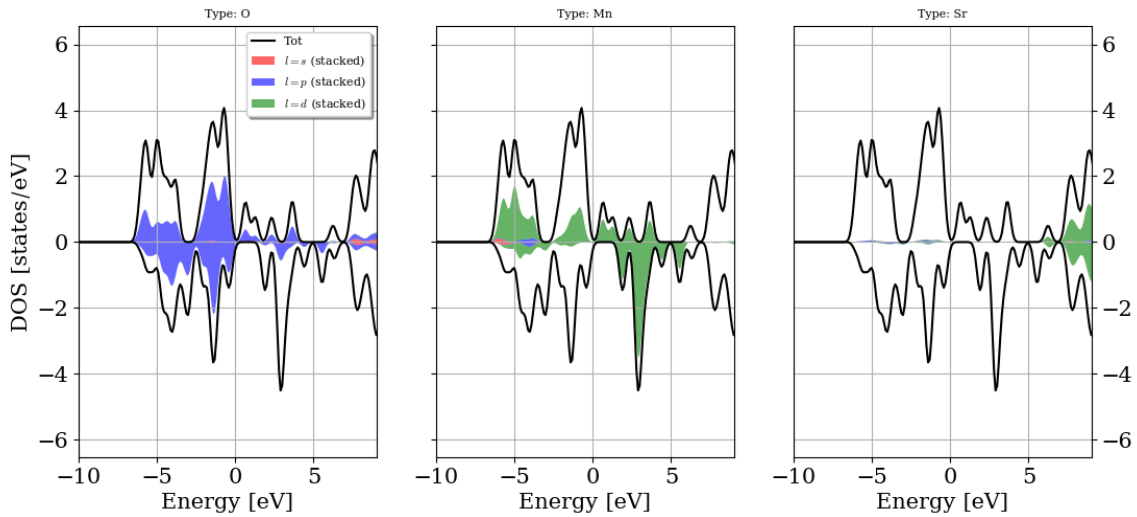
Tutorial: How to generate exchange parameters from DFT

This tutorial use cubic SrMnO3 as an example to show how to calculate the exchange parameters from DFT. Wannier functions (WF) Hamiltonians will be constructed with Wannier90. And TB2J will be used to calculate the exchange parameters. We assume the readers have the basic knowledge of WF and the Wannier90 package (see Maximally localized Wannier Functions, Wannier90).

Step 1. Find the orbitals and energy range to be used in the Wannier Function Hamiltonian.

First , calculate the electronic structure to find the energy windows for the WFs. To calculate the exchange parameters, perturbations to the spin polarized states are used. Therefore, we need to include the magnetic orbitals, and those which overlap with them. Therefore, we need to select the orbitals which has the energy near Fermi energy (E_F). We can calculate the density of states or the band structure to find the orbitals and energy range. We can see that the Mn 3d and O 2p orbitals should be included into the WF Hamiltonian.

Wannier90 make use of two energy windows to disentangle the bands. An outer window (the disentangle window), which contains all the required orbitals, and an inner window(the frozen window), which only contain the required orbitals, should be provided.



Step 2, construct WF Hamiltonian from DFT.

Beside the files usually needed for a non-scf calculation, we need another file (or two if spin-polarized) as input for wannier90, in which we define the initial projections, energy windows and so on. The names of the files are _w90_.win. For example, in the files file below, the output prefix is defined as "abinito", thus the Wannier90 input for spin up and down are "abinito_w90_up.win" and "abinito_w90_down.wout", respectively.

```
abinit.in
abinit.txt
abiniti
abinito
abinit.abinit
psp/Sr.GGA-PBESOL-JTH.xml
psp/Mn.GGA-PBESOL-JTH.xml
psp/O.GGA-PBESOL-JTH.xml
```

From the DOS we can find that the all the Mn 3d and O 2p bands are between -10 and 10 eV. There are some Sr 4d bands from 6 eV , which should be excluded from the frozen window. Thus we can select the energy window of (-10, 10) eV and the frozen window of (-9, 5) eV. Note that the energy defined in Wannier90 is not relative to E_F, so we need to add it (6.15 eV here) to the energies. And the Mn d and O p orbitals are used as initial guess for the WFs.

```
# Energy windows (Fermi energy is 6.15 eV)
dis_win_min = -3.85
dis_win_max = 16.15
dis_froz_min = 1.15
dis_froz_max = 11.15

# number of bands in DFT calculation
num_bands = 32

# number of WF
num_wann = 14

# parameters for w90
kmesh_tol = 1e-06
num_iter = 300
search_shells = 24
guiding_centres = true

# write the postitions of WF
write_xyz = true
# write the WF Hamiltonian (Note for W90 version>2.1, it is write_hr)
hr_plot = true

begin projections
Mn: d
O : p
end projections


begin unit_cell_cart
    3.8099846261953436  -0.0    -0.0
    0.0 3.8099846261953436  0.0
    0.0 0.0 3.8099846261953436
```

```
end unit_cell_cart


begin atoms_cart
Sr  0.0 0.0 0.0
Mn  1.9049923130976718  1.9049923130976718  1.9049923130976718
O   1.9049923130976718  1.9049923130976718  0.0
O   0.0 1.9049923130976718  1.9049923130976718
O   1.9049923130976718  0.0 1.9049923130976718
end atoms_cart

mp_grid =   4   4   4            # note this is too small.
begin kpoints
    0.125   0.125   0.125
    0.375   0.125   0.125
    -0.375  0.125   0.125
    -0.125  0.125   0.125
    0.125   0.375   0.125
    0.375   0.375   0.125
    -0.375  0.375   0.125
    ..............            # Do not simply copy this file. Here k-points are
end kpoints
```

The following lines need to be added to abinit input to generate WF's.

```
prtwant 2    # enable wannier90
w90iniprj 2  # use projection to orbitals instead of random.
w90prtunk 0  # use 1 if you want to visualize the WF's later.
```

Now the files below (for spin up) should be generated:

```
abinito_w90_up.amn          abinito_w90_up.chk  abinito_w90_up_hr.dat
abinito_w90_up.win   abinito_w90_up_wsvec.dat
abinito_w90_up_centres.xyz  abinito_w90_up.eig  abinito_w90_up.mmn
abinito_w90_up.wout
```

in which, the .dat file contains the Hamiltonian, the .xyz file contains the Wannier centres. The .wout files has a summary of the process of running wannier90, which will be used to calculate the exchange parameters.

To get localized WFs can be tricky sometimes. It is necessary to check if the WFs are localized by looking at the .wout file. For example, we have

```
 Final State
  WF centre and spread    1  (  1.904992,  1.904992,  1.904992 )     0.50185811
  WF centre and spread    2  (  1.904992,  1.904992,  1.904992 )     0.48650086
  WF centre and spread    3  (  1.904992,  1.904992,  1.904992 )     0.48650086
  WF centre and spread    4  (  1.904992,  1.904992,  1.904992 )     0.50185997
  WF centre and spread    5  (  1.904992,  1.904992,  1.904992 )     0.48650084
```

```
  WF centre and spread    6  (  1.904992,  1.904992, -0.000000 )     0.74591265
  WF centre and spread    7  (  1.904992,  1.904992,  0.000000 )     0.96557405
  WF centre and spread    8  (  1.904992,  1.904992, -0.000000 )     0.96557405
  WF centre and spread    9  ( -0.000000,  1.904992,  1.904992 )     0.96557489
  WF centre and spread   10  ( -0.000000,  1.904992,  1.904992 )     0.74589254
  WF centre and spread   11  (  0.000000,  1.904992,  1.904992 )     0.96557379
  WF centre and spread   12  (  1.904992,  0.000000,  1.904992 )     0.96557489
  WF centre and spread   13  (  1.904992, -0.000000,  1.904992 )     0.96557379
  WF centre and spread   14  (  1.904992, -0.000000,  1.904992 )     0.74589254
  Sum of centres and spreads ( 20.954915, 20.954915, 20.954915 )    10.49436382
```

Usually, the 3d orbitals has spread less than 1 Å , and O 2p has spread less than 2 Å .

Step 3. Run TB2J

Before running TB2J, an extra file, which contains the atomic structure, need to be prepared. It can be either a cif file, or a VASP POSCAR file. (For abinit, the abinit.in file is also fine if no fancy feature is used, like use of *, or units. cif or POSCAR file is recommended because they are simple.)

With the WF hamiltonian generated, we can calculate the exchange parameters now.

```
wann2J.py --efermi 6.15 --kmesh 4 4 4 --elements Mn --prefix_up abinito_w90_up --
prefix_down abinito_w90_down --rrange 1 1 1 --emin -10.0 --emax 0.0 --height 0.1
```

The parameters are:

- efermi: Fermi energy in eV
- kmesh: k-point mesh. Default is 5 5 5
- elements: the magnetic elements
- prefix_up: prefix for spin up channel of the Wannier90 output
- prefix_down: prefix for spin down channel of Wannier90 output.
- rrange: cutoff of supercell box. 1 1 1 means in each direction, 3 units from -1 to 1 will be considered.
- emin: the lower limit of the electron energy. (in eV, relative to Fermi energy.)
- emax: the upper limit of the electron energy. Should be close to zero.
- height: the smearing

Now we should have the files containing the J parameters in the TB2J_results directory.

```
TB2J_results/
├── exchange_distance.txt
├── exchange.out
├── exchange.xml
├── Multibinit
│   ├── exchange.xml
│   ├── mb.files
│   └── mb.in
├── TomASD
│   ├── exchange.exch
│   └── exchange.ucf
```

```
├── UppASD
│   ├── input
│   ├── jASD1
│   ├── momfile
│   └── posfile
└── Vampire
    ├── input
    ├── vampire.mat
    └── vampire.UCF
```

- exchange(_distance).out: A human readable file.
- exchange.xml : The xml file which can be used in Multibinit.
- Multibinit directory: the files file, input file and xml file, which can be used as template to run spin dynamics in Multibinit.
- The input for a few spin dynamics codes (Tom's ASD, Uppsala ASD, and Vampire) are also included.