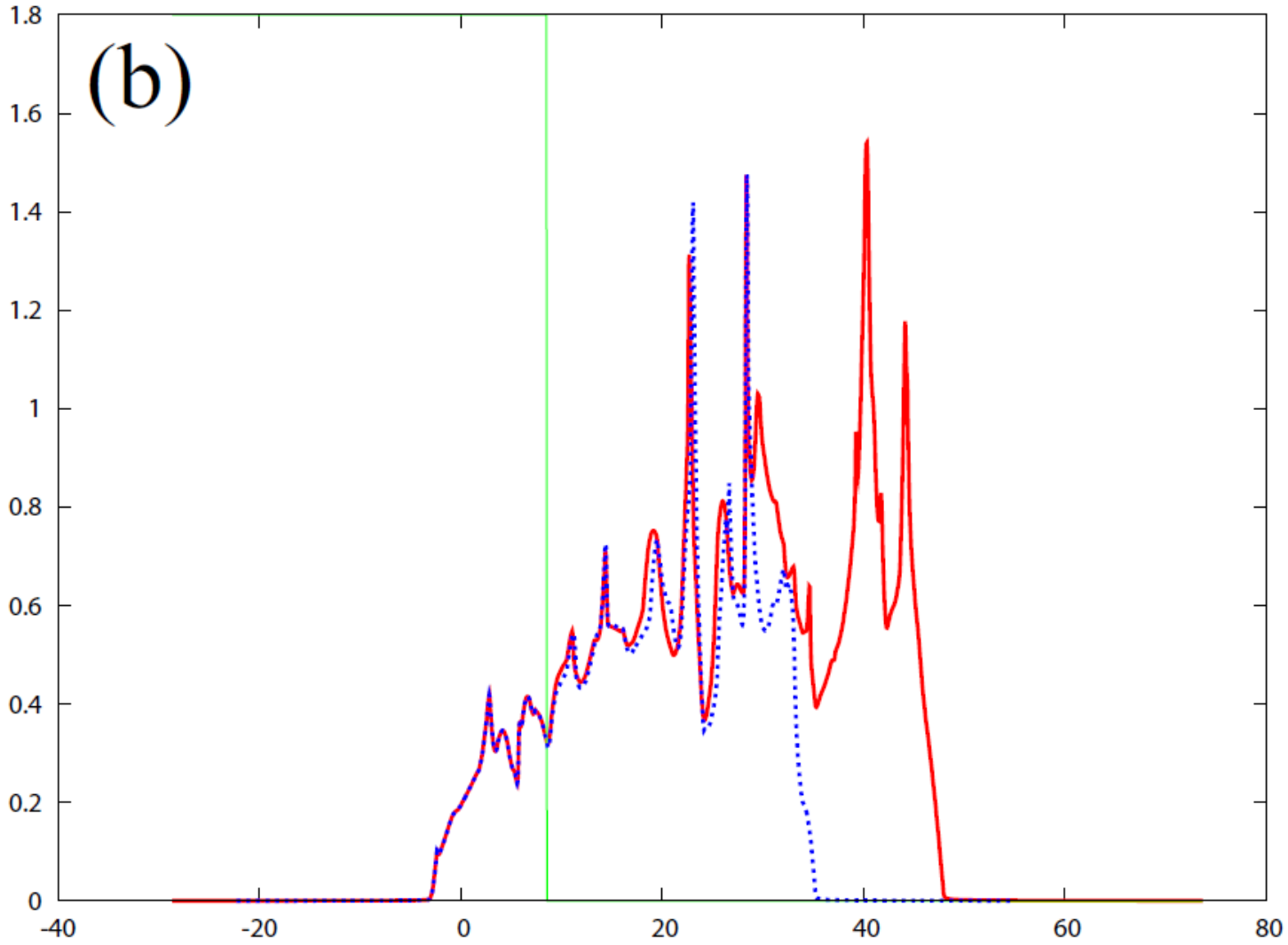
OUTPUT in wannier: Fermi surface

```
> cd dir-wan/
> fermisurfer dat.frmsf
```



OUTPUT in wannier: DOS

```
>cd dir-wan/
>gnuplot
gnuplot >plot 'dat.dos.global' , 'dat.dos.wannier'  u 1:3, 'dat.dos.wannier'
```



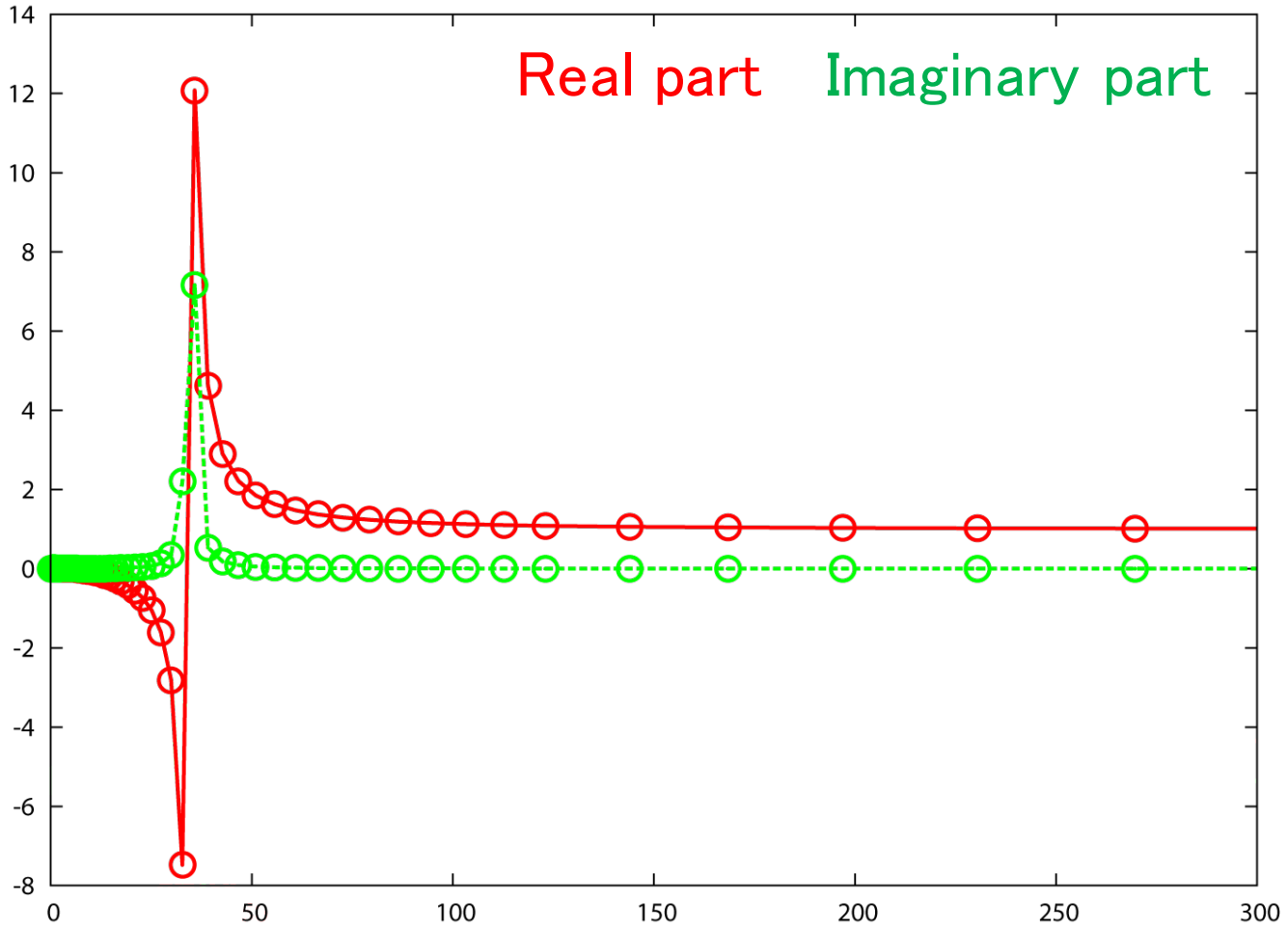
End check in chiqw

- dat.log.400 is end flag for chiqw calculation

```
> ls -al dir-eps/q0*/dat.log.400

-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q001/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q002/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q003/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q004/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q005/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q006/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q007/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q008/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q009/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q010/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q011/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q012/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q013/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q014/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q015/dat.log.400
-rw-r--r-- 1 kazuma users 47 Dec 12 18:43 dir-eps/q016/dat.log.400
```

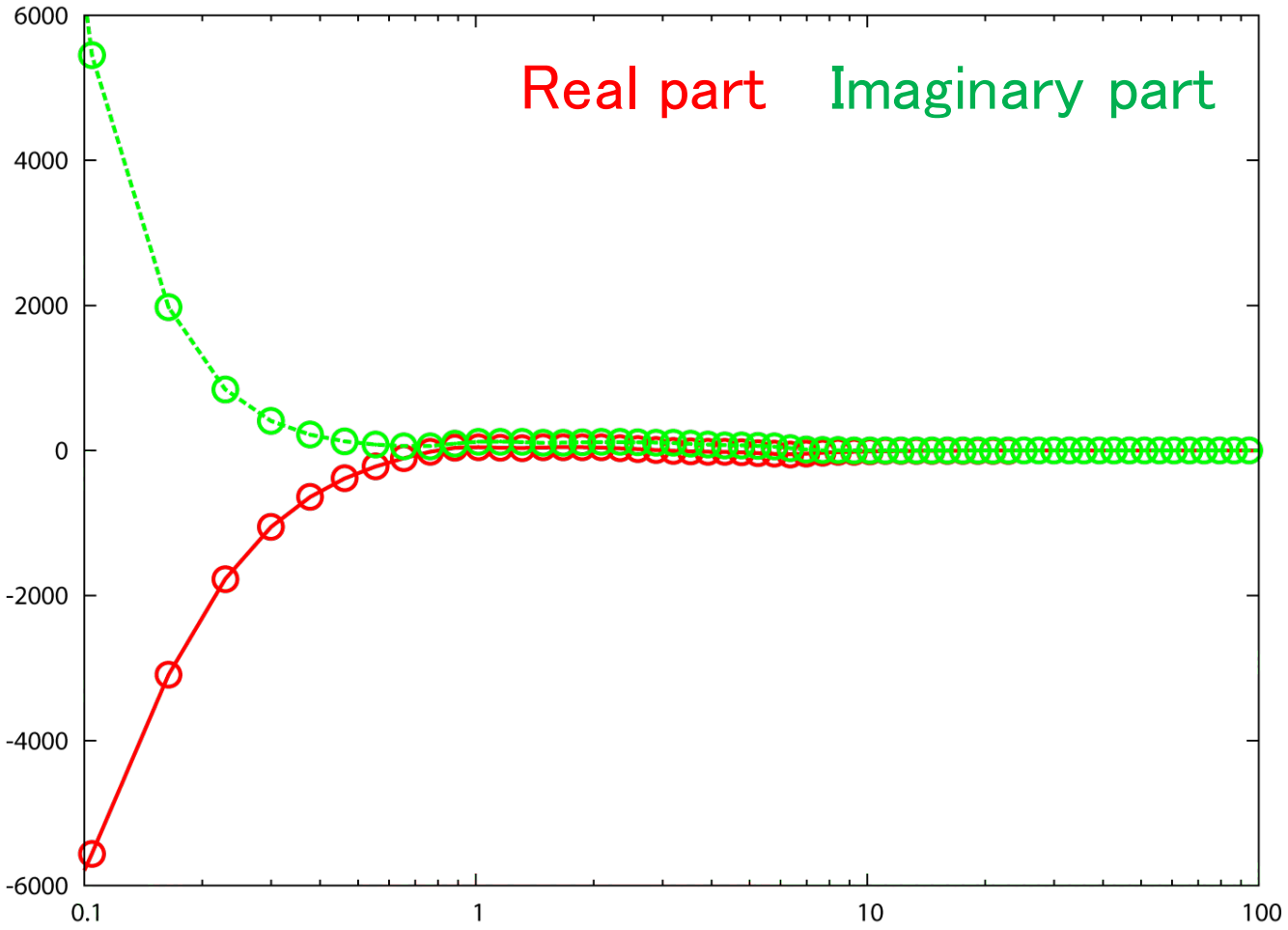
OUTPUT in chiqw (EELS)

```
> cd dir-eps/
> gnuplot
gnuplot> plot `dat.eels-x‘ u 1:2, `dat.eels’ u 1:3
```



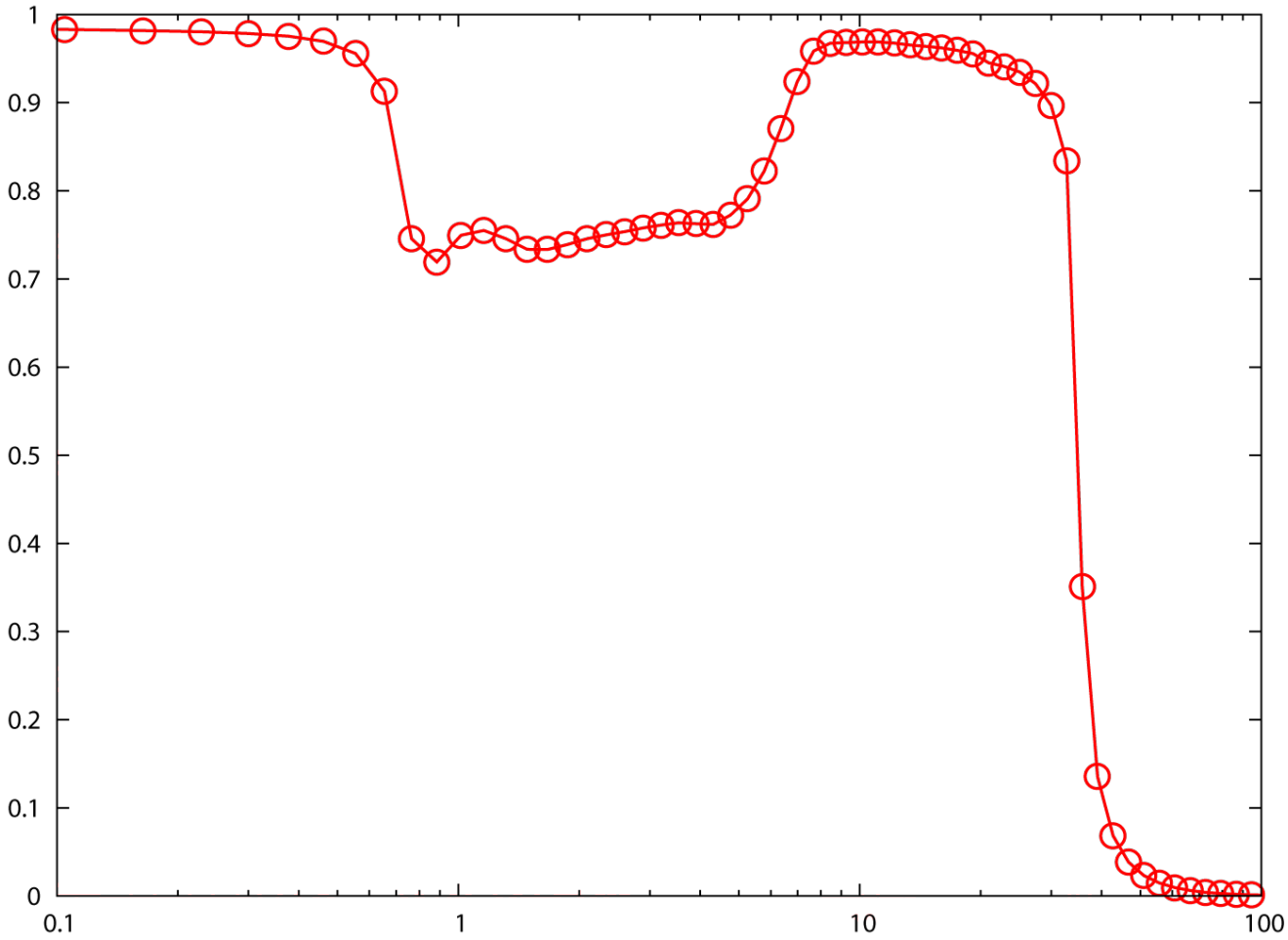
OUTPUT in chiqw (Optical conductivity)

```
> cd dir-eps/
> gnuplot
gnuplot> set logscale x; plot 'dat.optical_conductivity-x' u 1:2,
         'dat.optical_conductivity-x' u 1:3
```



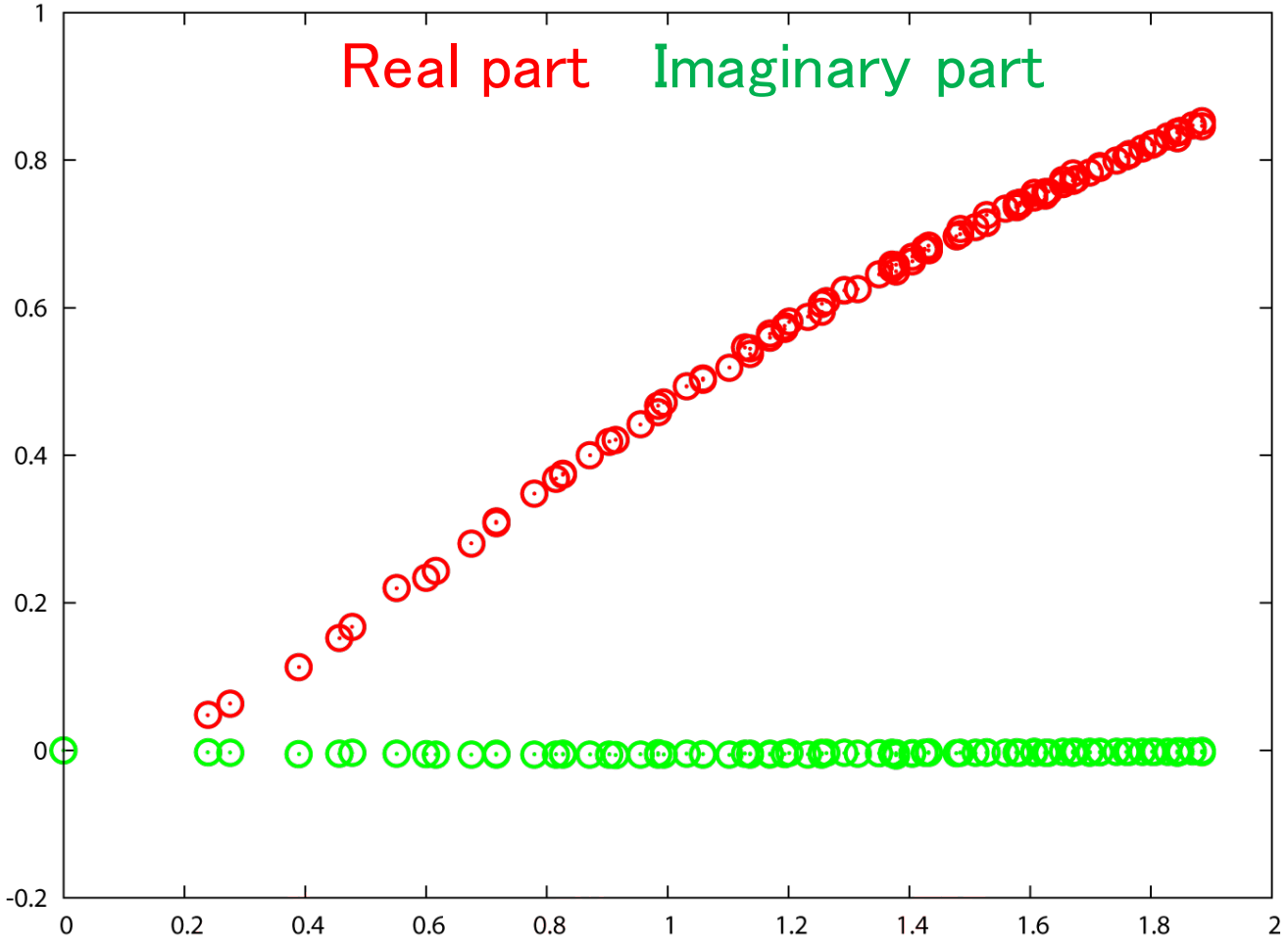
OUTPUT in chiqw (Reflectance)

```
> cd dir-eps/
> gnuplot
gnuplot> plot `dat.reflectivity-x'
```



OUTPUT in chiqw

```
> cat dir-eps/q0*/dat.epsqw.600001 > epsq0
> gnuplot
gnuplot> plot 'epsq0' u 1:2,'epsq0' u 1:3
```



OUTPUT in calc_int

Screened Coulomb integral

$$W_{ij}(\mathbf{R},\omega) = \int_V d\mathbf{r} \int_V d\mathbf{r}' w^*_{i\mathbf{0}}(\mathbf{r}) w_{i\mathbf{0}}(\mathbf{r}) W(\mathbf{r},\mathbf{r}',\omega) w^*_{j\mathbf{R}}(\mathbf{r}') w_{j\mathbf{R}}(\mathbf{r}')$$

> less log.Al-calc_w3d

!! $\omega = 0$

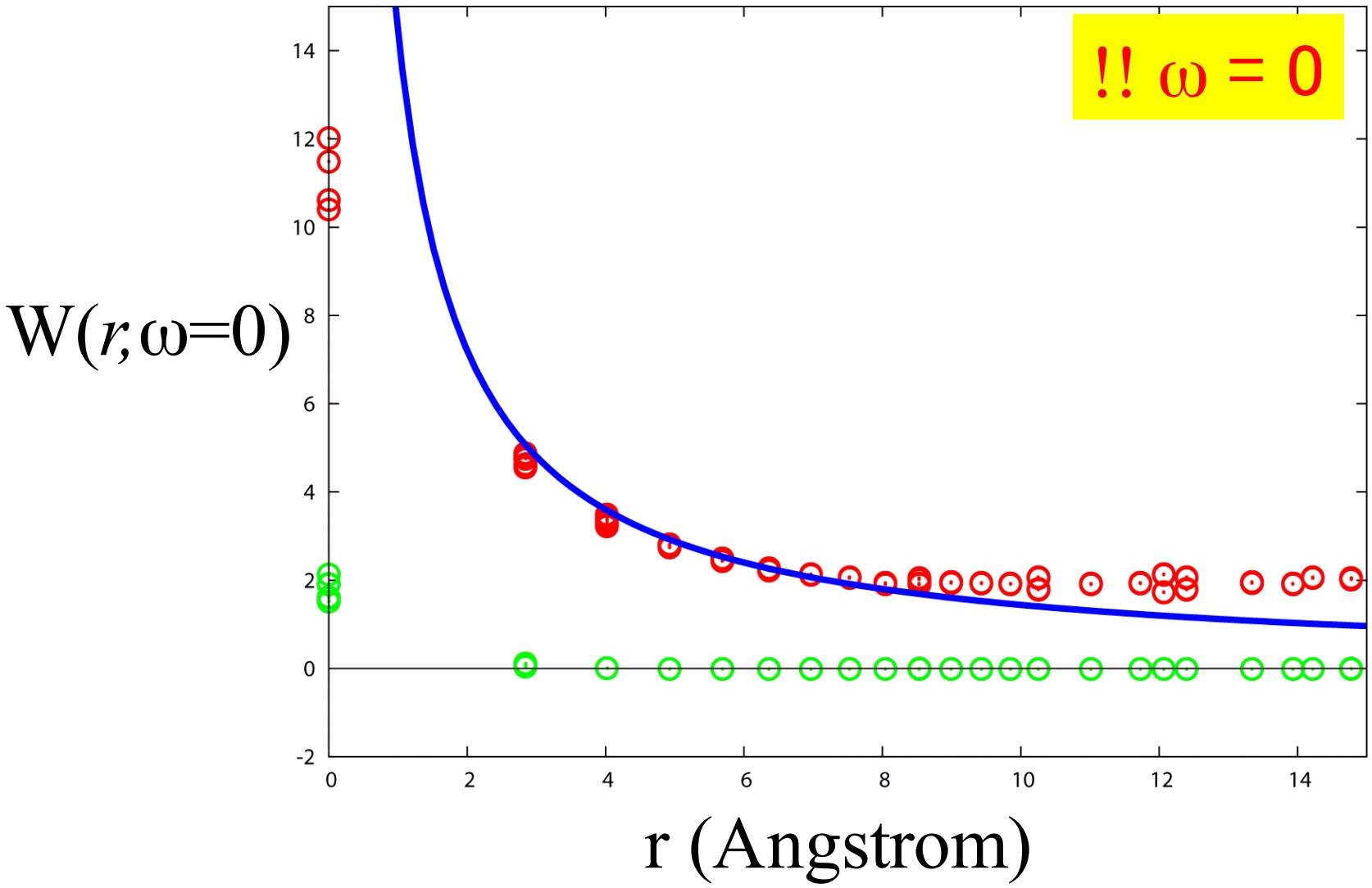
in eV

```
     0       0       0
 2.12878 1.91160 1.91129 1.91557 1.60892 1.61121 1.51849 1.61139 1.51439
 1.91160 2.53524 1.34343 1.34330 1.68691 1.05547 1.17082 1.68691 1.67226
 1.91129 1.34343 2.53453 1.34314 1.68657 1.68647 1.17065 1.05548 1.67192
 1.91557 1.34330 1.34314 2.53360 1.05545 1.68645 1.92002 1.68655 0.91746
 1.60892 1.68691 1.68657 1.05545 1.77622 1.17038 0.96019 1.17060 1.24700
 1.61121 1.05547 1.68647 1.68645 1.17038 1.77593 1.17401 1.17049 1.03039
 1.51849 1.17082 1.17065 1.92002 0.96019 1.17401 1.80037 1.17412 0.96096
 1.61139 1.68691 1.05548 1.68655 1.17060 1.17049 1.17412 1.77620 1.03060
 1.51439 1.67226 1.67192 0.91746 1.24700 1.03039 0.96096 1.03060 1.80556

     0       0       1
 0.06097 0.08081 0.03924 0.08056 0.05740 0.05726 0.08352 0.11886 0.06978
 0.08083 0.07827 0.05042 0.13360 0.06004 0.08269 0.14018 0.14446 0.06102
 0.03922 0.05039 0.02954 0.05039 0.04420 0.04417 0.05074 0.07851 0.04484
 0.08056 0.13359 0.05040 0.07810 0.08274 0.05993 0.08251 0.14438 0.11906
 0.05740 0.06003 0.04421 0.08274 0.05745 0.06993 0.08160 0.10210 0.05030
 0.05724 0.08266 0.04417 0.05992 0.06992 0.05736 0.06020 0.10203 0.07175
 0.08352 0.14016 0.05075 0.08251 0.08159 0.06021 0.10249 0.12832 0.13109
 0.11887 0.14446 0.07853 0.14439 0.10211 0.10205 0.12833 0.19369 0.11062
 0.06978 0.06101 0.04485 0.11906 0.05030 0.07176 0.13109 0.11061 0.04799
```

OUTPUT in calc_int

gnuplot> plot ‘dir-intW/dat.VvsR.001’,‘dir-intW/dat.WvsR.001’

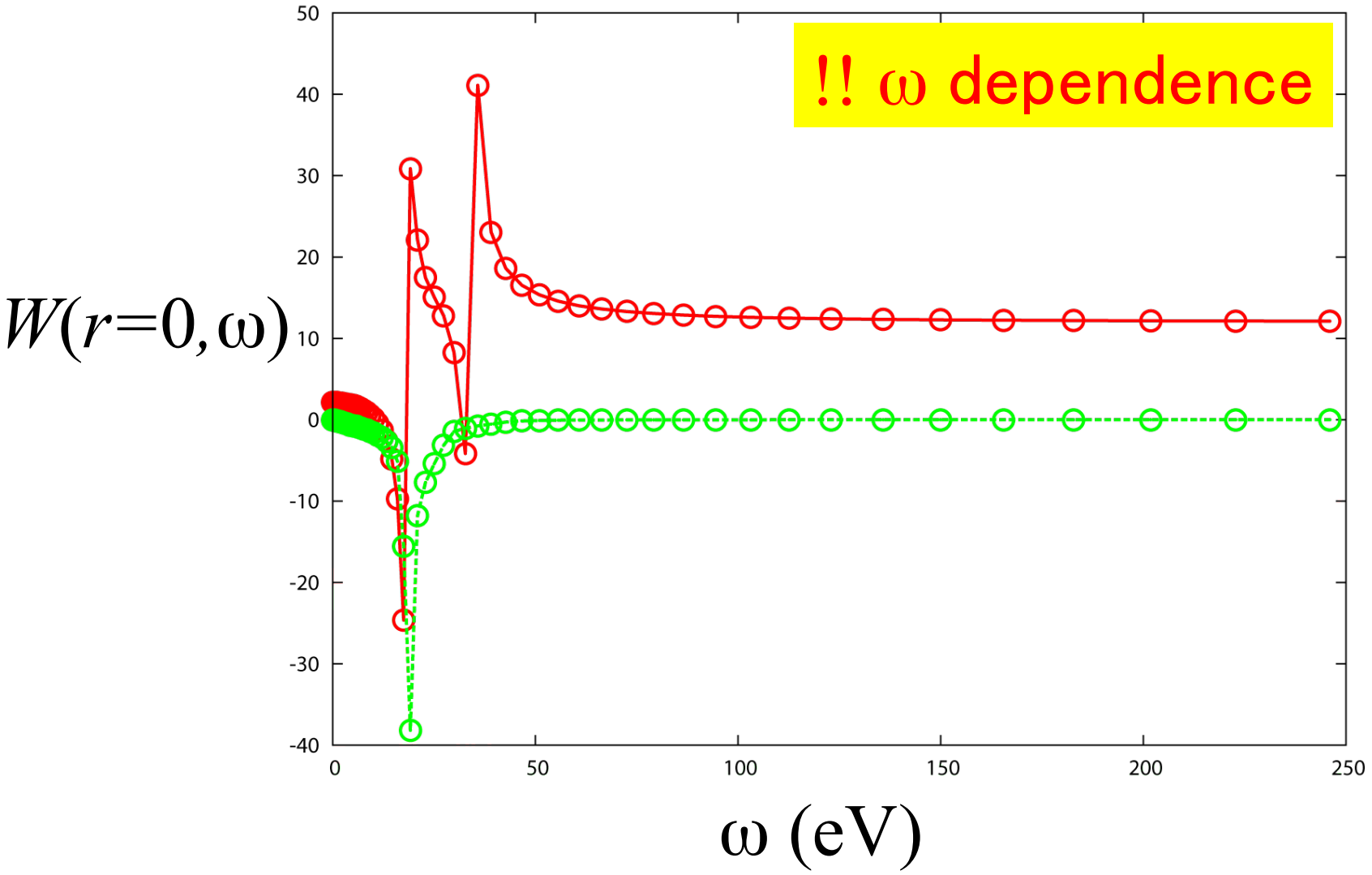
Bare Coulomb Screened Coulomb



OUTPUT in calc_int

gnuplot> plot ‘dir-intW/dat.UvsE.001-001’ u 1:3, ‘dir-intW/dat.UvsE.001-001’ u 1:4

Real part　　Imaginary part



OUTPUT in calc_int

Screened Exchange integral

$$J_{ij}(\mathbf{R},\omega) = \int_V d\mathbf{r} \int_V d\mathbf{r}' w^*_{i\mathbf{0}}(\mathbf{r}) w_{j\mathbf{R}}(\mathbf{r}) W(\mathbf{r},\mathbf{r}',\omega) w^*_{j\mathbf{R}}(\mathbf{r}') w_{i\mathbf{0}}(\mathbf{r}')$$

> less log.Al-calc_j3d

!! $\omega = 0$

in eV

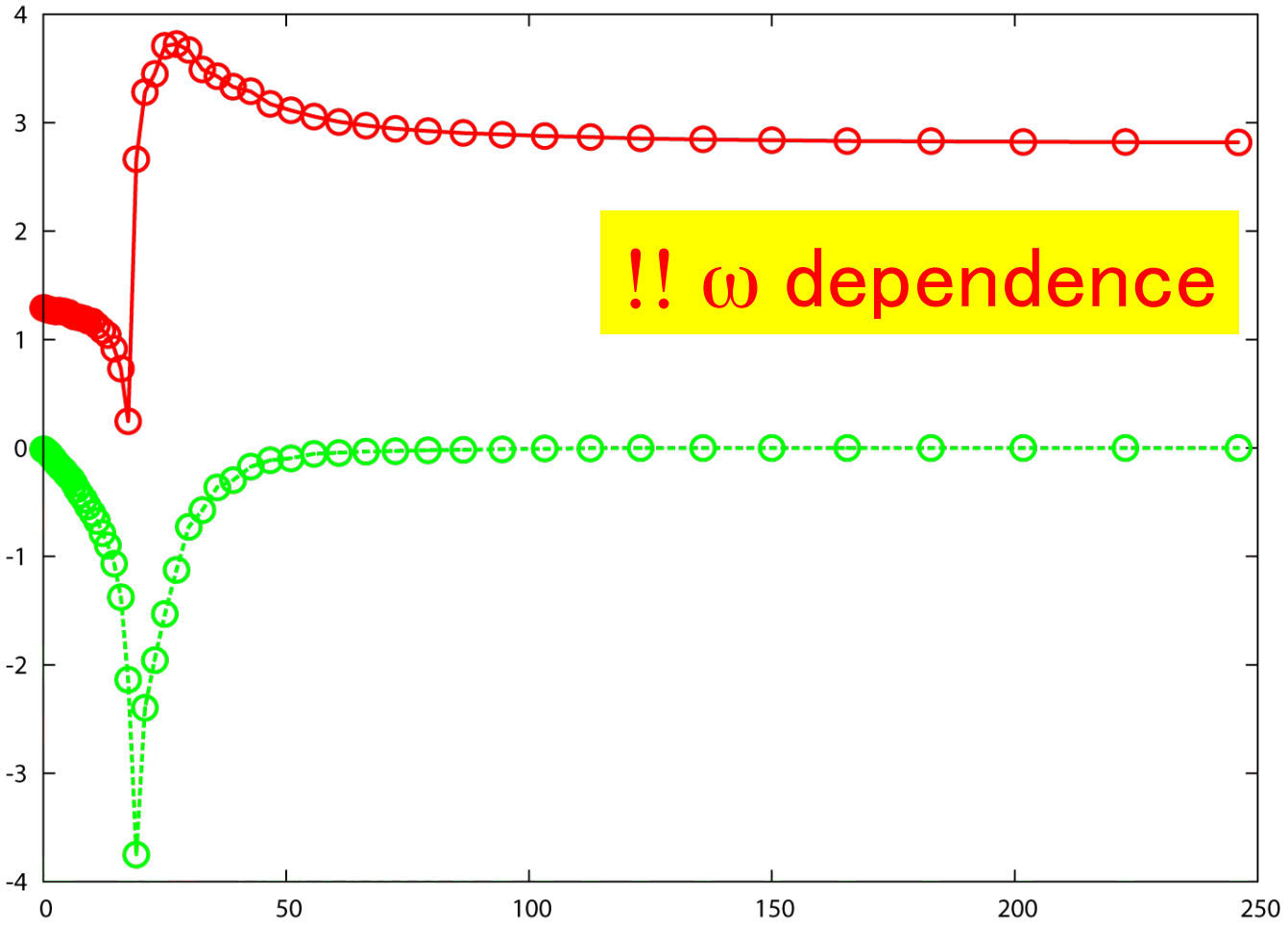
0	0	0						
2.12878	1.28938	1.28885	1.29494	0.79060	0.79294	0.76539	0.79304	0.76144
1.28938	2.53524	0.48554	0.48555	0.96892	0.24979	0.47109	0.96902	1.03490
1.28885	0.48554	2.53453	0.48549	0.96913	0.96893	0.47100	0.24979	1.03459
1.29494	0.48555	0.48549	2.53360	0.24988	0.96897	1.31316	0.96926	0.18624
0.79060	0.96892	0.96913	0.24988	1.77622	0.42483	0.31966	0.42481	0.25523
0.79294	0.24979	0.96893	0.96897	0.42483	1.77593	0.27011	0.42484	0.30228
0.76539	0.47109	0.47100	1.31316	0.31966	0.27011	1.80037	0.27013	0.42547
0.79304	0.96902	0.24979	0.96926	0.42481	0.42484	0.27013	1.77620	0.30231
0.76144	1.03490	1.03459	0.18624	0.25523	0.30228	0.42547	0.30231	1.80556

OUTPUT in calc_int

```
gnuplot> plot 'dir-intJ/dat.JvsE.001-001' u 1:3, 'dir-intJ/dat.JvsE.001-001' u 1:4
```

Real part　　Imaginary part

$J(r=0,\omega)$

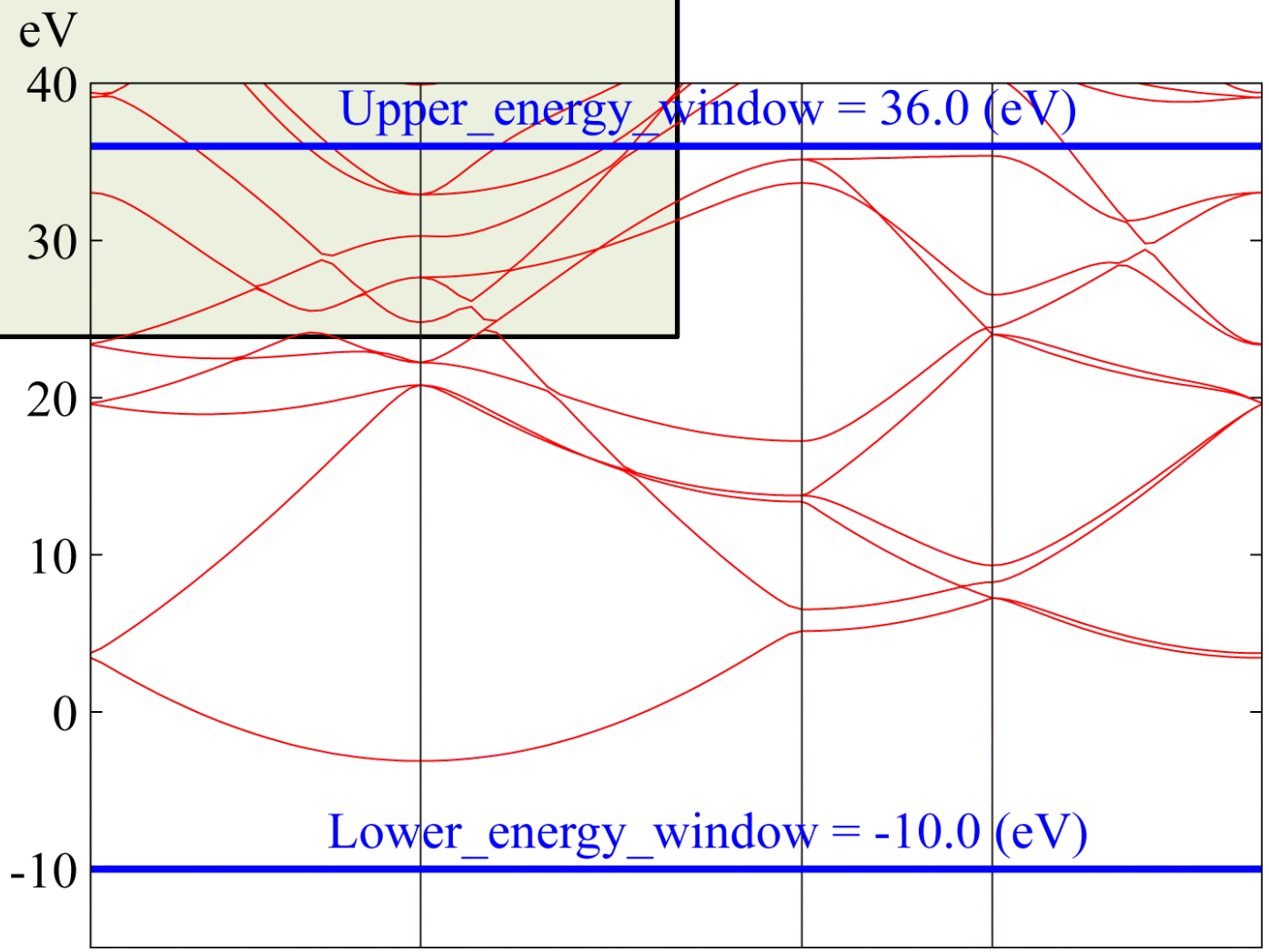


&param_wannier of Al

```
&param_wannier
N_wannier=9,                          !Total number of considerd band in wannier calc
Lower_energy_window=-10.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window= 36.0d0,  !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=9/                    !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
```

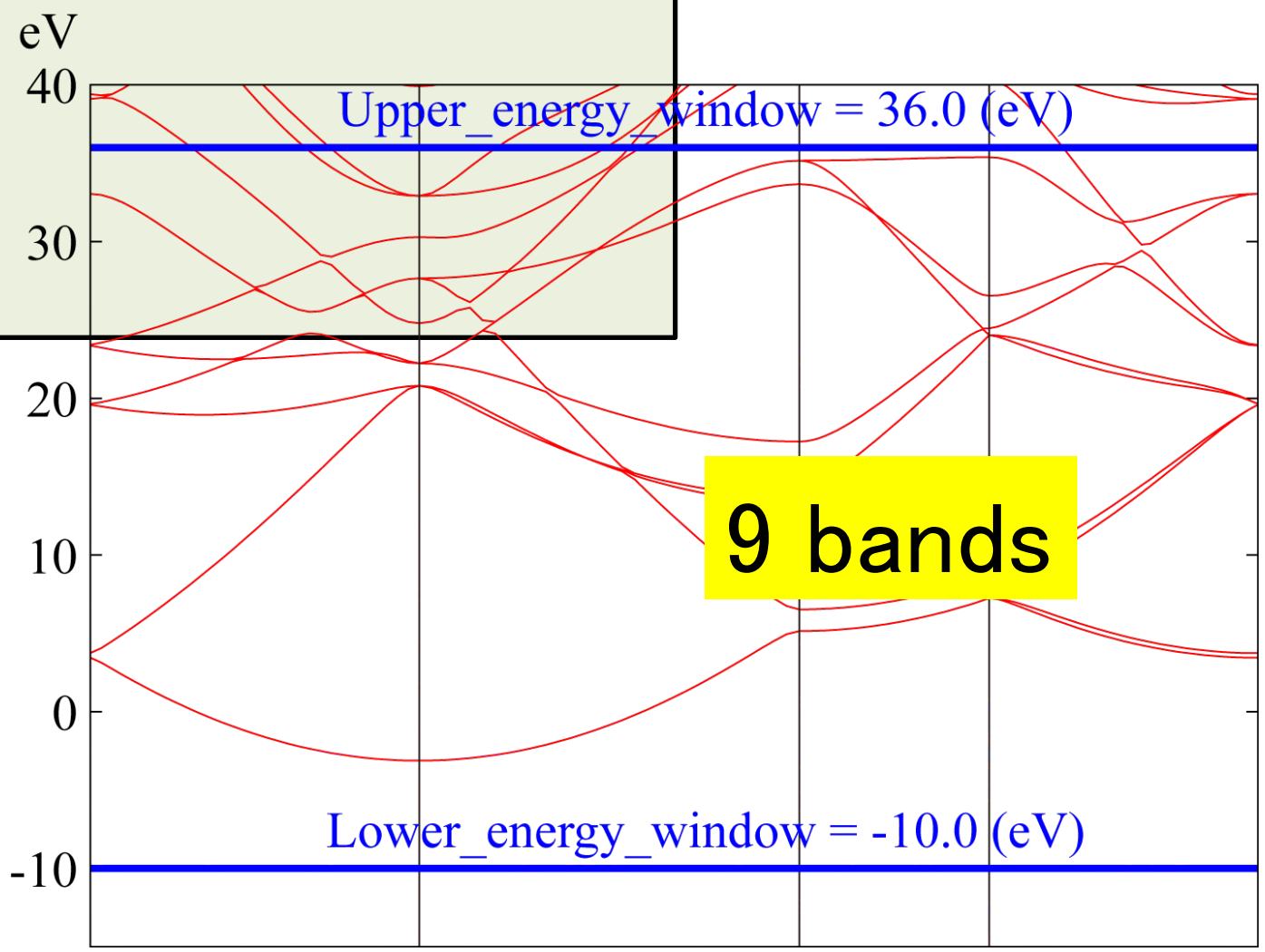
&param_wannier of Al

```
&param_wannier
N_wannier=9,                    !Total number of considerd band in wannier calc
Lower_energy_window=-10.0d0, !LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window= 36.0d0,  !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=9/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
```



&param_wannier of Al

```
&param_wannier
N_wannier=9,                    !Total number of considerd band in wannier calc
Lower_energy_window=-10.0d0, !LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window= 36.0d0,  !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=9/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
```

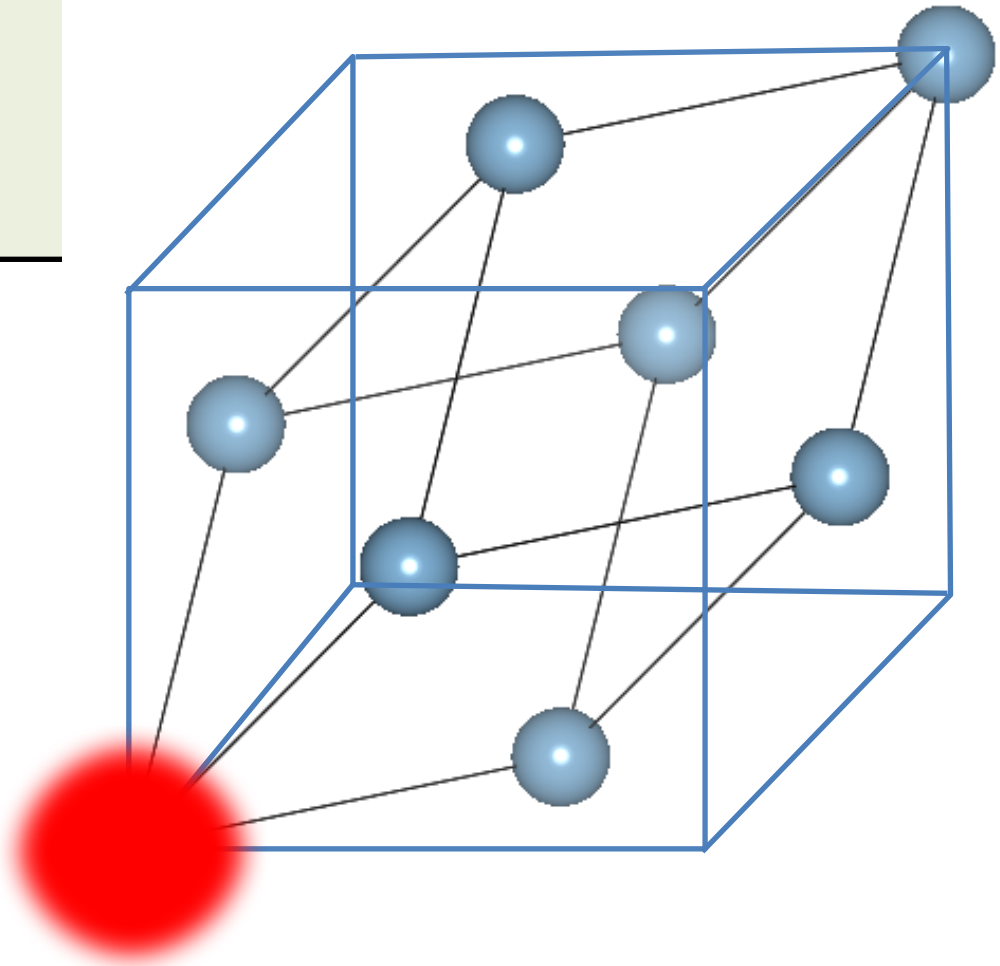


&param_wannier of Al

```
&param_wannier
N_wannier=9,                    !Total number of considerd band in wannier calc
Lower_energy_window=-10.0d0, !LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window= 36.0d0,  !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=9/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
```

$$\exp[-0.2(\boldsymbol{r} - \boldsymbol{r}_{\mathrm{g}})]$$

$$\boldsymbol{r}_g = 0.0\mathbf{a}_1 + 0.0\mathbf{a}_2 + 0.0\mathbf{a}_3$$

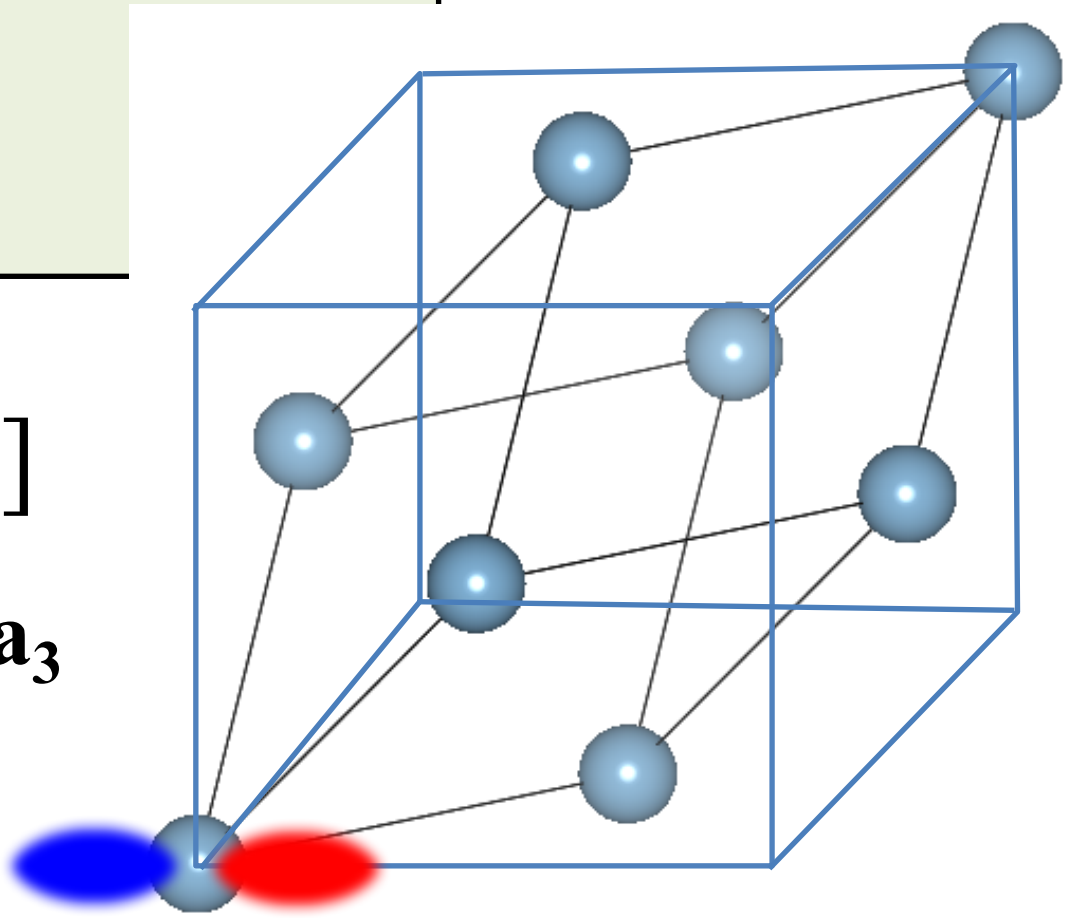


&param_wannier of Al

```
&param_wannier
N_wannier=9,                    !Total number of considerd band in wannier calc
Lower_energy_window=-10.0d0, !LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window= 36.0d0,  !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=9/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
```

$$x\exp[-0.2(\boldsymbol{r} - \boldsymbol{r}_g)]$$

$$\boldsymbol{r}_g = 0.0\mathbf{a}_1 + 0.0\mathbf{a}_2 + 0.0\mathbf{a}_3$$

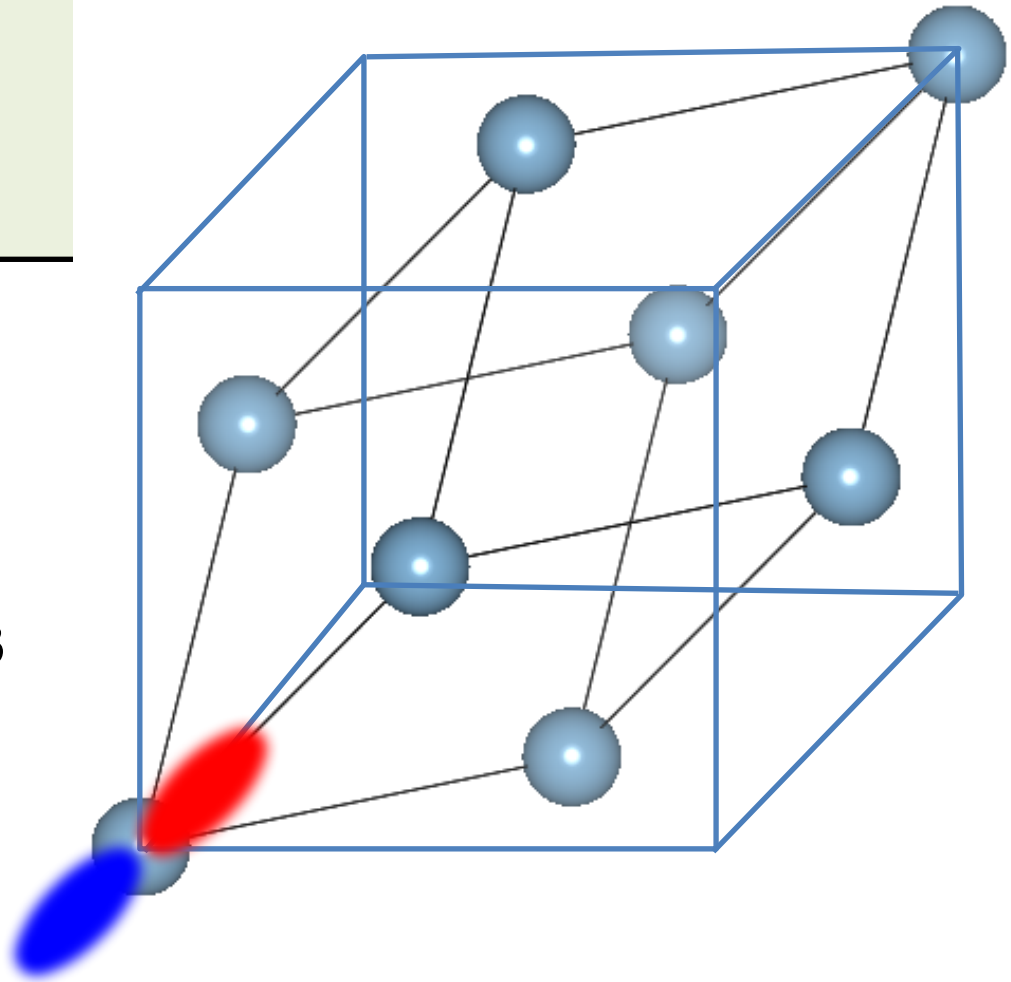


&param_wannier of Al

```
&param_wannier
N_wannier=9,                        !Total number of considerd band in wannier calc
Lower_energy_window=-10.0d0, !LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window= 36.0d0,  !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=9/                  !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
```

$$y\exp[-0.2(\boldsymbol{r} - \boldsymbol{r}_g)]$$

$$\boldsymbol{r}_g = 0.0\mathbf{a}_1 + 0.0\mathbf{a}_2 + 0.0\mathbf{a}_3$$

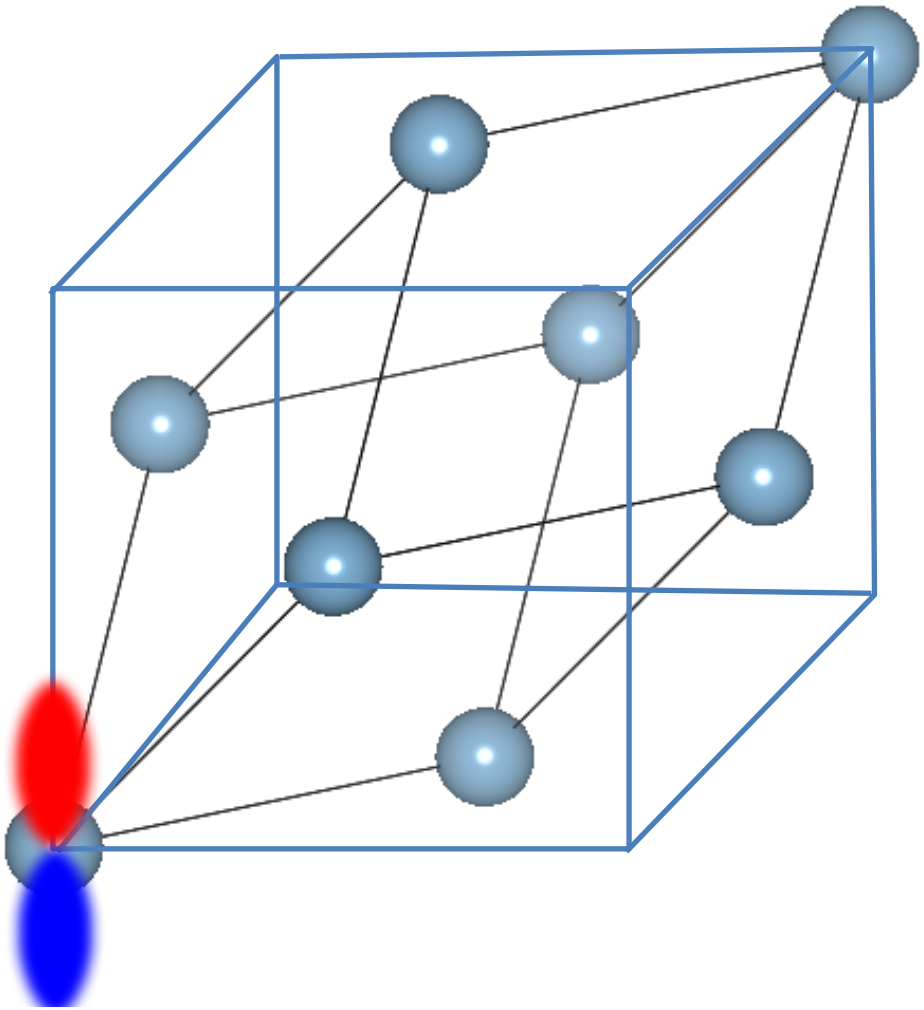


&param_wannier of Al

```
&param_wannier
N_wannier=9,                        !Total number of considerd band in wannier calc
Lower_energy_window=-10.0d0, !LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window= 36.0d0,  !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=9/                  !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
```

$$z\exp[-0.2(\boldsymbol{r} - \boldsymbol{r}_{\mathrm{g}})]$$

$$\boldsymbol{r}_g = 0.0\mathbf{a}_1 + 0.0\mathbf{a}_2 + 0.0\mathbf{a}_3$$

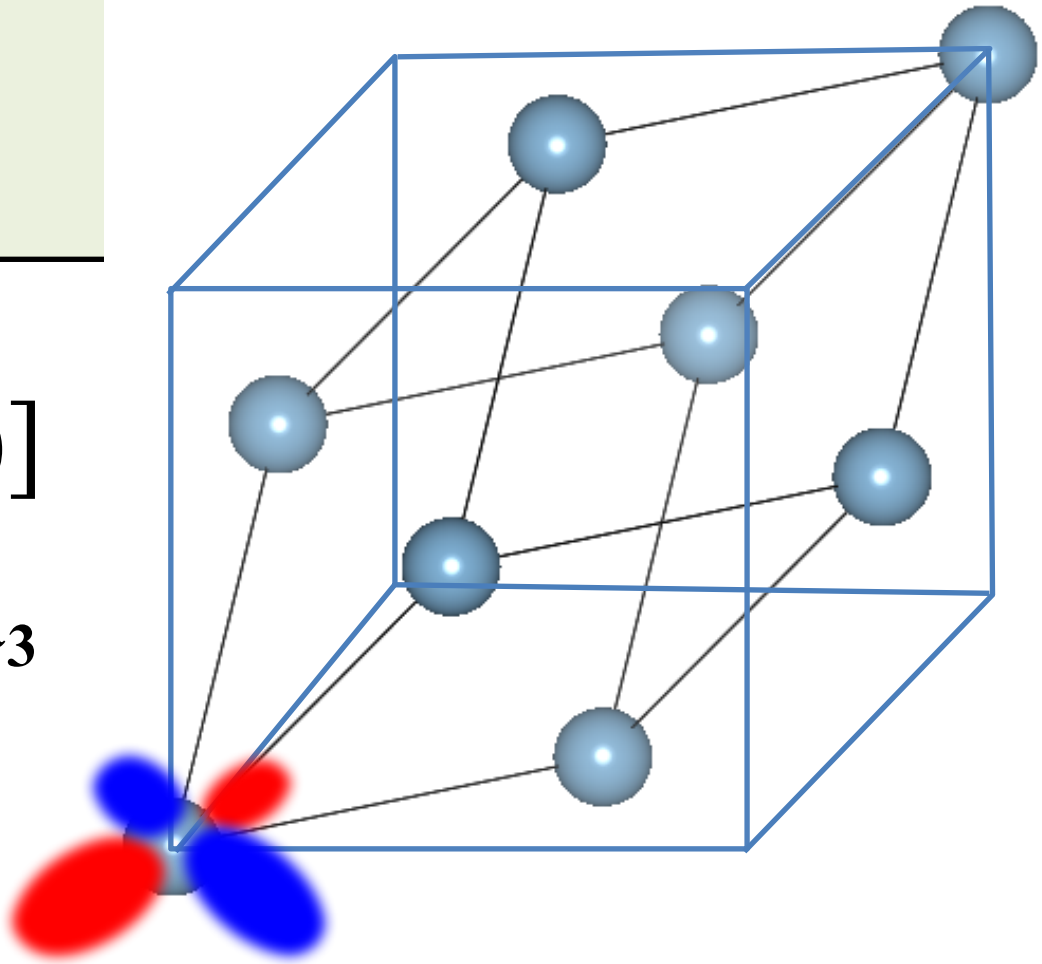


&param_wannier of Al

```
&param_wannier
N_wannier=9,                        !Total number of considerd band in wannier calc
Lower_energy_window=-10.0d0, !LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window= 36.0d0,  !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=9/                  !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
```

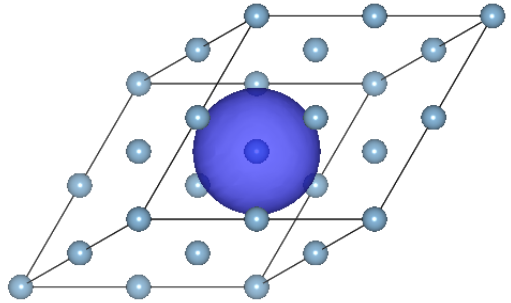
$$xy\exp[-0.2(\boldsymbol{r} - \boldsymbol{r}_g)]$$

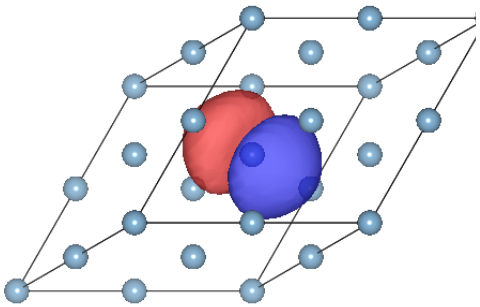
$$\boldsymbol{r}_g = 0.0\mathbf{a}_1 + 0.0\mathbf{a}_2 + 0.0\mathbf{a}_3$$

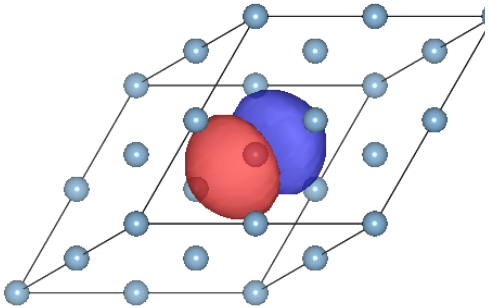


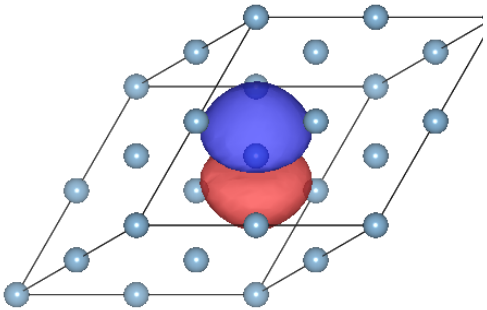
Results of Al

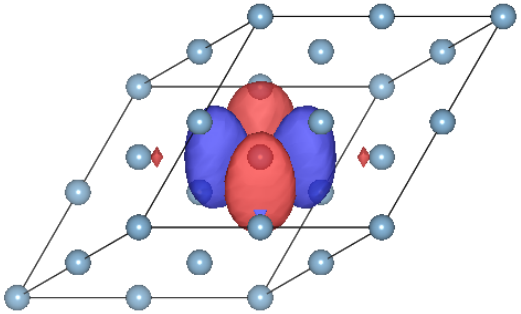
```
&param_wannier
N_wannier=9,                    !Total number of considerd band in wannier calc
Lower_energy_window=-10.0d0, !LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window= 36.0d0,  !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=9/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s   0.2d0  0.00d0  0.00d0  0.00d0
px  0.2d0  0.00d0  0.00d0  0.00d0
py  0.2d0  0.00d0  0.00d0  0.00d0
pz  0.2d0  0.00d0  0.00d0  0.00d0
dxy 0.2d0  0.00d0  0.00d0  0.00d0
dyz 0.2d0  0.00d0  0.00d0  0.00d0
dz2 0.2d0  0.00d0  0.00d0  0.00d0
dzx 0.2d0  0.00d0  0.00d0  0.00d0
dx2 0.2d0  0.00d0  0.00d0  0.00d0
```

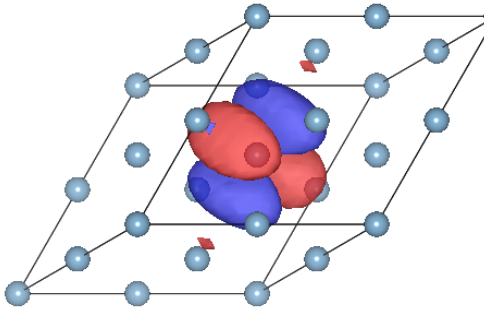


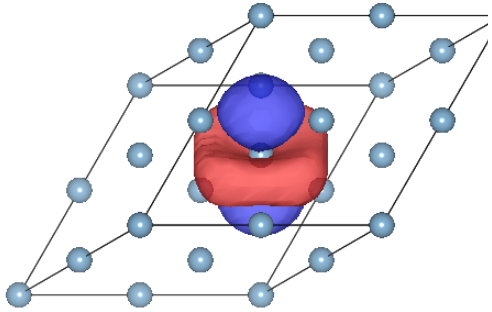


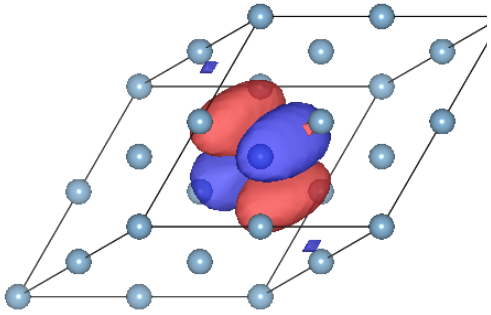


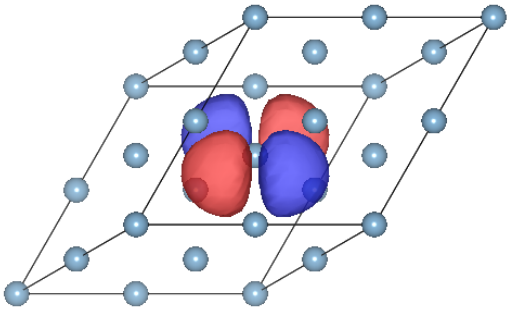










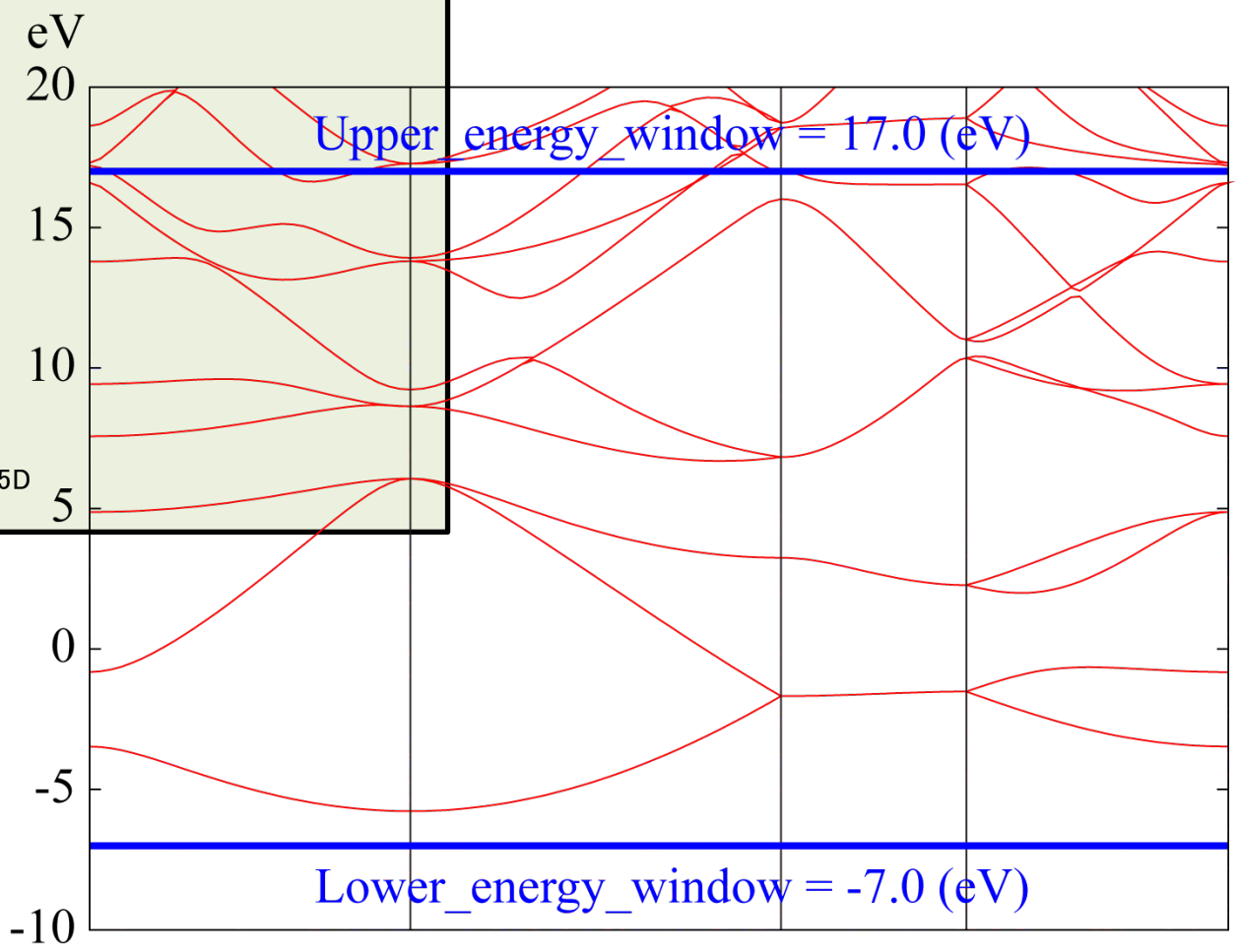


&param_wannier of Si

```
&param_wannier
N_wannier=8,                !Total number of considerd band in wannier calc
Lower_energy_window=-7.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=17.0d0,!UPPER BOUND OF ENERGY WINDOW (eV)
flg_BMAT=1,                 !0:BMAT=unit matrix, 1:reading BMAT
N_initial_guess=8/          !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s  0.5D0 0.00D0 0.00D0 0.00D0
px 0.5D0 0.00D0 0.00D0 0.00D0
py 0.5D0 0.00D0 0.00D0 0.00D0
pz 0.5D0 0.00D0 0.00D0 0.00D0
s  0.5D0 0.25D0 0.25D0 0.25D0
px 0.5D0 0.25D0 0.25D0 0.25D0
py 0.5D0 0.25D0 0.25D0 0.25D0
pz 0.5D0 0.25D0 0.25D0 0.25D0
0.50 -0.5D0  0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0 -0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50 -0.5D0 -0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0  0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0  0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0  0.5D0 -0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0 -0.5D0  0.5D0
0.00  0.0d0  0.0d0  0.0d0 -0.5D0  -0.5D0  -0.5D0  -0.5D
```

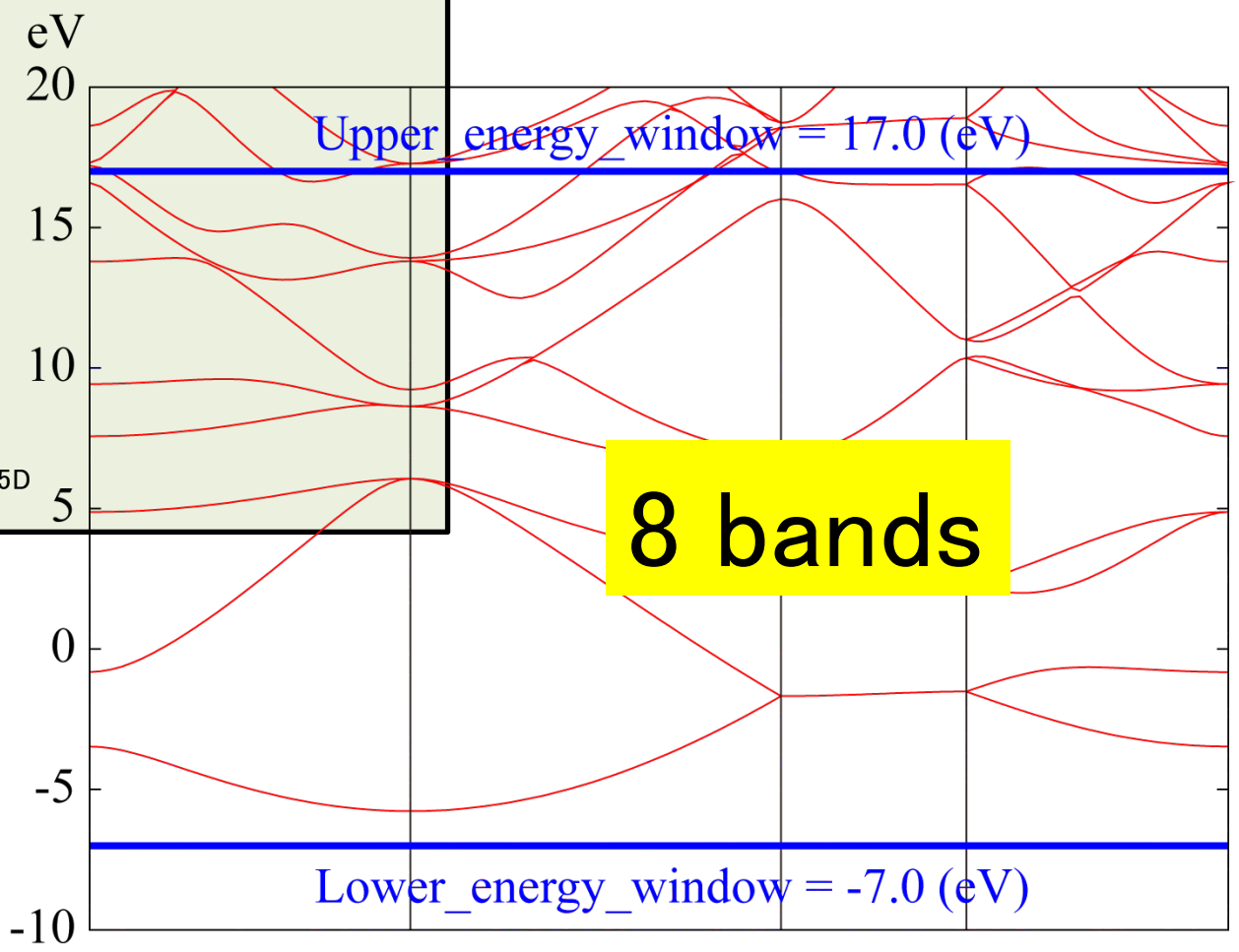
&param_wannier of Si

```
&param_wannier
N_wannier=8,              !Total number of considerd band in wannier calc
Lower_energy_window=-7.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=17.0d0,!UPPER BOUND OF ENERGY  WINDOW (eV)
flg_BMAT=1,               !0:BMAT=unit matrix, 1:reading BMAT
N_initial_guess=8/        !TOTAL  NUMBER OF INITIAL GUESS GAUSSIAN
s  0.5D0 0.00D0 0.00D0 0.00D0
px 0.5D0 0.00D0 0.00D0 0.00D0
py 0.5D0 0.00D0 0.00D0 0.00D0
pz 0.5D0 0.00D0 0.00D0 0.00D0
s  0.5D0 0.25D0 0.25D0 0.25D0
px 0.5D0 0.25D0 0.25D0 0.25D0
py 0.5D0 0.25D0 0.25D0 0.25D0
pz 0.5D0 0.25D0 0.25D0 0.25D0
0.50 -0.5D0  0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0 -0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50 -0.5D0 -0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0  0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0  0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0  0.5D0 -0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0 -0.5D0  0.5D0
0.00  0.0d0  0.0d0  0.0d0 -0.5D0  -0.5D0  -0.5D0  -0.5D
```

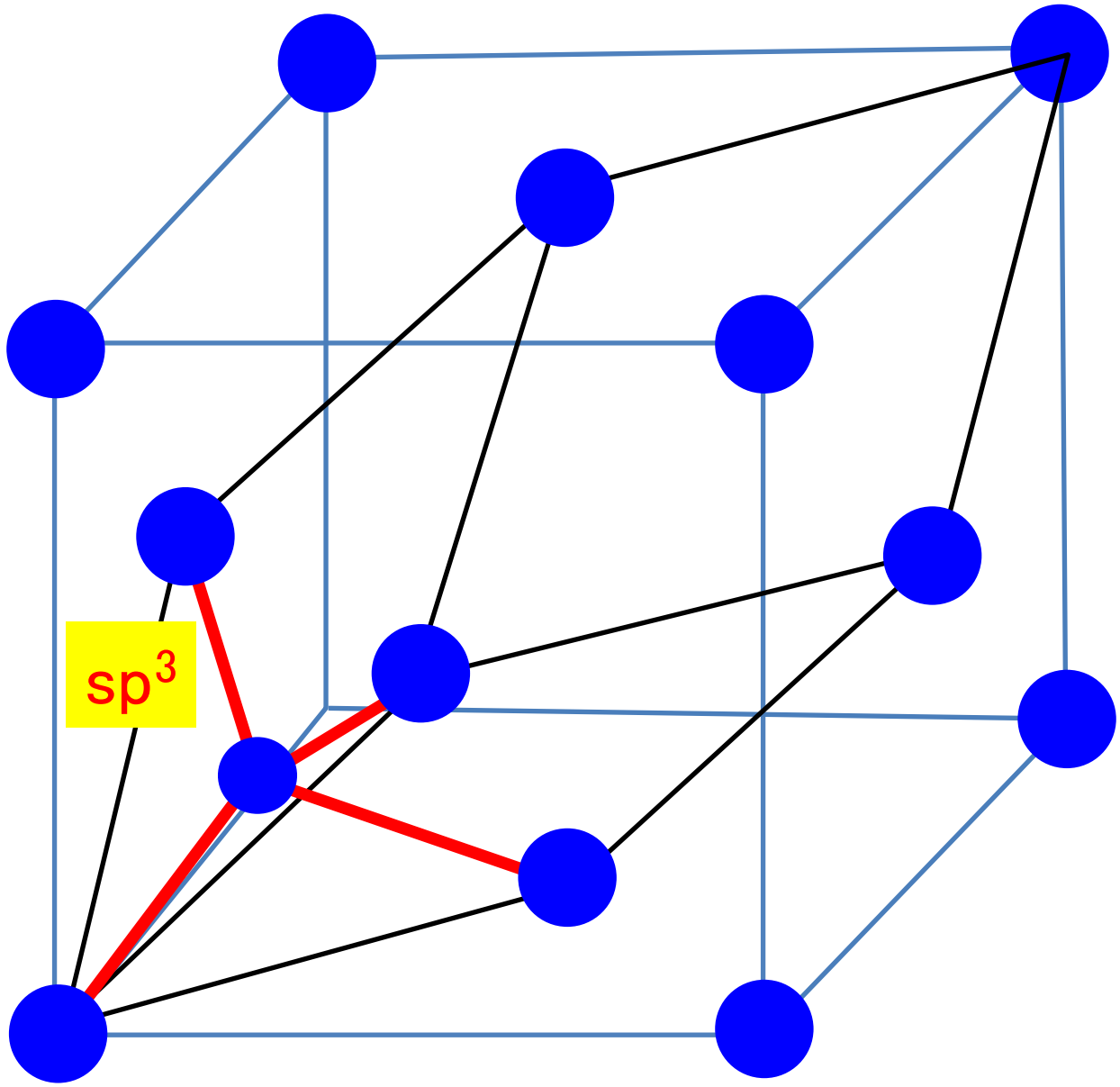


&param_wannier of Si

```
&param_wannier
N_wannier=8,              !Total number of considerd band in wannier calc
Lower_energy_window=-7.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=17.0d0,!UPPER BOUND OF ENERGY WINDOW (eV)
flg_BMAT=1,               !0:BMAT=unit matrix, 1:reading BMAT
N_initial_guess=8/        !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s  0.5D0 0.00D0 0.00D0 0.00D0
px 0.5D0 0.00D0 0.00D0 0.00D0
py 0.5D0 0.00D0 0.00D0 0.00D0
pz 0.5D0 0.00D0 0.00D0 0.00D0
s  0.5D0 0.25D0 0.25D0 0.25D0
px 0.5D0 0.25D0 0.25D0 0.25D0
py 0.5D0 0.25D0 0.25D0 0.25D0
pz 0.5D0 0.25D0 0.25D0 0.25D0
0.50 -0.5D0  0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0 -0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50 -0.5D0 -0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0  0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0  0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0  0.5D0 -0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0 -0.5D0  0.5D0
0.00  0.0d0  0.0d0  0.0d0 -0.5D0  -0.5D0  -0.5D0  -0.5D
```



sp^3 orbital of Si

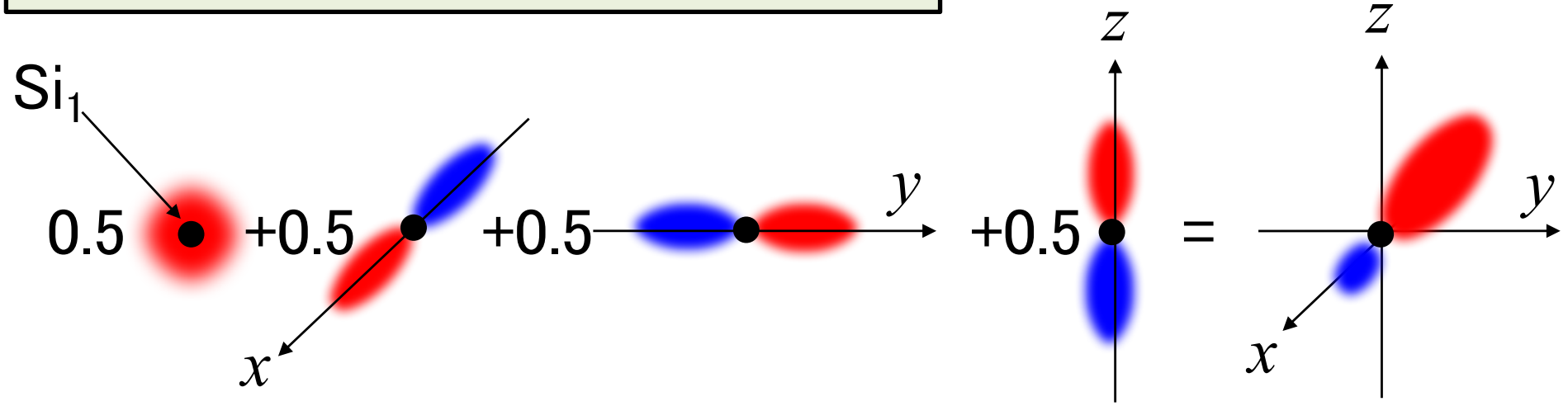


sp^3 orbital of Si

```
&param_wannier
N_wannier=8,              !Total number of considerd band in wannier calc
Lower_energy_window=-7.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=17.0d0,!UPPER BOUND OF ENERGY  WINDOW (eV)
flg_BMAT=1,               !0:BMAT=unit matrix, 1:reading BMAT
N_initial_guess=8/        !TOTAL  NUMBER OF INITIAL GUESS GAUSSIAN
s  0.5d0 0.00d0 0.00d0 0.00d0
px 0.5d0 0.00d0 0.00d0 0.00d0
py 0.5d0 0.00d0 0.00d0 0.00d0
pz 0.5d0 0.00d0 0.00d0 0.00d0
s  0.5d0 0.25d0 0.25d0 0.25d0
px 0.5d0 0.25d0 0.25d0 0.25d0
py 0.5d0 0.25d0 0.25d0 0.25d0
pz 0.5d0 0.25d0 0.25d0 0.25d0
0.50 -0.5D0  0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0 -0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50 -0.5D0 -0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0  0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0  0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0  0.5D0 -0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0 -0.5D0  0.5D0
0.00  0.0d0  0.0d0  0.0d0 -0.5D0  -0.5D0  -0.5D0  -0.5D
```

row: Gaussian

column: Wannier

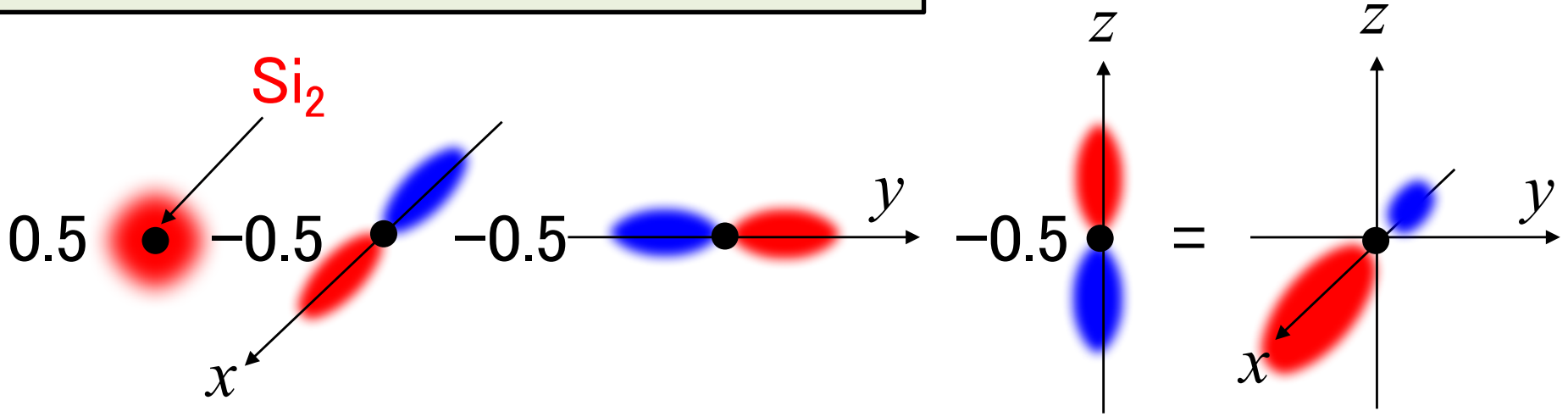


sp^3 orbital of Si

```
&param_wannier
N_wannier=8,              !Total number of considerd band in wannier calc
Lower_energy_window=-7.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=17.0d0,!UPPER BOUND OF ENERGY  WINDOW (eV)
flg_BMAT=1,               !0:BMAT=unit matrix, 1:reading BMAT
N_initial_guess=8/        !TOTAL  NUMBER OF INITIAL GUESS GAUSSIAN
s  0.5d0 0.00d0 0.00d0 0.00d0
px 0.5d0 0.00d0 0.00d0 0.00d0
py 0.5d0 0.00d0 0.00d0 0.00d0
pz 0.5d0 0.00d0 0.00d0 0.00d0
s  0.5d0 0.25d0 0.25d0 0.25d0
px 0.5d0 0.25d0 0.25d0 0.25d0
py 0.5d0 0.25d0 0.25d0 0.25d0
pz 0.5d0 0.25d0 0.25d0 0.25d0
0.50 -0.5D0  0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0 -0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50 -0.5D0 -0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0  0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0  0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0  0.5D0 -0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0 -0.5D0  0.5D0
0.00  0.0d0  0.0d0  0.0d0 -0.5D0  -0.5D0  -0.5D0  -0.5D0
```

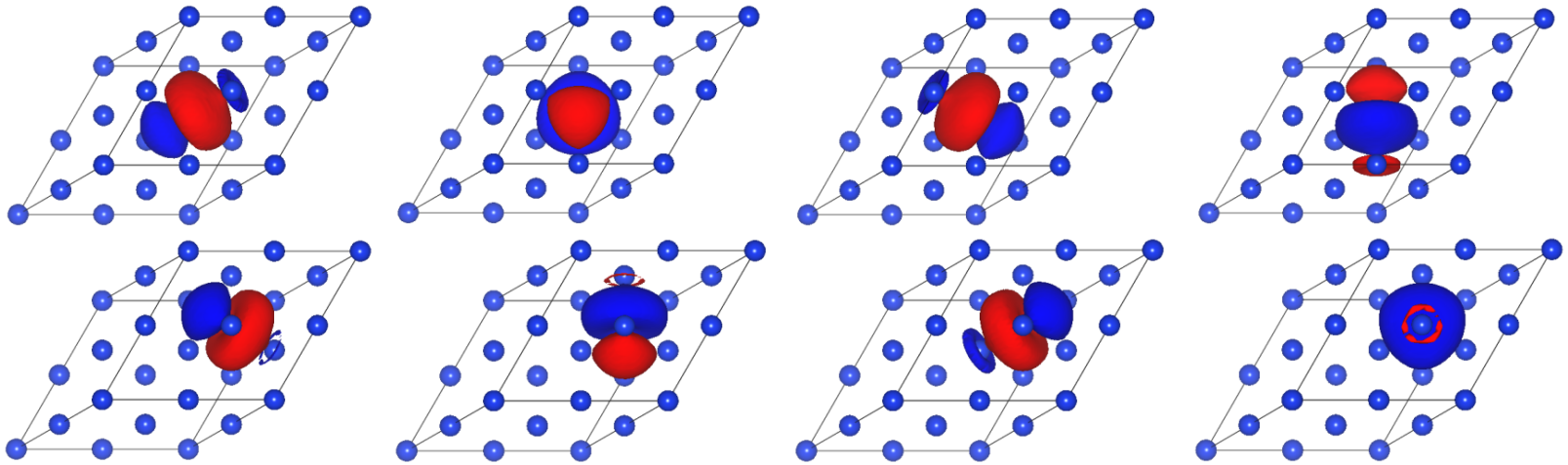
row: Gaussian

column: Wannier



Results of Si

```
&param_wannier
N_wannier=8,              !Total number of considerd band in wannier calc
Lower_energy_window=-7.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=17.0d0,!UPPER BOUND OF ENERGY WINDOW (eV)
flg_BMAT=1,               !0:BMAT=unit matrix, 1:reading BMAT
N_initial_guess=8/        !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
s  0.5D0 0.00D0 0.00D0 0.00D0
px 0.5D0 0.00D0 0.00D0 0.00D0
py 0.5D0 0.00D0 0.00D0 0.00D0
pz 0.5D0 0.00D0 0.00D0 0.00D0
s  0.5D0 0.25D0 0.25D0 0.25D0
px 0.5D0 0.25D0 0.25D0 0.25D0
py 0.5D0 0.25D0 0.25D0 0.25D0
pz 0.5D0 0.25D0 0.25D0 0.25D0
0.50 -0.5D0  0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0 -0.5D0 -0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50 -0.5D0 -0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.50  0.5D0  0.5D0  0.5D0 0.0d0  0.0d0  0.0d0  0.0d0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0  0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0  0.5D0 -0.5D0 -0.5D0
0.00  0.0d0  0.0d0  0.0d0 0.5D0 -0.5D0 -0.5D0  0.5D0
0.00  0.0d0  0.0d0  0.0d0 -0.5D0  -0.5D0  -0.5D0  -0.5D
```

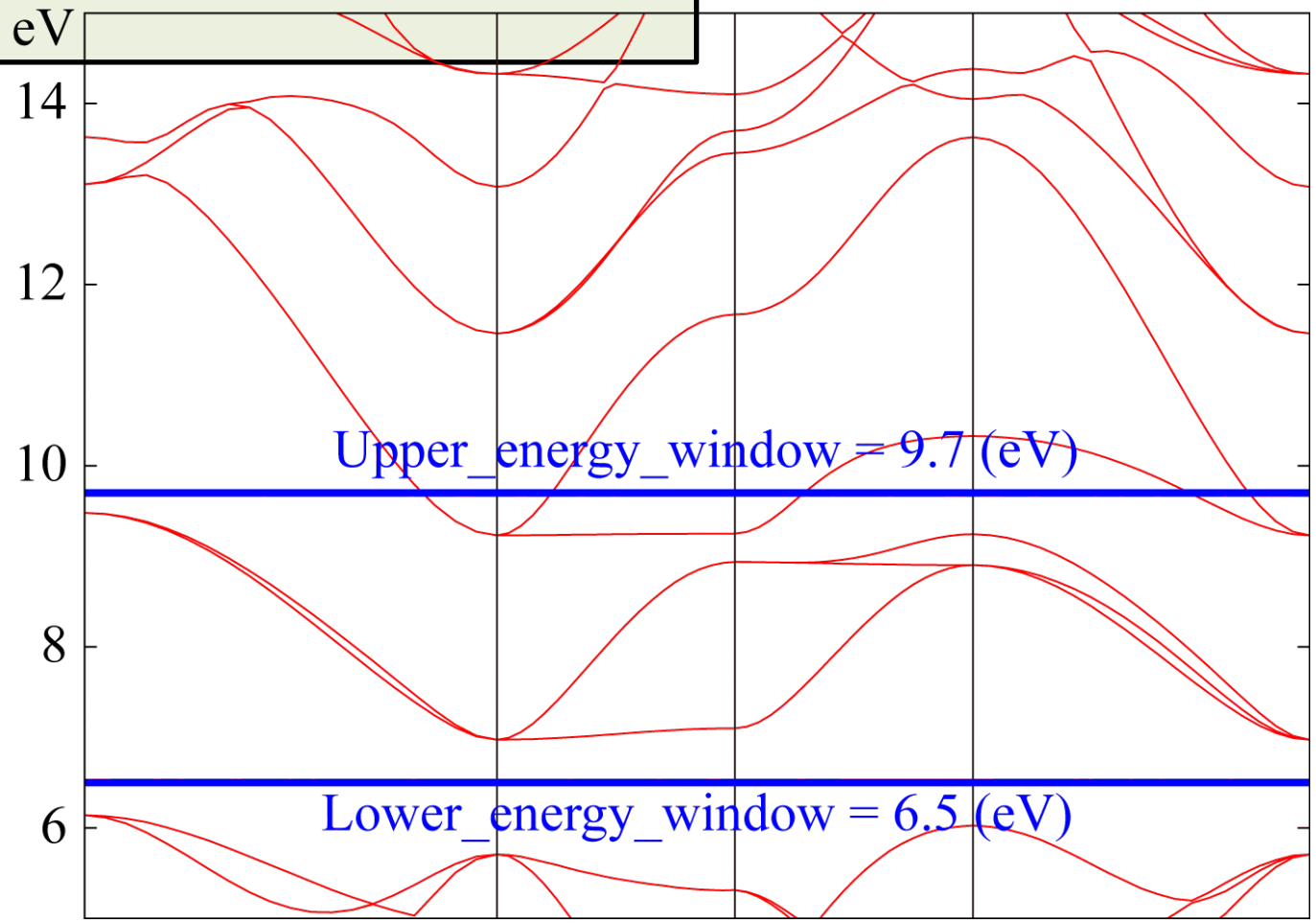


&param_wannier of SrVO3

```
&param_wannier
N_wannier=3,                    !Total number of considerd band in wannier calc
Lower_energy_window=6.5d0, !UPPER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=9.7d0, !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=3/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dxy 0.5d0 0.5d0 0.5d0 0.5d0
dyz 0.5d0 0.5d0 0.5d0 0.5d0
dzx 0.5d0 0.5d0 0.5d0 0.5d0
```

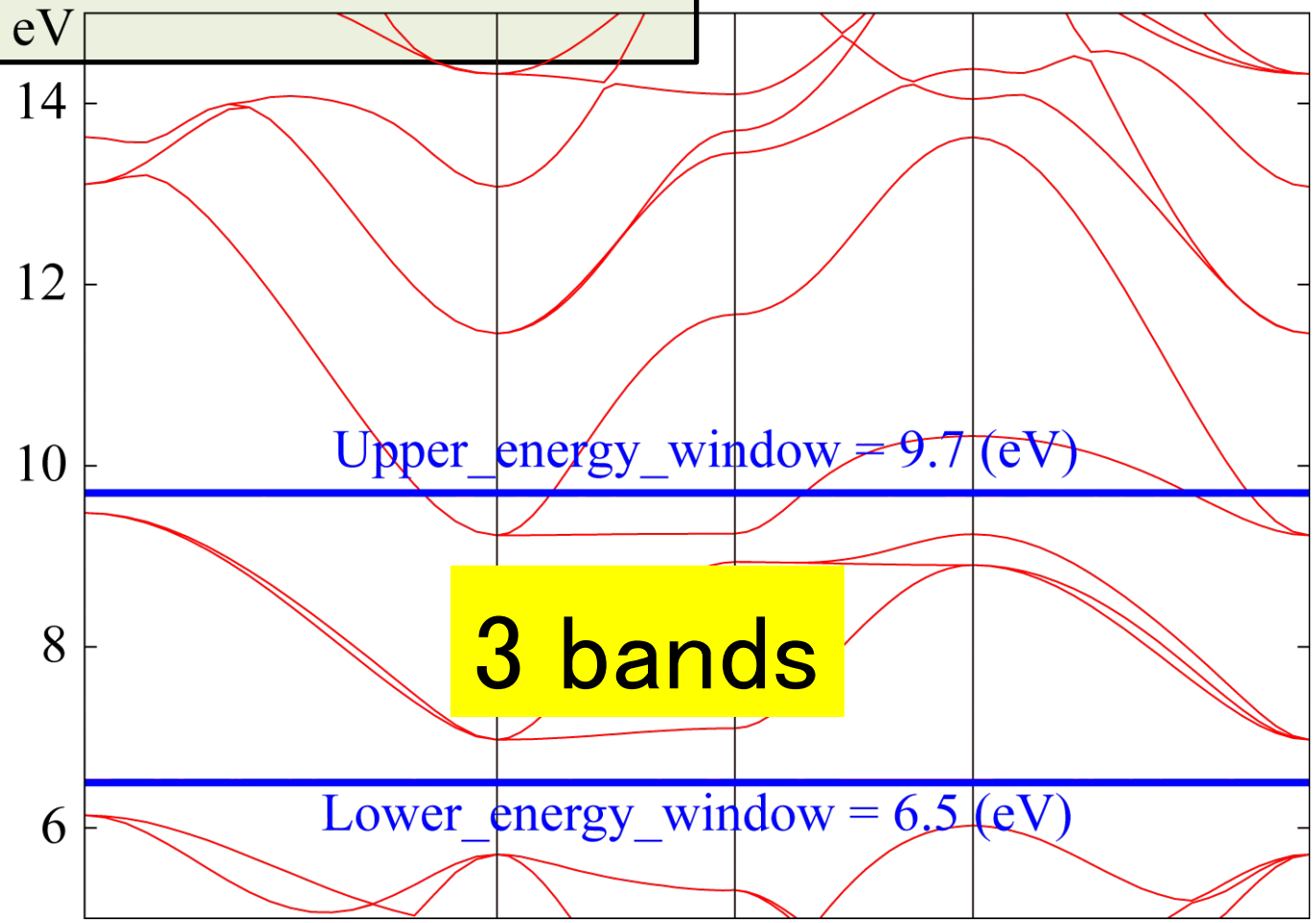
&param_wannier of SrVO3

```
&param_wannier
N_wannier=3,                    !Total number of considerd band in wannier calc
Lower_energy_window=6.5d0,!UPPER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=9.7d0,!UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=3/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dxy 0.5d0 0.5d0 0.5d0 0.5d0
dyz 0.5d0 0.5d0 0.5d0 0.5d0
dzx 0.5d0 0.5d0 0.5d0 0.5d0
```



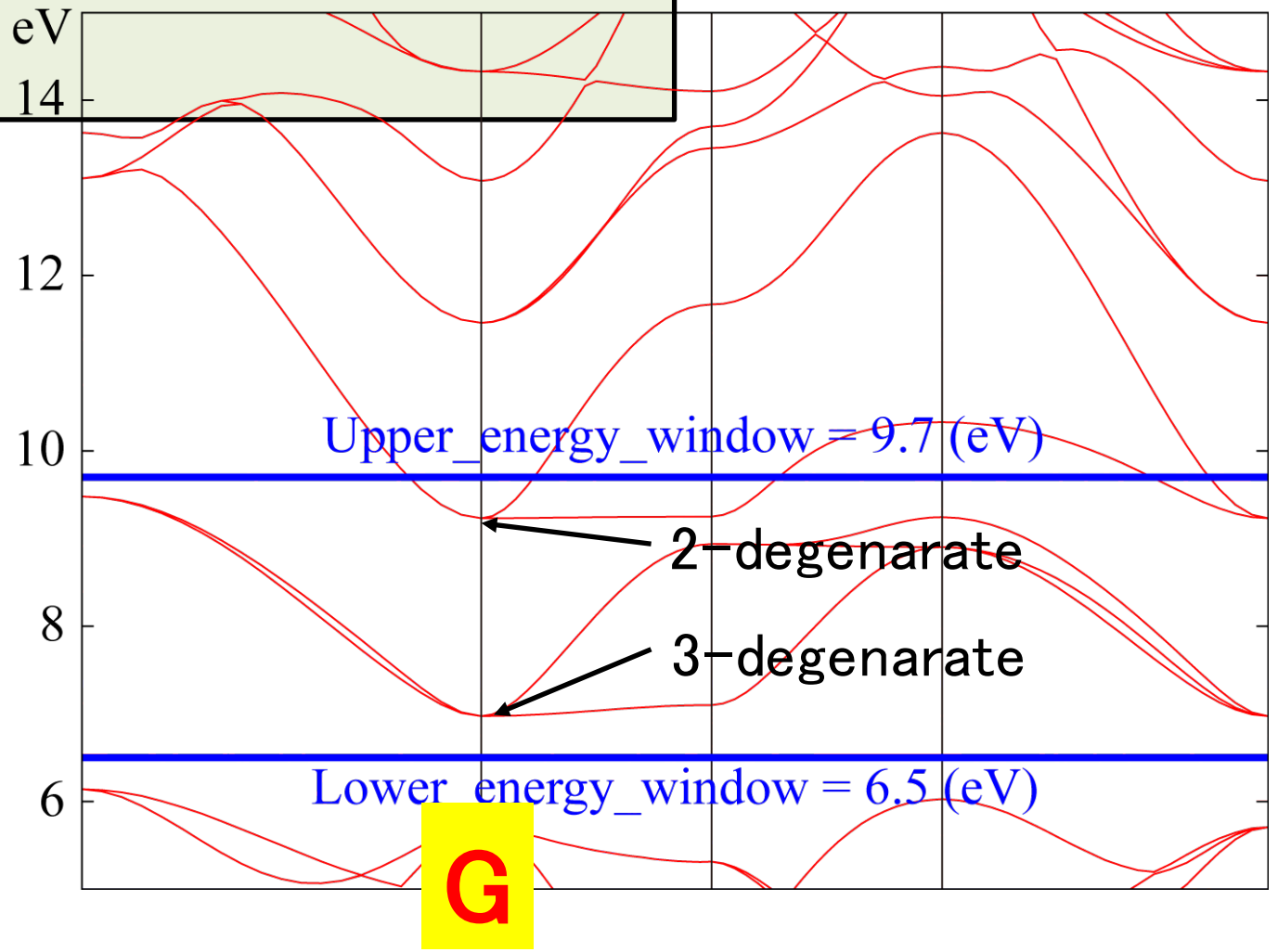
&param_wannier of SrVO3

```
&param_wannier
N_wannier=3,                    !Total number of considerd band in wannier calc
Lower_energy_window=6.5d0,!UPPER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=9.7d0,!UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=3/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dxy 0.5d0 0.5d0 0.5d0 0.5d0
dyz 0.5d0 0.5d0 0.5d0 0.5d0
dzx 0.5d0 0.5d0 0.5d0 0.5d0
```

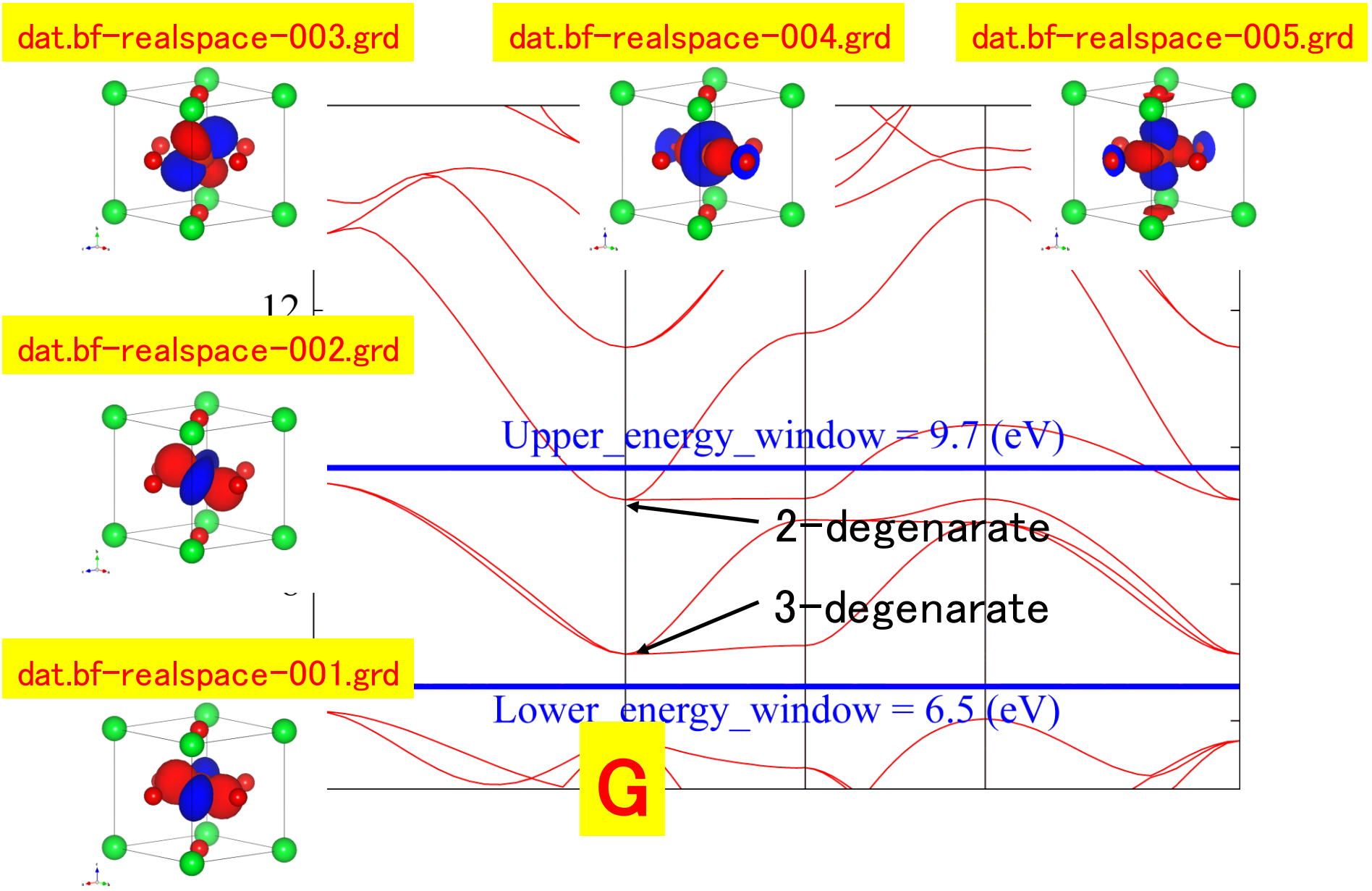


Visualize Bloch function at a k point

```
&param_wannier
N_wannier=3,                    !Total number of considerd band in wannier calc
Lower_energy_window=6.5d0,!UPPER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=9.7d0,!UPPER BOUND OF ENERGY WINDOW (eV)
flg_vis_Bloch = 1,              !visualize Bloch
calc_k = 0.0d0, 0.0d0, 0.0d0  !G
N_initial_guess=3/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dxy 0.5d0 0.5d0 0.5d0 0.5d0
dyz 0.5d0 0.5d0 0.5d0 0.5d0
dzx 0.5d0 0.5d0 0.5d0 0.5d0
```

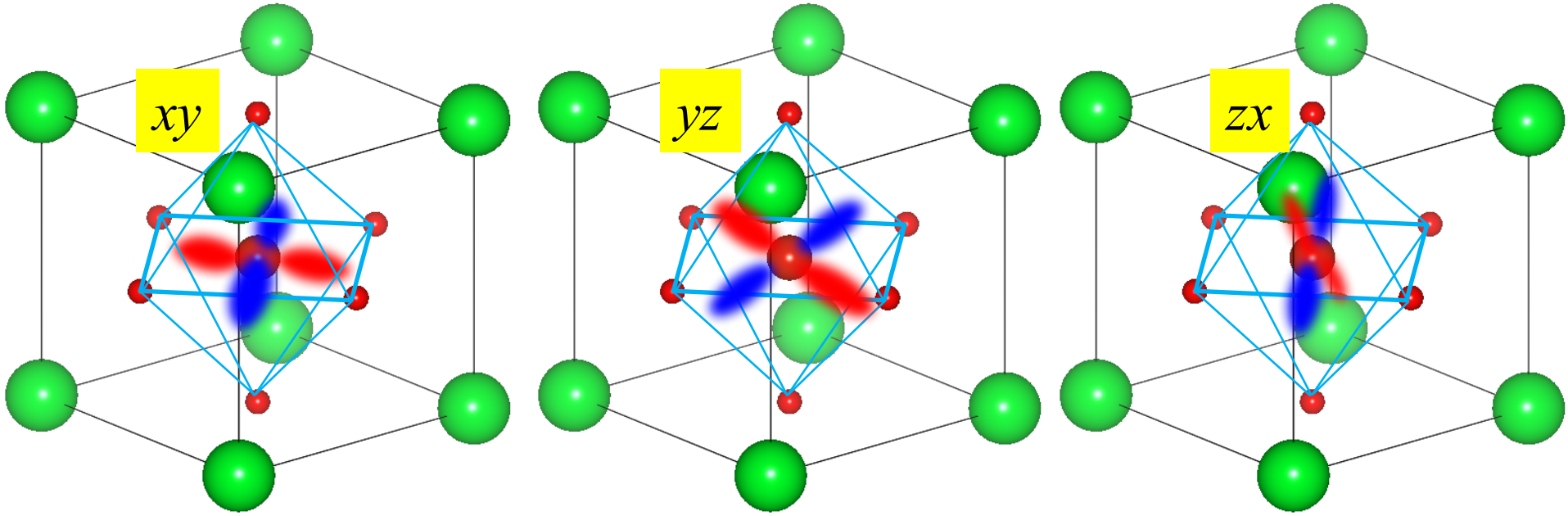


Visualize Bloch function at a k point



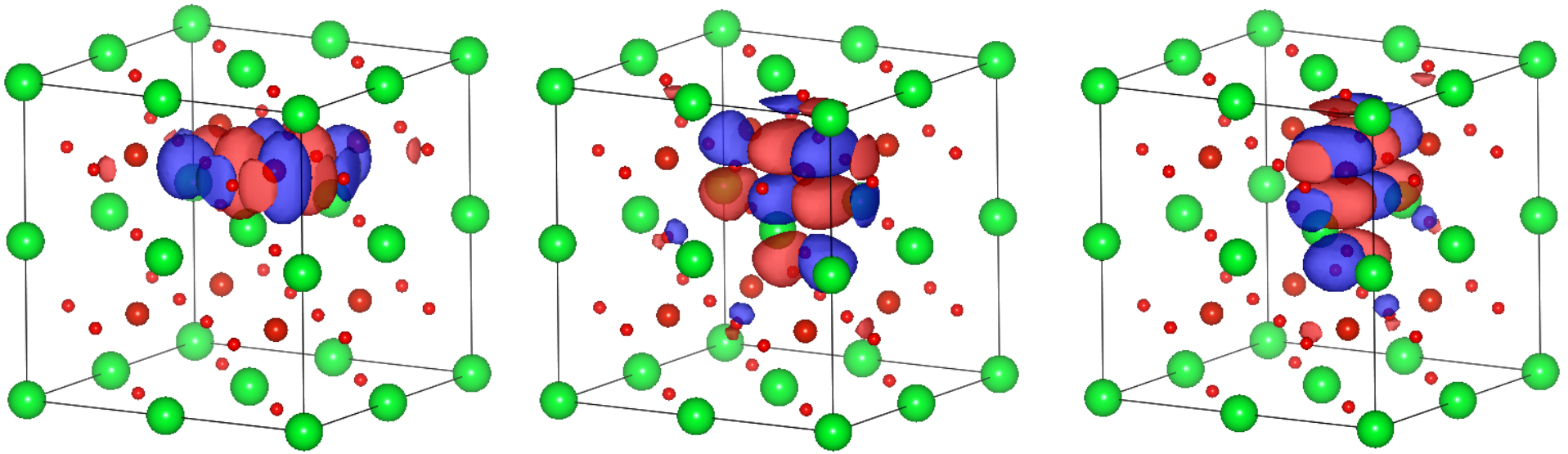
&param_wannier of SrVO3

```
&param_wannier
N_wannier=3,                    !Total number of considerd band in wannier calc
Lower_energy_window=6.5d0, !UPPER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=9.7d0, !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=3/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dxy 0.5d0 0.5d0 0.5d0 0.5d0
dyz 0.5d0 0.5d0 0.5d0 0.5d0
dzx 0.5d0 0.5d0 0.5d0 0.5d0
```



Result of SrVO3

```
&param_wannier
N_wannier=3,                    !Total number of considerd band in wannier calc
Lower_energy_window=6.5d0, !UPPER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=9.7d0, !UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=3/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dxy 0.5d0 0.5d0 0.5d0 0.5d0
dyz 0.5d0 0.5d0 0.5d0 0.5d0
dzx 0.5d0 0.5d0 0.5d0 0.5d0
```

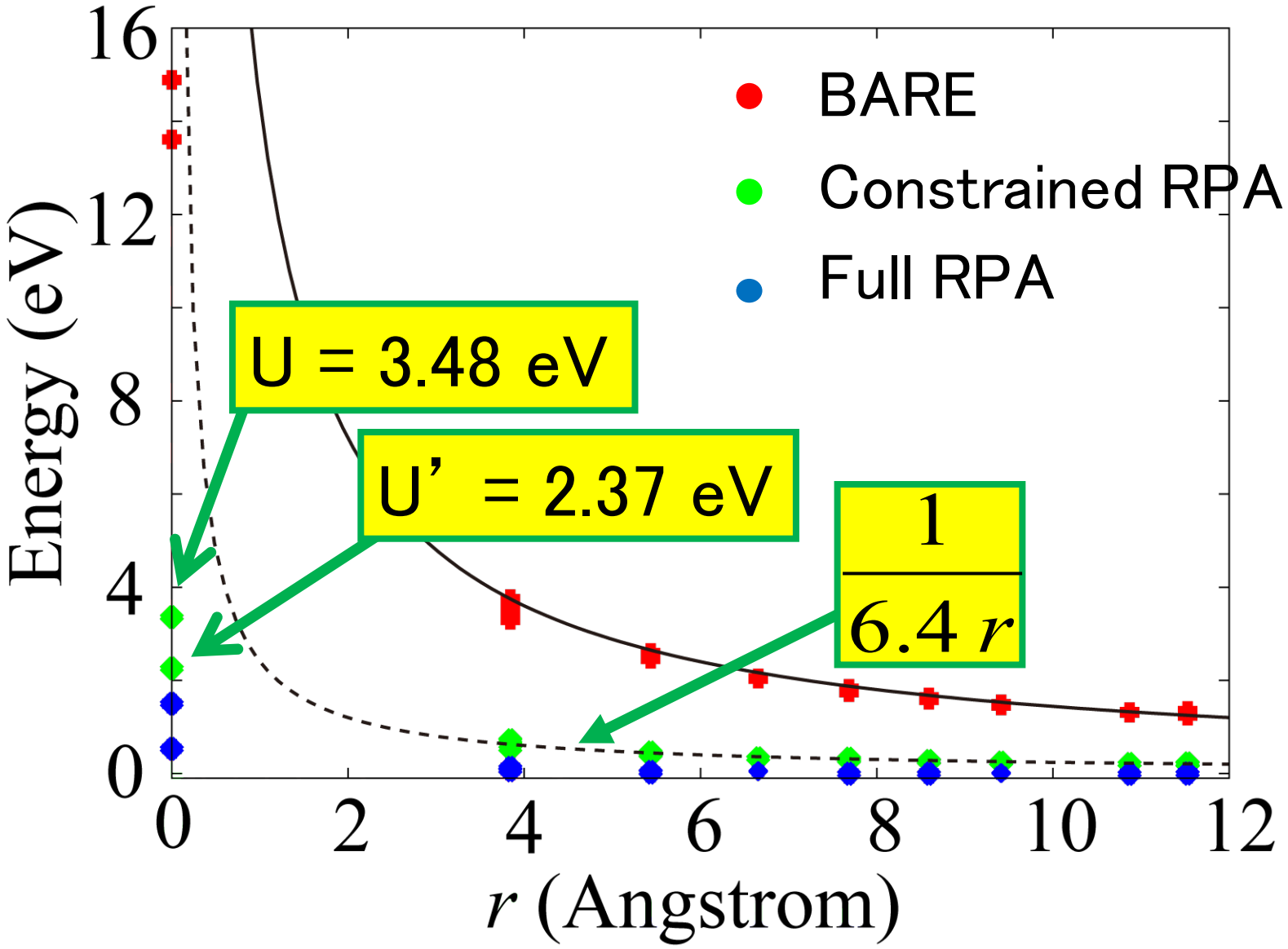


Input.in for constrained RPA –SrVO3–

```
&param_chiqw
flg_cRPA=1/  ! 0: full-RPA, 1: constrained RPA
&param_wannier
N_wannier=3, !Total number of considerd band in wannier calc
Lower_energy_window=6.5d0,!UPPER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=9.7d0,!UPPER BOUND OF ENERGY WINDOW (eV)
N_initial_guess=3/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dxy 0.50d0 0.50d0 0.50d0 0.50d0
dyz 0.50d0 0.50d0 0.50d0 0.50d0
dzx 0.50d0 0.50d0 0.50d0 0.50d0
&param_interpolation
N_sym_points=5/      !Number of symmetry points
0.50d0 0.50d0 0.50d0 !R
0.00d0 0.00d0 0.00d0 !G
…
&param_visualization
/
&param_calc_int
/
```

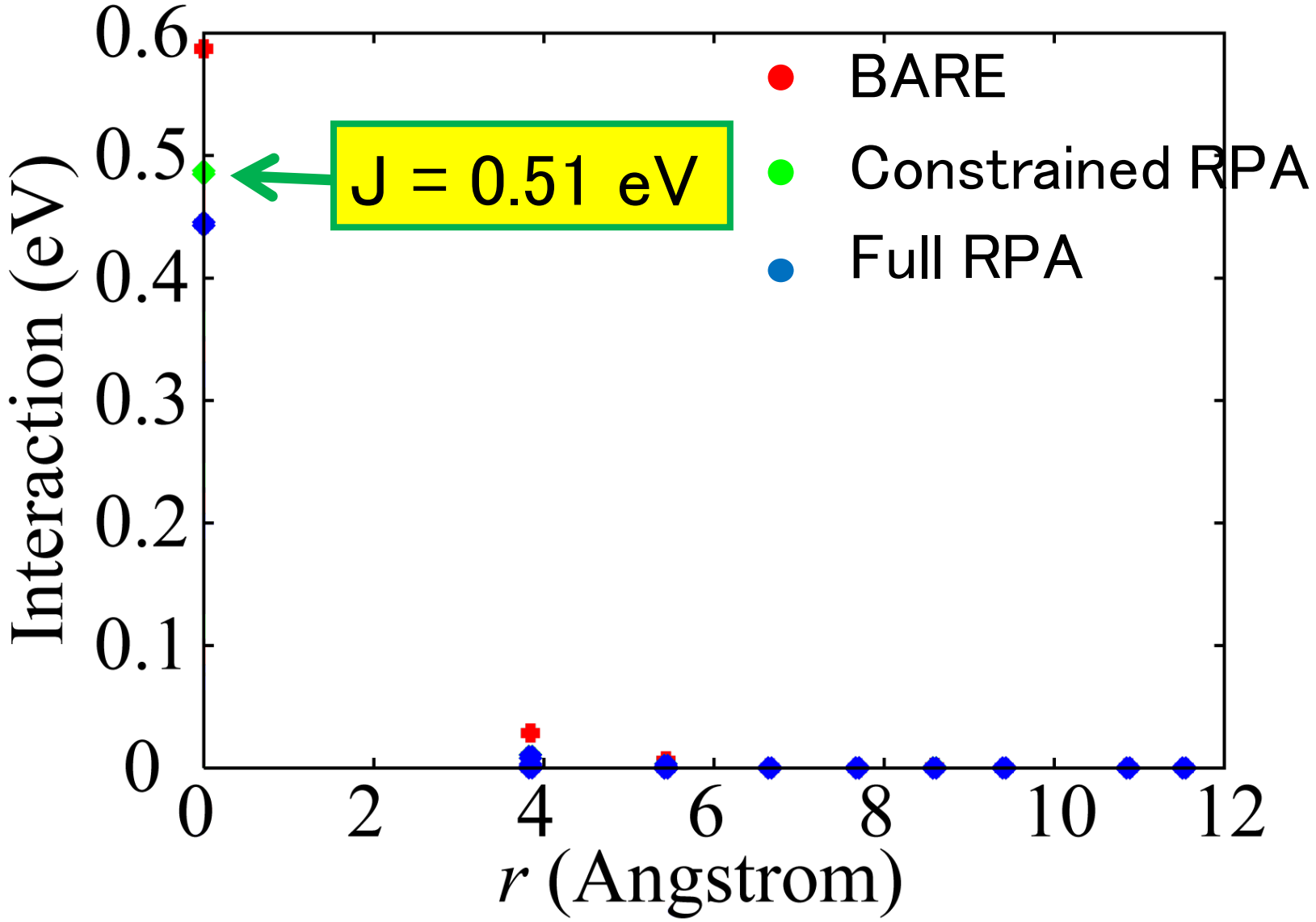
Diagonal part of Coulomb interaction

$$W_{ij}(r) = \langle w_{i\mathbf{0}} w_{i\mathbf{0}} | W(\omega = 0) | w_{j\mathbf{R}} w_{j\mathbf{R}} \rangle$$



Off-Diagonal part of Coulomb interaction

$$J_{ij}(r) = \left\langle w_{i\mathbf{0}} w_{j\mathbf{R}} \left| W(\omega = 0) \right| w_{j\mathbf{R}} w_{i\mathbf{0}} \right\rangle$$

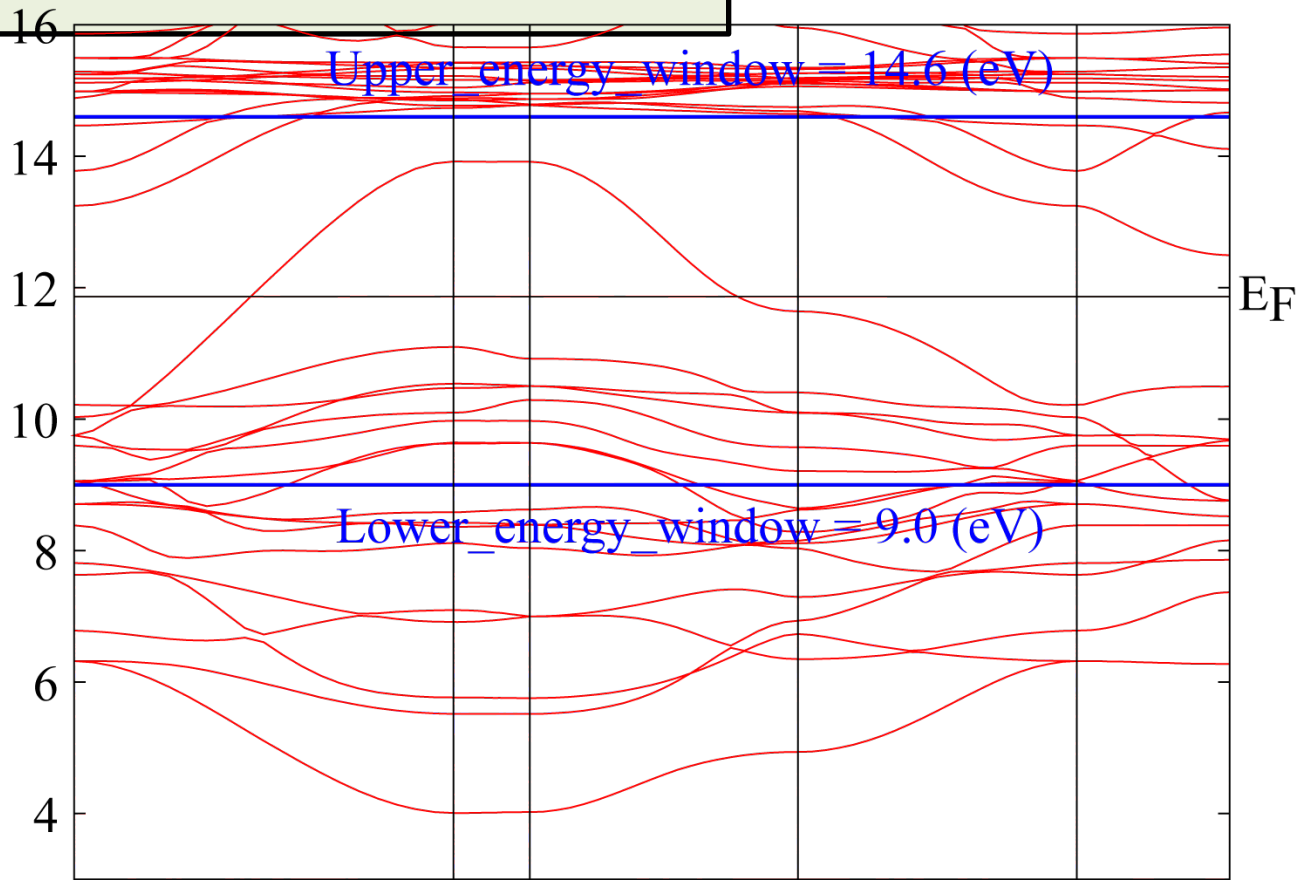


&param_wannier of La2CuO4

```
&param_wannier
N_wannier=1,                        !Total number of considerd band in wannier calc
Lower_energy_window= 9.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=14.6d0,!UPPER BOUND OF ENERGY WINDOW (eV)
set_inner_window=T,                 !flag for inner window
Lower_inner_window=11.60d0,!Lower inner energy window for wannier calc (eV)
Upper_inner_window=12.30d0,!Upper inner energy window for wannier calc (eV)
N_initial_guess=1/                  !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dx2 0.5d0  0.0d000  0.0d000  0.0d000
```

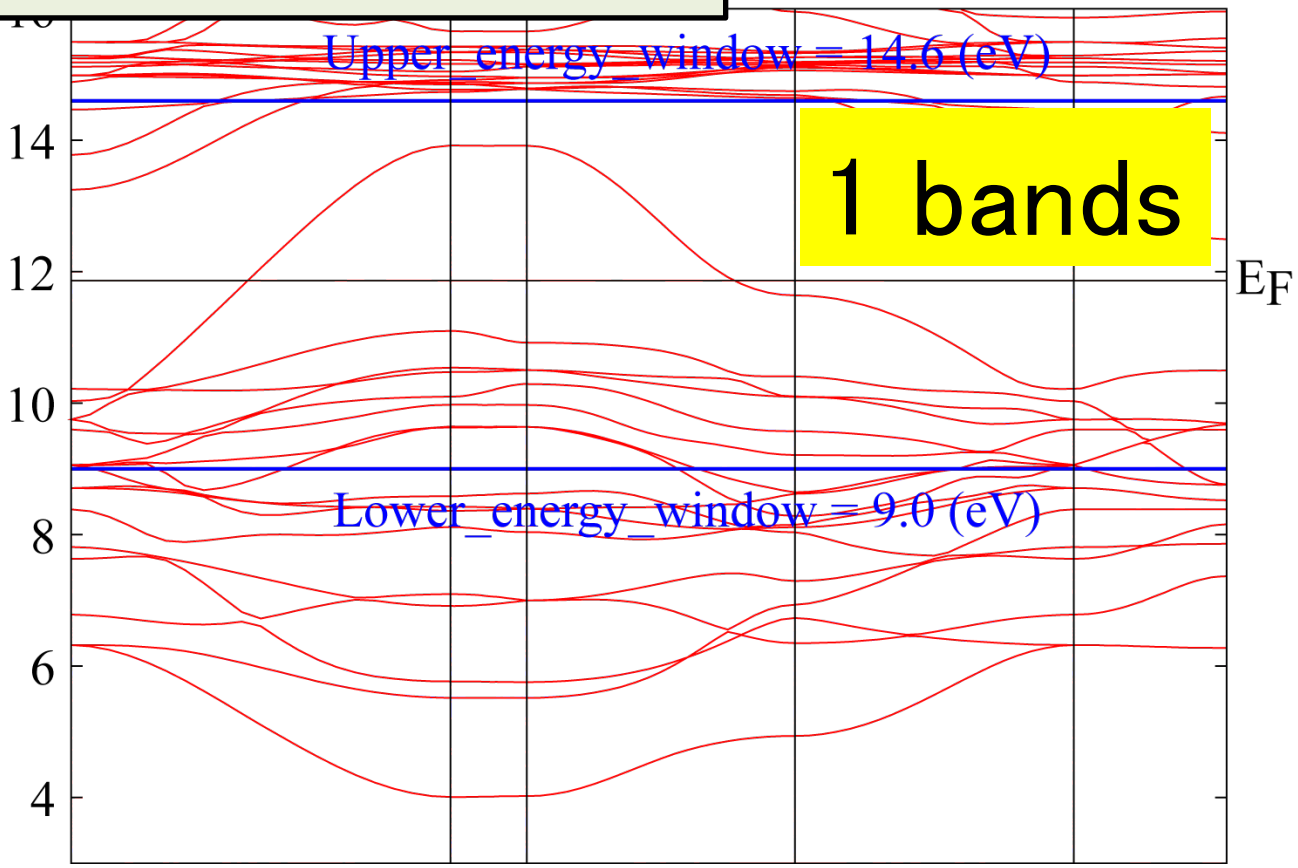
&param_wannier of La2CuO4

```
&param_wannier
N_wannier=1,                    !Total number of considerd band in wannier calc
Lower_energy_window= 9.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=14.6d0,!UPPER BOUND OF ENERGY WINDOW (eV)
set_inner_window=T,             !flag for inner window
Lower_inner_window=11.60d0,!Lower inner energy window for wannier calc (eV)
Upper_inner_window=12.30d0,!Upper inner energy window for wannier calc (eV)
N_initial_guess=1/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dx2 0.5d0  0.0d000  0.0d000  0.0d000
```



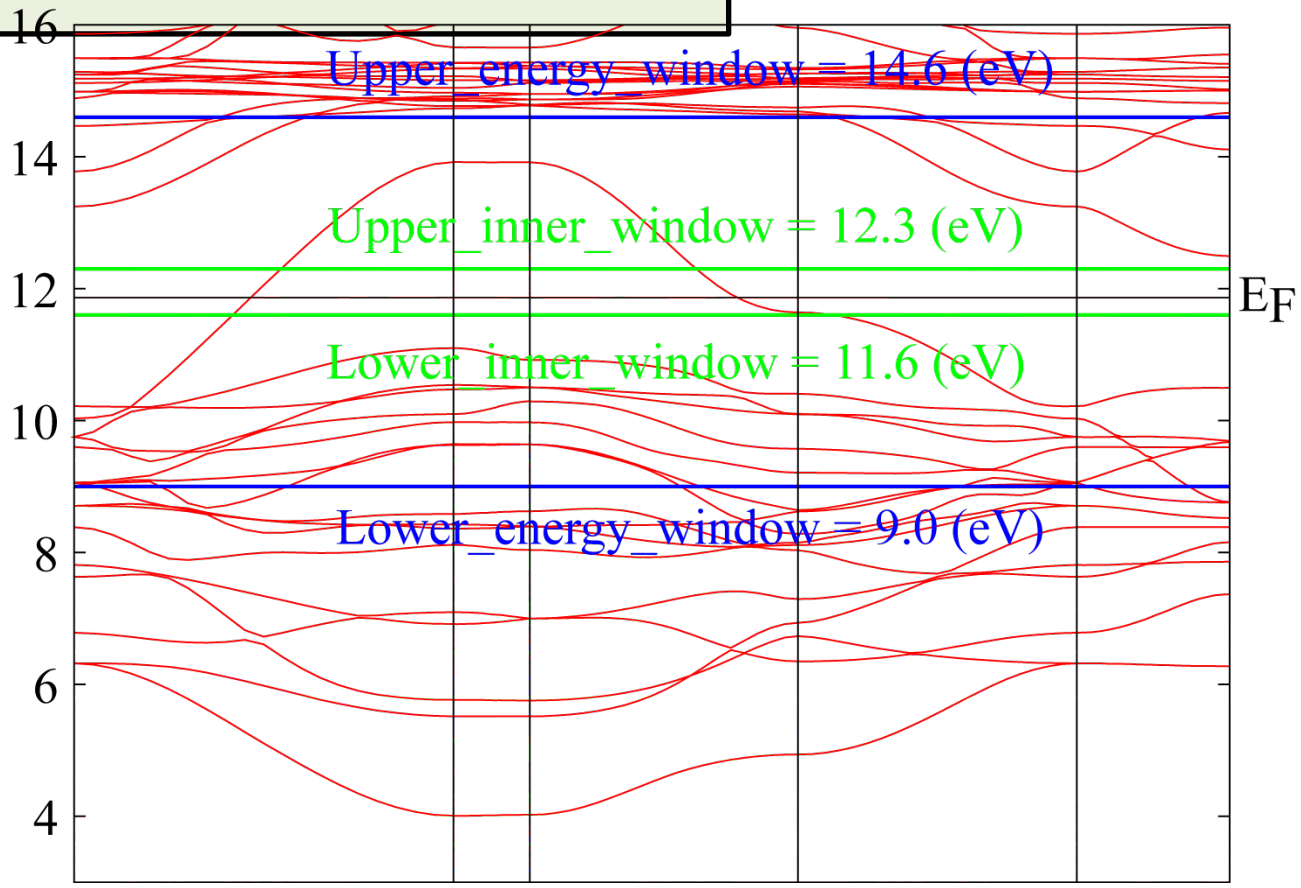
&param_wannier of La2CuO4

```
&param_wannier
N_wannier=1,                    !Total number of considerd band in wannier calc
Lower_energy_window= 9.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=14.6d0,!UPPER BOUND OF ENERGY WINDOW (eV)
set_inner_window=T,             !flag for inner window
Lower_inner_window=11.60d0,!Lower inner energy window for wannier calc (eV)
Upper_inner_window=12.30d0,!Upper inner energy window for wannier calc (eV)
N_initial_guess=1/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dx2 0.5d0  0.0d000  0.0d000  0.0d000
```



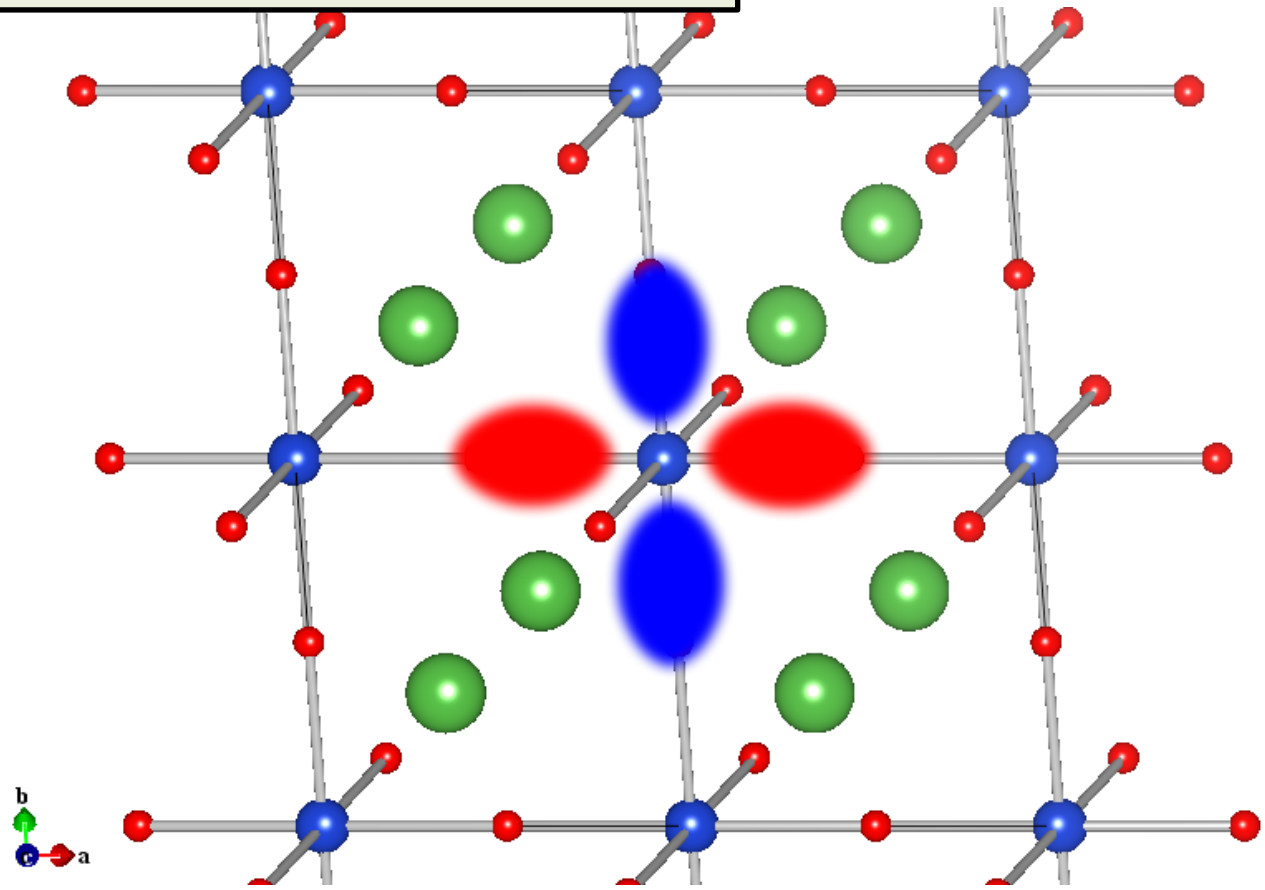
&param_wannier of La2CuO4

```
&param_wannier
N_wannier=1,                    !Total number of considerd band in wannier calc
Lower_energy_window= 9.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=14.6d0,!UPPER BOUND OF ENERGY WINDOW (eV)
set_inner_window=T,             !flag for inner window
Lower_inner_window=11.60d0,!Lower inner energy window for wannier calc (eV)
Upper_inner_window=12.30d0,!Upper inner energy window for wannier calc (eV)
N_initial_guess=1/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dx2 0.5d0  0.0d000  0.0d000  0.0d000
```



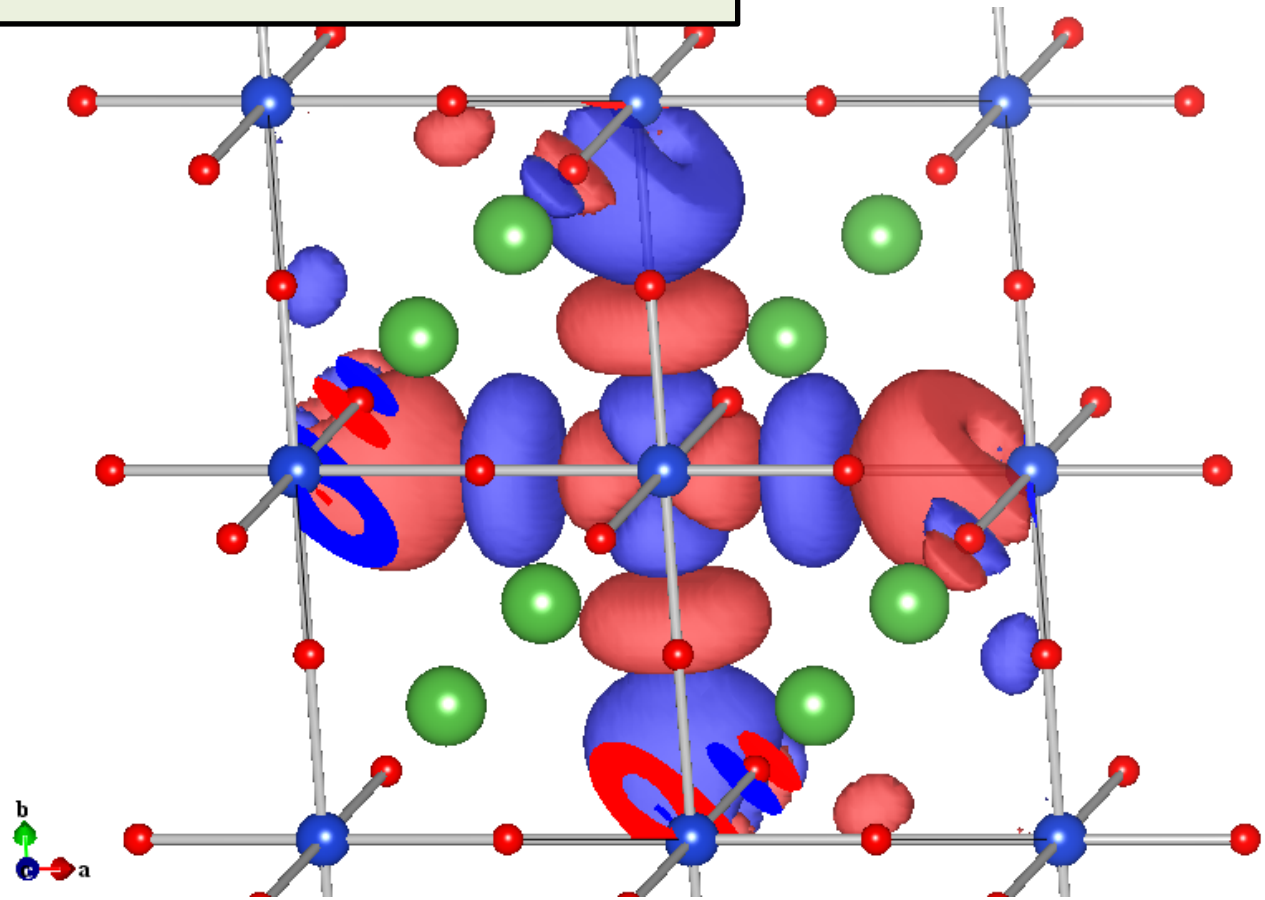
&param_wannier of La2CuO4

```
&param_wannier
N_wannier=1,                    !Total number of considerd band in wannier calc
Lower_energy_window= 9.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=14.6d0,!UPPER BOUND OF ENERGY WINDOW (eV)
set_inner_window=T,             !flag for inner window
Lower_inner_window=11.60d0,!Lower inner energy window for wannier calc (eV)
Upper_inner_window=12.30d0,!Upper inner energy window for wannier calc (eV)
N_initial_guess=1/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dx2 0.5d0  0.0d000  0.0d000  0.0d000
```



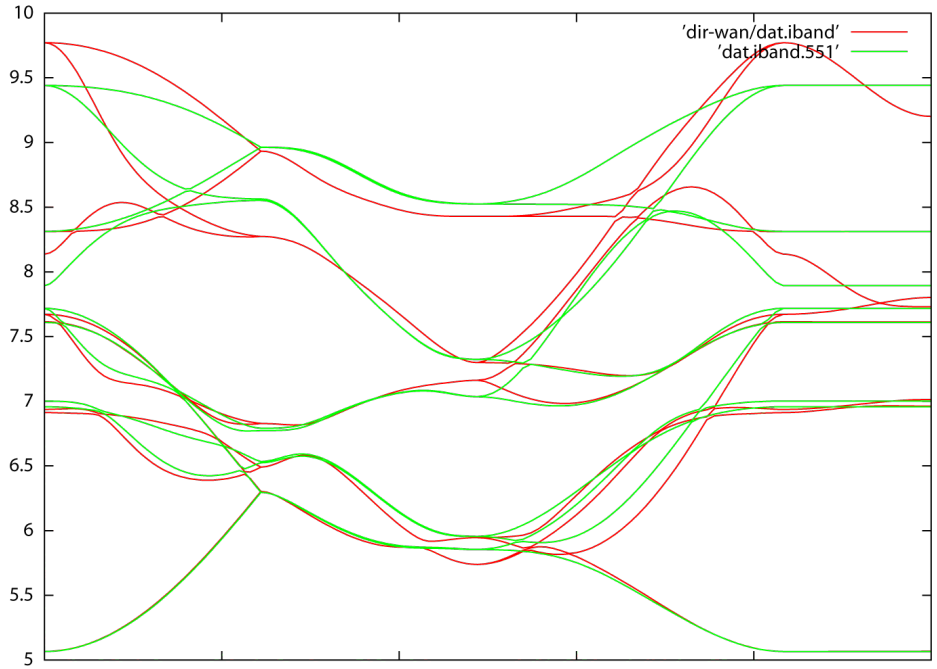
Result of La2CuO4

```
&param_wannier
N_wannier=1,                    !Total number of considerd band in wannier calc
Lower_energy_window= 9.0d0,!LOWER BOUND OF ENERGY WINDOW (eV)
Upper_energy_window=14.6d0,!UPPER BOUND OF ENERGY WINDOW (eV)
set_inner_window=T,             !flag for inner window
Lower_inner_window=11.60d0,!Lower inner energy window for wannier calc (eV)
Upper_inner_window=12.30d0,!Upper inner energy window for wannier calc (eV)
N_initial_guess=1/              !TOTAL NUMBER OF INITIAL GUESS GAUSSIAN
dx2 0.5d0  0.0d000  0.0d000  0.0d000
```



Transfer_analysis: FeSe (6x6x4 k)

> python tr.py --bnd --kgd='5 5 1'



> python tr.py --dos --kgd='5 5 1'