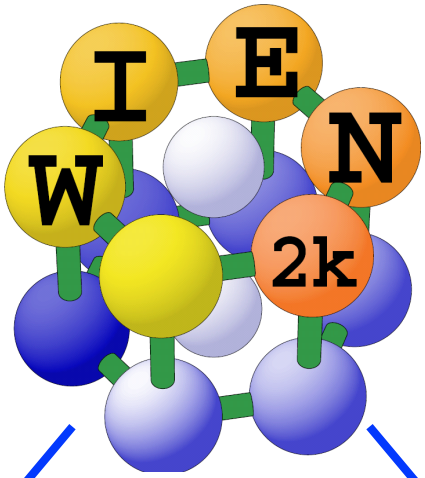
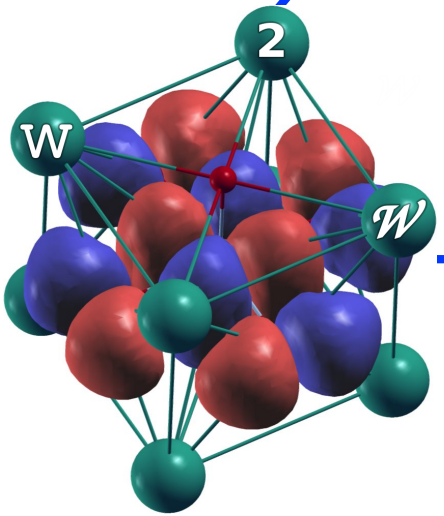


Wannier90 & Wien2Wannier Tutorial (08/Nov/2018)



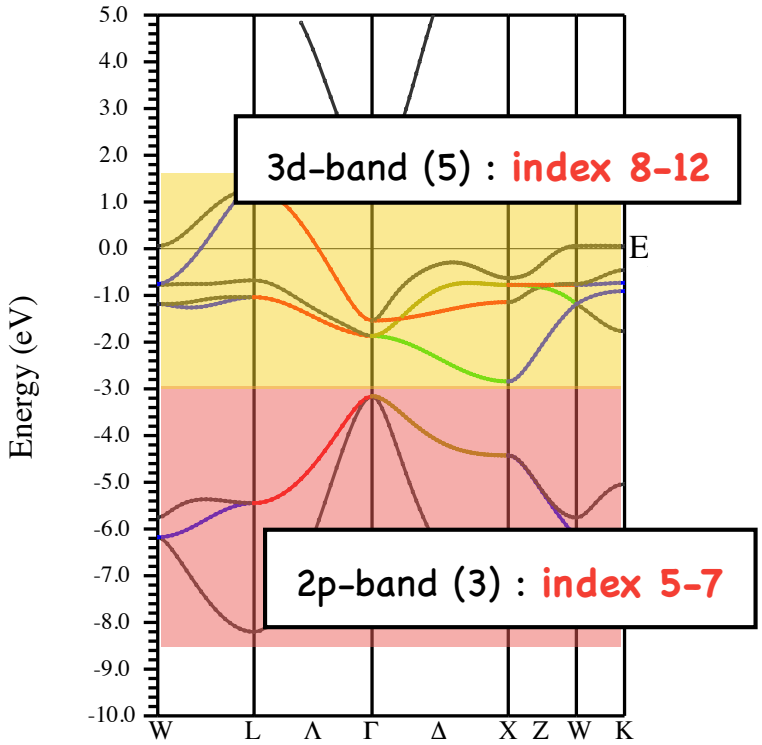
WANNIER90

STEP.1 :

1. Run LDA calculation for NiO with Wien2K and get band-structure date (from "task").
   Use lattice constant : 7.899055 Bohr & Ni (0.0,0.0,0.0) , O(0.5,0.5,0.5)
   or use "**NiO.cif**" on the top of cms16_30 server.
   (you can upload "case.cif" file on the first page of StructGen or put the file on "case" directly.)
2. Make "case.fermi" file with Fermi energy E_F on the first line.
   (Use "**grep :FER case.scf**" command to find E_F in Ry unit)
3. Make subdir and K-mesh in the whole BZ for wannierization
   (Use "prepare_w2wdir subdir" and "**x kgen -fbz**" command with no-shift ("0"))

STEP.2 : Write "case.inwf" file

Find the number of target bands (to be wannierized, d-only or d-p ?) and the indices of these bands defined in Wien2K calculation.



Find band index using ...
"case.output1" file
or
"x findbands -emin ** -emax ** -efermi **" command
(note : emin and emax in eV, efermi in Ry unit)
which writes the band index in the energy window to "case.outputfind" file

Example of "case.outputfind"

```
Bloch bands in the interval
at all k:    5     12      8
at any k:    5     13      9
```

Example of "case.inwf" file (dp-model)

```
BOTH                  # AMN, MMN, or BOTH
 5  12                # min band, max band
 3   8                # LJMAX in exp(ibr) expansion, #WF
 2                    # 1:d-eg -> 1:dx2-y2
 2 2 -2    0.70710678    0.00000000   # iat, l, m, Re(coeff), Im(coeff)
 2 2  2    0.70710678    0.00000000
 1                    # 1:d-eg -> 1:d3z2-r2
 2 2  0    1.00000000    0.00000000
 2                    # 1:d-t2g -> 1:dxy
 2 2 -2    0.00000000    0.70710678
 2 2  2    0.00000000   -0.70710678
 2                    # 1:d-t2g -> 1:dxz
 2 2 -1    0.70710678    0.00000000
 2 2  1   -0.70710678    0.00000000
 2                    #  1:d-t2g -> 1:dyz
 2 2 -1    0.00000000    0.70710678
 2 2  1    0.00000000    0.70710678
 2                    # 5:p -> 5:px
 1 1 -1    0.70710678    0.00000000
 1 1  1   -0.70710678    0.00000000
 2                    # 5:p -> 5:py
 1 1 -1    0.00000000    0.70710678
 1 1  1    0.00000000    0.70710678
 1                    # 5:p -> 5:pz
 1 1  0    1.00000000    0.00000000
```

The number of terms used to approximate exp(-ikb) (use 3~4)

Min and max of band index

The number of Wannier functions

Atom index

$$|d_{x^2-y^2}\rangle = \frac{1}{\sqrt{2}}(|d_2\rangle + |d_{-2}\rangle)$$
$$|d_{3z^2-r^2}\rangle = |d_0\rangle$$

E_g

$$|d_{xy}\rangle = \frac{-i}{\sqrt{2}}(|d_2\rangle - |d_{-2}\rangle)$$
$$|d_{yz}\rangle = \frac{i}{\sqrt{2}}(|d_1\rangle + |d_{-1}\rangle)$$
$$|d_{zx}\rangle = \frac{-1}{\sqrt{2}}(|d_1\rangle - |d_{-1}\rangle)$$

T_{2g}

$$|p_x\rangle = \frac{-1}{\sqrt{2}}(|p_1\rangle - |p_{-1}\rangle)$$
$$|p_y\rangle = \frac{1}{\sqrt{2}}(|p_1\rangle + |p_{-1}\rangle)$$
$$|p_z\rangle = |p_0\rangle$$

You can use "init_w2w" to check the atom index

The number of expansion coefficients

STEP.3 : Run interface

1. Command "**write_win**" to make "case.win" using "case.inwf" file
   ("case.win" file is input file for wannier90)
2. Command "**x wannier90 -pp**"
   (write a list of nn k-points to "case.nnkp" on the basis on "case.win")
3. Run "**x lapw1**"
   (compute eigen states and vectors for the new k-mesh prepared in STEP.1)
4. Command "**x w2w**" → Output : "case.mmn" and "case.amn"

   (compute overlaps M_{mn} and initial projections A_{mn})

Example of "case.win" file

```
num_bands       = 8
num_wann        = 8

!!! Disentanglement parameters !!!
!dis_froz_min     = 7.
!dis_froz_max     = 9.
!dis_mix_ratio    = 0.5

!!! Iterations &c. !!!
 iprint                 = 1
 num_iter               = 10000
 num_print_cycles       =   100
 conv_window            = 3
!conv_tol               = 1e-10
 dis_num_iter           = 10000
!dis_conv_window        = 3
!dis_conv_tol           = 1e-10
!restart                = default | wannierise | plot | transport
```

Option for disentanglement
(num_bands > num_wann case)
dis_froz_min : bottom of the frozen energy window
dis_froz_max : top of the frozen energy window
dis_mix_ratio : mixing ratio during minimization of Ω_I

Maximum number of iterations for minimization

"Restart" option
Wannierise : Restart from the beginning of the wannierization
Plot : Go directly to plotting phase
(Use this "restart" option in Q.1 to save time)

```
!!! Post-processing options !!!
 write_proj              = .true.
 write_xyz               = .true.
 translate_home_cell     = .true.
 hr_plot                 = .true.
!fermi_surface_plot      = .true.

!!! Band structure !!!
!!! needs `kpoint_path' block
!bands_plot              = .true.
 bands_num_points        = 50
!bands_plot_format       = gnuplot xmgrace
!bands_plot_project      = 1-3
!bands_plot_mode         = s-k | cut [Slater-Koster | truncate Hamiltonian]
!dist_cutoff             = 1.0
```

"dist_cutoff" option :
put "bands_plot_mode = cut" and
enter the largest distance between WFs for which
the Hamiltonian matrix element is retained.
(use Å unit)

```
bands_plot = .true.
begin kpoint_path
  R  0.50  0.50  0.50   L  0.28  0.28  0.28
  L  0.28  0.28  0.28   G  0.00  0.00  0.00
  G  0.00  0.00  0.00   D  0.00  0.12  0.12
  D  0.00  0.12  0.12   X  0.00  0.25  0.25
  X  0.00  0.25  0.25   Z  0.12  0.25  0.38
  Z  0.12  0.25  0.38   M  0.25  0.25  0.50
  M  0.25  0.25  0.50   S  0.12  0.12  0.25
  S  0.12  0.12  0.25   G  0.00  0.00  0.00
end kpoint_path
```

SETP.4 : Run Wannierization

1. Command "**x wannier90**" to make "case.win" on the basis on "case.inwf"
   ("case.win" file is input file for wannier90)
2. Check the result of wannierization written to "case.wout" file
   (especially, convergence of the spread, which is (usually) smaller than the unit cell)

Wannierization Fin !!

SETP.5 : Analysis and Visualization

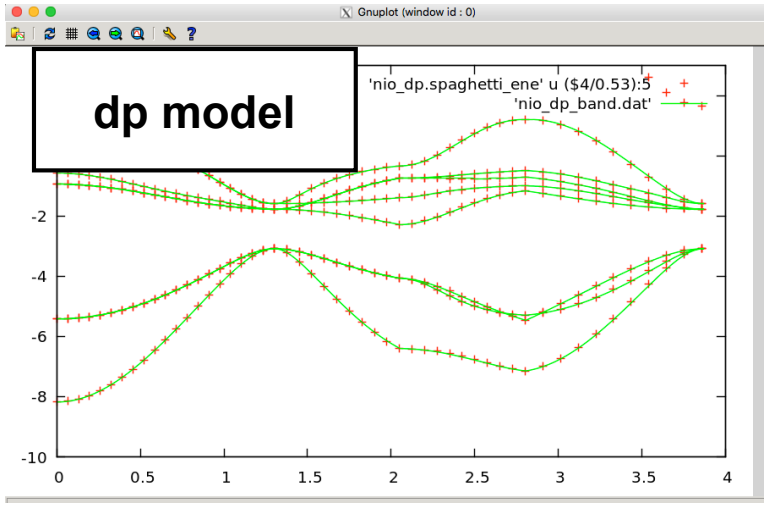
1. Compare band-structures

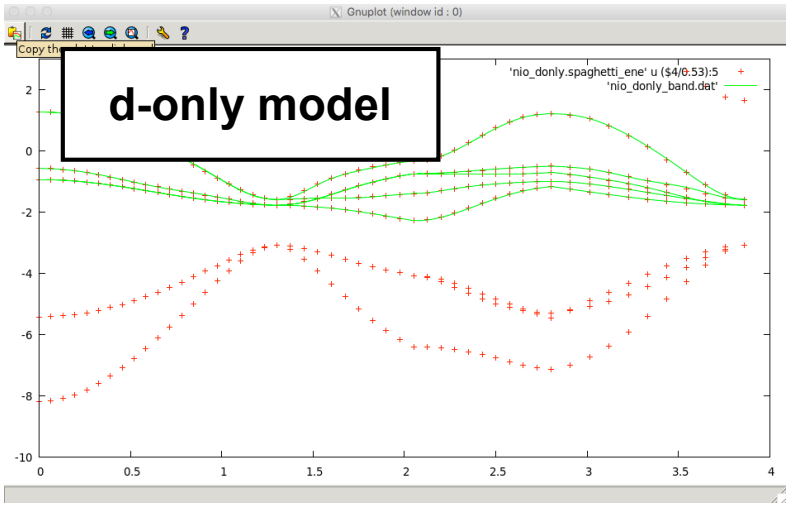
Wannier90 writes a band structure derived from the Wannier-interpolated H(k) to "case_band.dat". One can compare it to the one computed in STEP.1 (Wien2K) ("case.spaghetti" file).

GNUPLOT COMAND : p 'case.spaghetti_ene' u ($4/0.53):5, 'case_band.dat' w l

for conversion from Bohr^{-1} to Å^{-1} unit

1 Bohr = 0.5291772083Å





Question.1

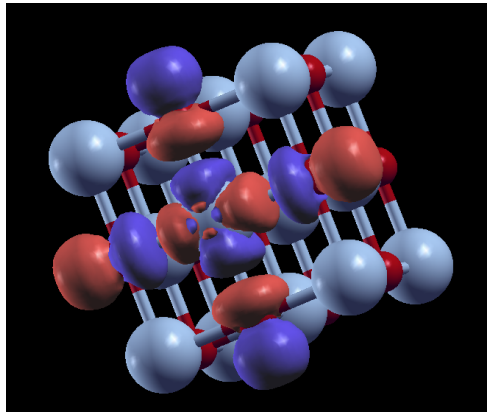
Find the diameters of nn, nnn, ... shells of Ni from "case.outputnn".
Then, use wannier90 to calculate band-structures with no hopping, nn, nnn ... hopping and compare them with the original band structure.
(use the "dist_cutoff" parameter and "restart" option to save time.)

2. Plot Wannier Functions

1. write "**case.inwplot**" as follows (see HINTS for details of this input file),

```
3D ORTHO
-1 -1 -1  1
 1 -1 -1  1
-1  1 -1  1
-1 -1  1  1
 40 40 40 0 0 0     # grid points and echo increments
NO
WAN ANG LARGE
1 2
```

"m"-th WF you want to plot



2. Command "**x wplot -wf -m**" (it may take a few minutes depending on your grid points)
   (evaluate m-th WF on the real-space grid and write density to "case_m.psink")
3. Run "**wplot2xsf**"
   (converts files to "xsf" files which can be opened by XCrySDen.)
4. Command "**xcrysden --xsf case_m.xsf**"
   : Pick "Tools→Date Grid" from the menu and press OK

   (set "isovalue" to 2 and check the "Render +/- isovalue" box)

Question.2

Plot "xy" and "$3z^2-r^2$" wannier functions for d-only and dp models

Question.3

Find out H(R=(0,0,1)) part in "case_hr.dat" file and which n-shell it corresponds to.
(use "XCRySDen" and "Modify → # of unit cells drawn" to find out.)
Then, analyze the symmetry of H(R=(0,0,1)) and H(R=(0,0,0)).
(ex. find out the reason for ZERO values from the viewpoint of symmetry)

Structure of "case_hr.dat" file

This file contains the hopping integrals <m,R |H|n,0> between the n-th wannier function |n,0> in the home unit cell and the m-th wannier function |m, R> in the unit cell at R.

−6	0	3	1	1	0.000040	0.000000
−6	0	3	2	1	0.000000	−0.000000
−6	0	3	3	1	−0.000000	0.000000
−6	0	3	4	1	0.000047	−0.000000
−6	0	3	5	1	−0.000047	−0.000000
−6	0	3	1	2	0.000000	−0.000000
−6	0	3	2	2	0.000041	−0.000000
(R_1, R_2, R_3)			(m, n)		Real(T_{mn})	Im(T_{mn})

orbital label

where R is given as $\vec{R} = R_1\vec{a_1} + R_2\vec{a_2} + R_3\vec{a_3}$

Question.4

What is the largest nn and nnn hopping element $T_{\alpha\beta}$ (values and orbitals) ?

HINTS

2.9.12 character(len=20) :: bands_plot_mode

To interpolate the band structure along the k-point path, either use the Slater-Koster interpolation scheme or truncate the Hamiltonian matrix in the WF basis. Truncation criteria are provided by `hr_cutoff` and `dist_cutoff`.

The valid options for this parameter are:

- `s-k` (default)
- `cut`

2.9.42 real(kind=dp) :: hr_cutoff

The absolute value of the smallest matrix element of the Hamiltonian in the WF basis. If $h_{mn}(\mathbf{R}) >$ `hr_cutoff`, then the matrix element $h_{mn}(\mathbf{R})$ is retained and used in the band structure interpolation (when `bands_plot_mode` = `cut`) or in the transport calculation. Otherwise it is deemed to be insignificant and is discarded. Units are eV.

The default value is 0.0.

2.9.43 real(kind=dp) :: dist_cutoff

The largest distance between two WFs for which the Hamiltonian matrix element is retained and used in the band interpolation (when `bands_plot_mode` = `cut`) or in the transport calculation. Units are Å.

The default value is 1000.0.

2.9.11 integer :: bands_plot_project(:)

If present wannier90 will compute the contribution of this set of WF to the states at each point of the interpolated band structure. The WF are numbered according to the seedname.wout file. The result is written in the seedname_band.dat file, and a corresponding gnuplot script to seedname_band_proj.dat .

For example, to project on to WFs 2, 6, 7, 8 and 12:

```
bands_plot_project : 2, 6-8, 12
```

2.6.7 character(len=20) :: restart

If restart is present the code will attempt to restart the calculation from the seedname.chk file. The value of the parameter determines the position of the restart

The valid options for this parameter are:

- default. Restart from the point at which the check file seedname.chk was written
- wannierise. Restart from the beginning of the wannierise routine
- plot. Go directly to the plotting phase
- transport. Go directly to the transport routines

case.inwplot

```
-------------------- top of file: case.inwplot --------------------
3D ORTHO         # mode O(RTHOGONAL)|N(ON-ORTHOGONAL)
-1 -1 -1 1      #x, y, z, divisor of orig
 0 -1 -1 1      #x, y, z, divisor of x-end
-1  0 -1 1      #x, y, z, divisor of y-end
-1 -1  0 1      #x, y, z, divisor of z-end
 20 20 20 0 0 0 # grid points and echo increments
NO               # DEP(HASING)|NO (POST-PROCESSING)
WAN ANG LARGE    # switch ANG|ATU|AU LARGE|SMALL
1  1             # k-point, band index
------------------------- bottom of file -------------------------
```

Interpretive comments on this file are as follows:

line 1: A3, A1
mode flag

MODE	3D	a three-dimensional grid will be specified
	nD	with $n = 0, 1, 2$ exist in `lapw7`, but are untested with `wplot`
	ANY	read arbitrary grid from *`case`*`.grid` (untested)
flag	O	grid axes will be checked for mutual orthogonality
	N	axes may be non-orthogonal

line 2: free format

ix,iy,iz,idv	Coordinates of the origin of the grid, where x=ix/idv etc. in units of the *conventional* lattice vectors

line 3: free format

ix,iy,iz,idv	Coordinates of the end points of each grid axis

>>> **line 3** must be given for each direction (i.e., n times in total for an nD grid).
line 6: free format nx, ny, nz; N N N

nx,ny,nz	number of mesh points in each direction; the additional input on this line is unused