ABCAP : advanced — qsub sh —

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Purpose:

(1) Study the symmetry of crystal (symmetry operations).

(2) Study the symmetry of wavefunction (irreducible representations).

(3) Study the optical transition between valence and conduction bands (dipole allowed).

(4) Calculate the optical absorption spectrum.

(5) Treat magnetic materials.

(6) Use the +U method.

1 Environment variables

Let's use bash.

In order to set some environment variables, execute the following commands:

```
---------------------------------------------
cat /home/CMD/teac02/Bash_envs >> ~/.bash_profile
source ~/.bash_profile
---------------------------------------------
```

The content of this `Bash_envs` file is

```
######### Bash_envs ############
  export ABCAP='/home/CMD/teac02/abcap1707'

  export FC_TYPE='gen'
  export      FC='ifort'
  export      FO=
  export   MPIFC='mpif90'
  export   MPIFO=

  export PATH=.:$HOME/bin:$PATH
  export HOSTNAME=`hostname`
######### Bash_envs ############
```

2 Preparation

Make a directory, e.g., abc, for the ABCAP calculation. Copy a shell-script file, `Setnew.sh`, as follows.

```
----------------------------
cd ~
mkdir abc
cp $ABCAP/samples/Setnew.sh abc/
----------------------------
```

The shell-script file, `Setnew.sh`, is used on starting a new calculation: Files needed for ABCAP calculation are copied from the directory,
`$ABCAP/samples/LaMnO3c_f_6/`.

3 Band Structure Calculation

3.1 Ferromagnetic Fe

Prepare a directory for the calculation:

```
----------------------------
cd ~/abc
mkdir Fe
cd Fe
../Setnew.sh
----------------------------
```

Enter a command, `H`, which shows a procedure of the calculation.
The procedure consists of

- Edit a file, ???.data.
- Execute a shell-script file, ???.sh.

[1] Edit the file, `ab_prp.data` by using the following information:

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
Fe
  a=2.87A (229, Oh9, Im-3m)
  body-centered (il=3) cubic lattice
  generators   5  (0, 0, 0)
              19  (0, 0, 0)
              25  (0, 0, 0)
  atomic position (0.0, 0.0, 0.0)
  magnetic (jmag=2)
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```

```
----------------------------
(ab_prp.data)    ab_prp.qsub
----------------------------
```

Execute `ab_prp.qsub`: This is used for executing `ab_prp.sh`.
It makes a file, `ab_input.data`, which is a real input file for the ABCAP calculation.

The file, `ab_input.data`, is made from the informations of `ab_prp.data` and `atom.data`. The `atom.data` file is a data base for atoms from H to U.

[2] Calculate the initial charge density:

```
----------------------------
(ab_input.data)  ab_in.qsub
----------------------------
```

In `ab_in.qsub`, the following programs run.

- `ab_in.exe` checks the crystal structure, and makes totally-symmetric basis functions.
- `ab_inch.exe` makes the initial charge density as the superposition of atomic charge densities.
- `ab_kpgn.exe` generates the k points used in the calculation.

- `ab_size.exe` estimates the size of calculation.
- `ab_ospw.exe` calculates the overlap integral among the totally symmetric basis functions.
- `fl_dm00.exe` sets the initial value of the local density matrix. (diagonal elements are 1/2)

[3] Iteration for the selfconsistent calculation. Edit `fl06.sh` and set the number of iteration at the parameter, `ITER_MAIN`.

```
-----------------------------
(ab_input.data) fl06.qsub
-----------------------------
```

In `fl06.qsub`, the following programs run:

- `fl_pot.exe` makes the potential from the charge densty.
- `fl_potuj.exe` makes the +U potential from the local density matrix.
- `fl_bnd.exe` calculates eigen functions through a standard diagonalization.
- `fl_chg.exe` determines the Fermi energy and calculate the charge desity from the eigen functions.
- `fl_dmmx.exe` calculates the local density matrix.
- `fl_pot.exe` calculates the total energy.
- `fl_mx5.exe` calculates the next input of charge density.

Here, `fl_ptuj.exe` works only with lda+u> 0.

A summary on each cycle of the iterative calculation is written in the file, `iter.log`. The summary is shown on the display by the commnad,

```
-----------------------------
  check.sh
-----------------------------
```

[4] Drawing of the crystal structure

- Edit `bn_atps.data`. Give the region of drawing in the file.
- Run `bn_atps.sh` and `p3_atps.sh`.
- A postscript file, `plot.ps`, is obtained.

[5] Drawing of the band structure (e-k curve)

- Edit `bnpl.data`. Give paths in the k space to be drawn.
- Run `bnpl.sh`.
- `plot.ps` is obtained for the nonmagnetic case (jmag=0) or the antiferromagnetic case (jmag=1); `plot1.ps` and `plot2.ps` are obtained for the magnetic case (jmag=2).

[6] Drawing of the k-space path

- Run `brzone.sh`.
- `plot.ps` is obtained, which shows he k-space path in the e-k curve.

[7] Drawing of the density of states (DOS)

- Edit `bn_pdos.data`. Give the energy region to be drawn.
- Run `bn_pdos.sh`.
- Edit `p2_dos.data`. Select the total DOS, the s, p, d, and f partial DOS.
- Run `p2_dos.sh`
- `plot.ps` is obtained for the nonmagnetic case (jmag=0) or the antiferromagnetic case (jmag=1); `plot1.ps` and `plot2.ps` are obtained for the magnetic case (jmag=2).

3.2 Nonmagnetic Si

```
>>>>>>>>> ab_prp.data >>>>>>>>>>>
Si (227, Oh7, Fd-3m)
  a=5.4296 A
  face-centered (il=2) cubic lattice
  generators   5  (0/1, 0/1, 0/1)
              19  (1/4, 1/4, 1/4)
              25  (1/4, 1/4, 1/4)
  atomic position (0.0, 0.0, 0.0)
  nonmagnetic (jmag=0)
>>>>>>>>> ab_prp.data >>>>>>>>>>>
```

In 'magnetic state' section in the `ab_prp.data` file, the jmag0 parameter should be 0, namely,

```
magnetic state    -2----*----3----*----4----*-
 2              !jmag0 !noSO:(0(N),1(AF),2(M))
-------------------------------------------
```

3.3 Antiferromagnetic Cr

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
Cr andiferromagnetic (221, Oh1, Pm-3m)
  a=2.88A (bcc)
  simple (il=1) cubic lattice for AFM
  generators   5  (0, 0, 0)
              19  (0, 0, 0)
              25  (0, 0, 0)
  atomic positions (0.0, 0.0, 0.0)
                   (0.5, 0.5, 0.5)
  antiferromagnetic (jmag=1)
    operation  1  (1/2, 1/2, 1/2)
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```

In 'magnetic state' section in the `ab_prp.data` file, the jmag0 parameter should be 1, followed by the antiferromagnetic operation code, namely

```
magnetic state    -2----*----3----*----4----*-
 1              !jmag0 !noSO:(0(N),1(AF),2(M))
    1   1 2  1 2  1 2  !igen,jgen(2,3) for AF
-------------------------------------------
```

Here, the antiferromagnetic operation means the symmetry operation which shows the relation between the up-spin state and the down-spin state.

4 The k group

[1] Irreducible representations for the k group

- Edit `ab_irep.data`: Give k points to be calculated.

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
abcap-ab_irep.data
1           ! the number of k
0 0 0  1    ! k point
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```

- Run `ab_irep.sh`.
- See `ab_irep.log`.

[2] Compatibility in k space

- Edit `ab_compat.data`: Give a series of k points for which you want to know the compatibility between the successive k points.

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
abcap-ab_compat.data
2           ! the number of k points
0 0 0  1    ! k point
1 0 0  8    ! k point
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```

- Run `ab_compat.sh`.
- See `ab_compat.log`.

[3] Optical transition (dipole allowed)

- Edit `optsel.data`: Give k points to be calculated.

```
>>>>>>>>>> optsel.data >>>>>>>>>>>>
0         ! jpr (std output control)
0         ! idoub (0: noSOi or 1: SOi)
0 0 0 1   ! k-point
6         ! irrep. of vector (r or p)
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```

- Run `optsel.sh`.
- See `optsel.txt`.

5 LDA+U method

The LDA+U calculation is done by the input data in the 'exchange-correlation potential' section of `ab_input.data` file, namely,

```
exchange-correlation potential ---------------
vwn
    1    1.000000         lda+u, amix_u
    1    3   10.7   0.7  kind, l, U[eV], J[eV]
-----------------------------------------------
```

This is an example for the calculation of $LaMnO_3$, in which kind=1 means La, and U-J=10eV, J=0.7eV.

Typical values of U are 2eV – 5eV for the 3d (l=2) orbital, and 5eV – 10eV for the 4f (l=3) orbital.

For example, please check the value of the band gap and the feature of valence band top for NiO.

- Nonmagnetic NiO
- Ferromagnetic NiO
- Type II AFM NiO

5.1 Nonmagnetic and ferromagnetic NiO

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
NiO
  a=4.17A,   NaCl structure
  face-centered (il=2) cubic lattie
  generators   5  (0, 0, 0)
              19  (0, 0, 0)
              25  (0, 0, 0)
  atomic positions (0.0, 0.0, 0.0) Ni
                   (0.5, 0.5, 0.5) O
  nonmagnetic   (jmag=0)
  ferromagnetic (jmag=2)
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```

5.2 Antiferromagnetic NiO

- Type I AFM

```
  >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
  NiO [a(cubic)=4.17A]
    a=2.948635A, c=4.17A
    simple (il=1) tetragonal lattice
    generators   2  (0, 0, 0)
                21  (0, 0, 0)
                25  (0, 0, 0)
    atomic positions (0.0, 0.0, 0.0) Ni-up
                     (0.5, 0.5, 0.5) Ni-down
                     (0.5, 0.5, 0.0) O
                     (0.0, 0.0, 0.5) O
    antiferromagnetic (jmag=1)
                  1  (1/2, 1/2, 1/2)
  >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```

- Type II AFM NiO

```
  >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
  NiO [a(cubic)=4.17A]
    a=2.948635A, c=14.445304A
    Rhombohedral (il=-1) lattie
    generators   3  (0, 0, 0)
                10  (0, 0, 0)
                13  (0, 0, 0)
    atomic positions (0.0, 0.0, 0.0) Ni-up
                     (0.0, 0.0, 0.5) Ni-down
                     (2/3, 1/3, 1/12) O
    antiferromagnetic (jmag=1)
                  1  (0, 0, 1/2)
  >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```

6 Optical property

- Calculate the dielctric function within the dipole interband transition.

- Calculate the optical constants.
- Calculate the optical property of thin film.

[1] Preparation

Use a command, Setopt.sh, to prepare a directory for the optical-spectrum calculation. We assume that the band structure calculation has been done at the directory, `NiOr_a2_u6`.

```
-----------------------------
  cd ~/abc
  cp $ABCAP/samples/Setopt.sh .
  Setopt.sh NiOr_a2_u6
-----------------------------
```

This makes a directory, `NiOr_a2_u6_s`, and copies some files from `$ABCAP/samples/ZnO_5_s0` and `NiOr_a2_u6` to this directory.

[2] Initial check

```
-----------------------------
  cd ~/abc/NiOr_a2_u6_s
  H
  bnpl.sh  ;  gs plot.ps
  bngap.sh ;  cat bngap.log
           ;  cat bngap.txt
-----------------------------
```

[3] Adjustment of the band gap

```
-----------------------------
  (bn_scis.data)  bn_scis.sh
  bngap.sh ;  cat bngap.log
-----------------------------
```

`bn_scis.sh` makes a scissors operation.

[4] Carrier doping

```
-----------------------------
  (bn_dope.data)  bn_dope.sh
  (bnpl.data)     bnpl.sh
-----------------------------
```

[5] Calculation of the dielectric function

```
-----------------------------
  (df01.data)  df01.qsub
-----------------------------
```

[6] Contribution of plasma oscillation

```
-----------------------------
  (wpw.data)  wpw.sh
              bn_efp2.sh
  (df_total.data) df_total.sh
-----------------------------
```

[7] Drawing of optical constants

```
-----------------------------
  (p2_dielec.data)  p2_dielec.sh
  (p2_optnk.data)   p2_optnk.sh
  (p2_absorb.data)  p2_absorb.sh
-----------------------------
```

[8] Drawing of optical property of the thin film

```
-----------------------------
  (optra.data)    optra.sh
  (p2_optra.data) p2_optra.sh
-----------------------------
```

7 Space group information

- generators:
  File: `generator.data`
- Wycoff positions:
  File: `wycoff.data`
- To make `ab_prp.data`,
  there is a tool, `ab_crystal.sh`.

8 Some other materials

8.1 AlP

```
>>>>>>>>> ab_prp.data >>>>>>>>>>>
AlP (216, Td2, F-43m) zinc blende
  a=5.45 A
  face-centered (il=2) cubic lattice
  generators   5  (0, 0, 0)
              43  (0, 0, 0)
  atomic positions
           (0.0,  0.0,  0.0 )  Al
           (0.25, 0.25, 0.25)  P
  nonmagnetic (jmag=0)
>>>>>>>>> ab_prp.data >>>>>>>>>>>
```

8.2 Al

```
>>>>>>>>> ab_prp.data >>>>>>>>>>>
Al (225, Oh5, Fm-3m) fcc
  a=4.05 A
  face-centered (il=2) cubic lattice
  generators   5  (0, 0, 0)
              19  (0, 0, 0)
              25  (0, 0, 0)
  atomic position (0.0, 0.0, 0.0)
  nonmagnetic (jmag=0)
>>>>>>>>> ab_prp.data >>>>>>>>>>>
```

9 Crystal structures

NIMS database:

`http://crystdb.nims.go.jp/crystdb/search-materials`

- Search 'nims' and 'atomwork' by using internet.
- Click "Enter AtomWork"
- login.
- Input elements of the compound
  (example: Al P)
  Click "Search materials".
- Choose a structure.
- Choose a paper from the refernce list.
- See crystal structure (standardized).