2nd-6th September 2019

ABCAP: advanced course

ABCAP(All electron BAnd Calculation Package): FLAPW code

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Purpose

①Study the symmetry of crystal and electronic structure (symmetry operations).

②Study the symmetry of wavefunction (irreducible representations).

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

④Calculate the optical absorption spectrum.

⑤Treat magnetic materials.

⑥Use the +*U* method.

1-1. Environment variables

Let's use bash.
In order to set some environment variables, execute
the following commands:

```
cat /home/CMD/teac02/abcap1707/Bash_envs >> ~/.bash_profile
source ~/.bash_profile
```


```
#---------------------------------
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`
#---------------------------------
```

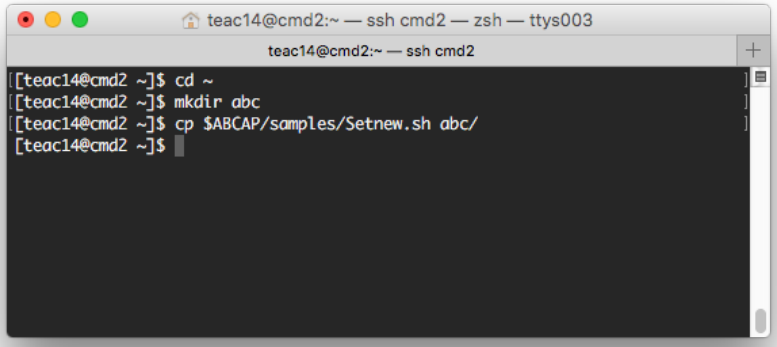
contents: /home/CMD/teac02/abcap1707/Bash_envs

1-2. 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/***.

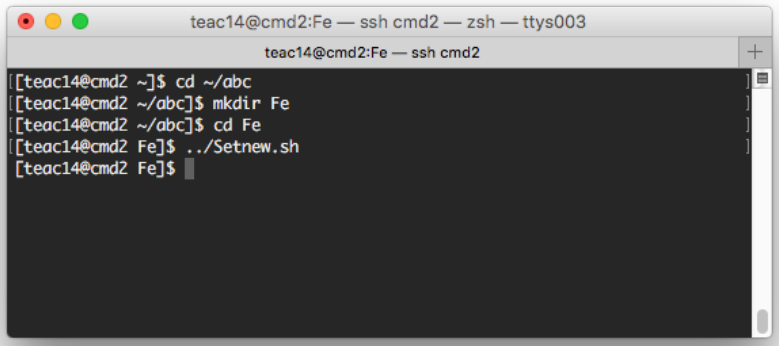
Hands on DFT simulation

- Ferromagnetic Fe
- Nonmagnetic Si

2-1. Ferromagnetic Fe

Prepare a directory for the calculation:

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



Enter a command, ***Hqc***, which shows a procedure of the calculation.

The procedure consists of

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

Attention

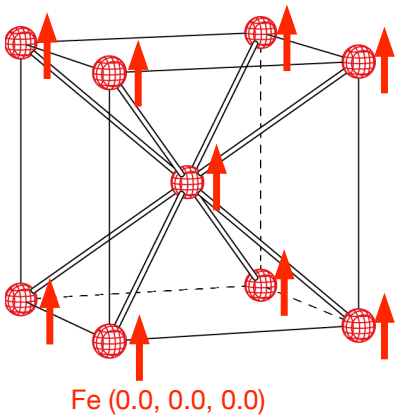
In this workshop, you must replace "*.qc" to "*.qsub"

e.g.

ab_prp.qc -> ab_prp.qsub

```
teac14@cmd2:Fe — ssh cmd2 — zsh — ttys003
[teac14@cmd2 Fe]$ Hqc
-----------------------------------------------------------------
(0) (ab_prp.data, atom.data)   ab_prp.qc
(1) (ab_input.data)            ab_in.qc
-----------------------------------------------------------------
(2) Hu (for +U calculation)
-----------------------------------------------------------------
(3) (ab_input.data)            fl06.qc or fl06b.qc
                               check.sh
-----------------------------------------------------------------
(4a) (bn_atps.data)  bn_atps.sh  (p3_atps.data)  p3_atps.sh
-----------------------------------------ghostview plot.ps ------
(4b) <noSOi>  (bnpl.data)      bnpl.sh
     <noSOi>  (angle.data)     brzone.sh --> brzone.ps
       <SOi>  cd bndraw_so  (bndraw.data)     bndraw.sh
-----------------------------------------ghostview plot?.ps ------
(4c) (bndraw.data)             bndraw.sh
-----------------------------------------ghostview plot.ps ------
(4d) (bn_pdos.data)  bn_pdos.sh  (p2_dos.data)  p2_dos.sh
-----------------------------------------ghostview plot?.ps ------
(4e) cd force; make; cd ../;   force.sh
-----------------------------------------------------------------
-----------------------------------------------------------------
(1') (ab_input.data)  ab_kpgn.sh  --> (2)
-----------------------------------------------------------------
(1") (ab_input.data)  ab_in2.sh   --> (2)
-----------------------------------------------------------------

[teac14@cmd2 Fe]$
```

Edit the file, ***ab_prp.data*** by using the following information:



Body Centered Cubic (BCC) Structure

$\mathrm{Im}\bar{3}\mathrm{m}(O_h^9, \#229)$

Lattice Type

Point group O_h has full cubic symmetry.

3-fold rotation

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
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)
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```

Space Group

periodicity: 14 Bravais Lattice

point symmetry: 32 point group

point group
rotation(including reflection)
+
translational group
→ **space group**

7 crystal systems		Point Group
Cubic	P,F,I	O_h, O, T_d, T_h, T
Tetragonal	P,I	$D_{4h}, D_4, D_{2d}, C_{4v}, C_{4h}, S_4, C_4$
Orthorhombic	P,F,I,C	D_{2h}, D_2, C_{2v}
Hexagonal	P	$D_{6h}, D_6, D_{3h}, C_{6v}, C_{6h}, C_{3h}, C_6$ $D_{3d}, D_3, C_{3v}, S_6, C_3$
Trigonal	R	$D_{3d}, D_3, C_{3v}, S_6, C_3$
Monoclinic	P,C	C_{2h}, C_S, C_2
Triclinic	P	C_i, C_1

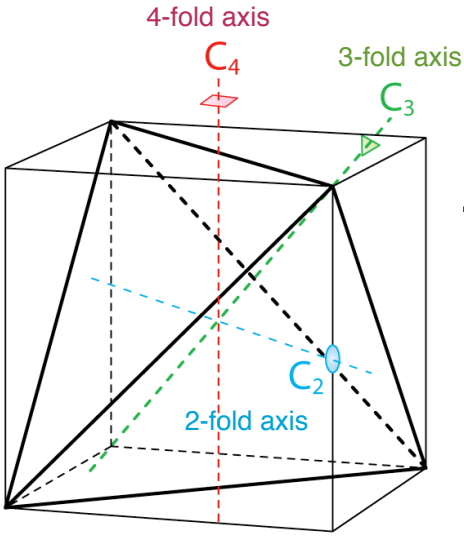
Subgroup of O_h / D_{6h}

P... simple
F...Face Centered
I ... Body Centered
C...Base Centered
R... Rhombohedlal

symmetry Operation

$$\left(\alpha|\vec{t}+\vec{u}_\alpha\right)=\alpha\vec{u}+\vec{t}+\vec{u}_\alpha$$
$$(\alpha|\vec{a})\left(\beta|\vec{b}\right)=\left(\alpha\beta|\alpha\vec{b}+\vec{a}\right)$$
$$\left(\alpha|\vec{b}\right)^{-1}=\left(\alpha^{-1}|-\alpha^{-1}\vec{b}\right)$$

Point Group: $\mathrm{O_h}$



Cubic Symmetry $\mathrm{O_h}$

$\mathrm{E}\cdots\cdots 1$ identity operation

$\mathrm{C_4}\cdots\cdots 6$	$\pm\pi/2$
$\mathrm{C_4^2}\cdots\cdots 3$	
$\mathrm{C_2}\cdots\cdots 6$	$\pm\pi$
$\mathrm{C_3}\cdots\cdots 8$	$\pm 2\pi/3$

24 rotational operation

+ inversion, rotation inversion, reflection and rotational reflection

→ **48 symmetry Operation**

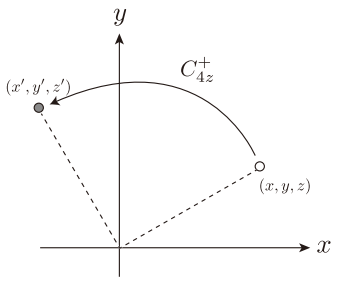
subgroup of $\mathrm{O_h}$

example
Tetrahedral Symmetry → $\mathrm{T_d}$

$$\mathrm{T_d}\otimes\mathrm{C_4}=\mathrm{O_h}$$

Rotational Operation

example: C_{4z}^{+}



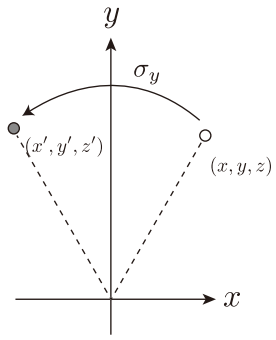
$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -y \\ x \\ z \end{bmatrix}$$

matrix representation of C_{4z}^{+}

```
C4z+     (-y,  x,  z)
```

reflectional Operation

example: σ_{yz}



$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ y \\ z \end{bmatrix}$$

matrix representation of σ_{yz}

$$= \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

space inversion(I) C_{2x} ← x-axis is the normal direction of yz-plane

```
IC2x     (-x,  y,  z)
```

Generally speaking, reflectional operation is written as production between space inversion and 2-hold rotation,C_2

rotational operation code for O_h and subgroup in TSPACE

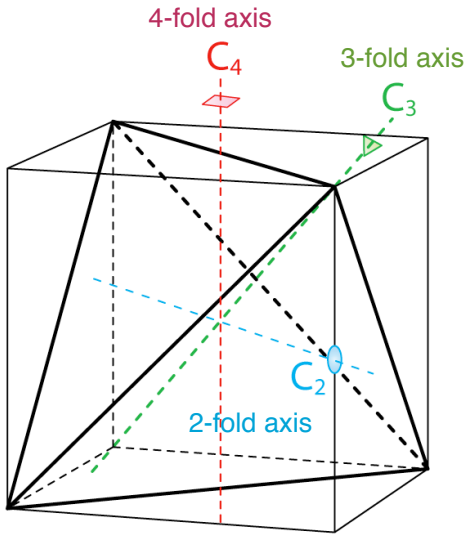
identity

(1)	E	(x, y, z)
(2)	C2x	(x, -y, -z)
(3)	C2y	(-x, y, -z)
(4)	C2z	(-x, -y, z)
(5)	C31+	(z, x, y)
(6)	C32+	(-z, x, -y)
(7)	C33+	(-z, -x, y)
(8)	C34+	(z, -x, -y)
(9)	C31-	(y, z, x)
(10)	C32-	(y, -z, -x)
(11)	C33-	(-y, z, -x)
(12)	C34-	(-y, -z, x)
(13)	C2a	(y, x, -z)
(14)	C2b	(-y, -x, -z)
(15)	C2c	(z, -y, x)
(16)	C2d	(-x, z, y)
(17)	C2e	(-z, -y, -x)
(18)	C2f	(-x, -z, -y)
(19)	C4x+	(x, -z, y)
(20)	C4y+	(z, y, -x)
(21)	C4z+	(-y, x, z)
(22)	C4x-	(x, z, -y)
(23)	C4y-	(-z, y, x)
(24)	C4z-	(y, -x, z)

C_4^2 $C_3^{\pm}$ C_2 $C_4^{\pm}$

(25)	IE	(-x, -y, -z)
(26)	IC2x	(-x, y, z)
(27)	IC2y	(x, -y, z)
(28)	IC2z	(x, y, -z)
(29)	IC31+	(-z, -x, -y)
(30)	IC32+	(z, -x, y)
(31)	IC33+	(z, x, -y)
(32)	IC34+	(-z, x, y)
(33)	IC31-	(-y, -z, -x)
(34)	IC32-	(-y, z, x)
(35)	IC33-	(y, -z, x)
(36)	IC34-	(y, z, -x)
(37)	IC2a	(-y, -x, z)
(38)	IC2b	(y, x, z)
(39)	IC2c	(-z, y, -x)
(40)	IC2d	(x, -z, -y)
(41)	IC2e	(z, y, x)
(42)	IC2f	(x, z, y)
(43)	IC4x+	(-x, z, -y)
(44)	IC4y+	(-z, -y, x)
(45)	IC4z+	(y, -x, -z)
(46)	IC4x-	(-x, -z, y)
(47)	IC4y-	(z, -y, -x)
(48)	IC4z-	(-y, x, -z)

space inversion



We can identify the space group as rotational, inversion and reflectional operation with translation operation.

production between group elements

e.g. $C_{2b} \cdot C_{2x} = ?$

```
( 2)    C2x     ( x, -y, -z)
(14)    C2b     (-y, -x, -z)
```

$$\mathcal{O}(C_{2b}) \cdot \mathcal{O}(C_{2x}) = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$
$$= \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
$$= \mathcal{O}(C_{4z}^{-})$$

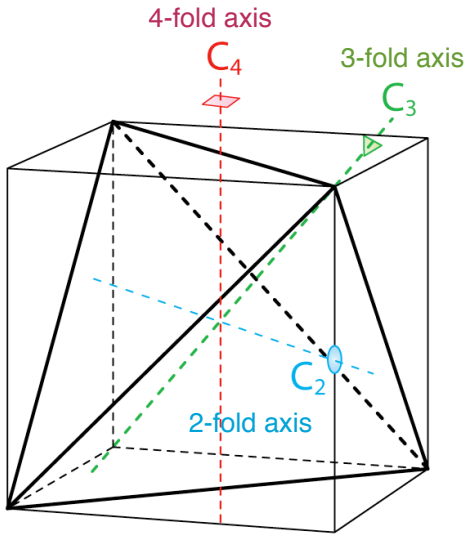
rotational operation code for O_h and subgroup in TSPACE

identity

	(1)	E	(x, y, z)
C_4^2	(2)	C2x	(x, -y, -z)
	(3)	C2y	(-x, y, -z)
	(4)	C2z	(-x, -y, z)
$C_3^{\pm}$	(5)	C31+	(z, x, y)
	(6)	C32+	(-z, x, -y)
	(7)	C33+	(-z, -x, y)
	(8)	C34+	(z, -x, -y)
	(9)	C31-	(y, z, x)
	(10)	C32-	(y, -z, -x)
	(11)	C33-	(-y, z, -x)
	(12)	C34-	(-y, -z, x)
C_2	(13)	C2a	(y, x, -z)
	(14)	C2b	(-y, -x, -z)
	(15)	C2c	(z, -y, x)
	(16)	C2d	(-x, z, y)
	(17)	C2e	(-z, -y, -x)
	(18)	C2f	(-x, -z, -y)
$C_4^{\pm}$	(19)	C4x+	(x, -z, y)
	(20)	C4y+	(z, y, -x)
	(21)	C4z+	(-y, x, z)
	(22)	C4x-	(x, z, -y)
	(23)	C4y-	(-z, y, x)
	(24)	C4z-	(y, -x, z)

	(25)	IE	(-x, -y, -z)
	(26)	IC2x	(-x, y, z)
	(27)	IC2y	(x, -y, z)
	(28)	IC2z	(x, y, -z)
	(29)	IC31+	(-z, -x, -y)
	(30)	IC32+	(z, -x, y)
	(31)	IC33+	(z, x, -y)
	(32)	IC34+	(-z, x, y)
	(33)	IC31-	(-y, -z, -x)
	(34)	IC32-	(-y, z, x)
	(35)	IC33-	(y, -z, x)
	(36)	IC34-	(y, z, -x)
	(37)	IC2a	(-y, -x, z)
	(38)	IC2b	(y, x, z)
	(39)	IC2c	(-z, y, -x)
	(40)	IC2d	(x, -z, -y)
	(41)	IC2e	(z, y, x)
	(42)	IC2f	(x, z, y)
	(43)	IC4x+	(-x, z, -y)
	(44)	IC4y+	(-z, -y, x)
	(45)	IC4z+	(y, -x, -z)
	(46)	IC4x-	(-x, -z, y)
	(47)	IC4y-	(z, -y, -x)
	(48)	IC4z-	(-y, x, -z)

inversion



group table (not including space inversion)

C_{2x}

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
2	2	1	4	3	8	7	6	5	10	9	12	11	24	21	20	18	23	16	22	15	14	19	17	13
3	3	4	1	2	6	5	8	7	11	12	9	10	21	24	17	22	15	19	18	23	13	16	20	14
4	4	3	2	1	7	8	5	6	12	11	10	9	14	13	23	19	20	22	16	17	24	18	15	21
5	5	6	7	8	9	12	10	11	1	3	4	2	23	17	22	24	18	14	13	16	15	21	19	20
6	6	5	8	7	11	10	12	9	3	1	2	4	20	15	16	14	19	24	21	22	17	13	18	23
7	7	8	5	6	12	9	11	10	4	2	1	3	15	20	18	21	22	13	14	19	23	24	16	17
8	8	7	6	5	10	11	9	12	2	4	3	1	17	23	19	13	16	21	24	18	20	14	22	15
9	9	12	10	11	1	2	3	4	5	7	8	6	19	18	21	20	14	17	23	24	22	15	13	16
10	10	11	9	12	2	1	4	3	8	6	5	7	22	16	14	15	21	23	17	13	19	20	24	18
11	11	10	12	9	3	4	1	2	6	8	7	5	18	19	13	23	24	15	20	14	16	17	21	22
12	12	9	11	10	4	3	2	1	7	5	6	8	16	22	24	17	13	20	15	21	18	23	14	19
13	13	21	24	14	22	19	18	16	20	23	15	17	1	4	11	8	12	7	6	9	2	5	10	3
14	14	24	21	13	18	16	22	19	17	15	23	20	4	1	10	6	9	5	8	12	3	7	11	2
15	15	23	17	20	24	14	13	21	19	16	18	22	7	6	1	10	3	11	9	4	8	12	2	5
16	16	18	19	22	23	15	20	17	21	14	24	13	12	10	6	1	8	2	3	7	9	4	5	11
17	17	20	15	23	14	24	21	13	18	22	19	16	8	5	3	12	1	9	11	2	7	10	4	6
18	18	16	22	19	17	20	15	23	14	21	13	24	11	9	7	2	5	1	4	6	10	3	8	12
19	19	22	16	18	15	23	17	20	24	13	21	14	9	11	8	4	6	3	2	5	12	1	7	10
20	20	17	23	15	13	21	24	14	22	18	16	19	6	7	2	9	4	12	10	3	5	11	1	8
21	21	13	14	24	16	18	19	22	23	20	17	15	3	2	9	7	10	8	5	11	4	6	12	1
22	22	19	18	16	20	17	23	15	13	24	14	21	10	12	5	3	7	4	1	8	11	2	6	9
23	23	15	20	17	21	13	14	24	16	19	22	18	5	8	4	11	2	10	12	1	6	9	3	7
24	24	14	13	21	19	22	16	18	15	17	20	23	2	3	12	5	11	6	7	10	1	8	9	4

C_{2b}

e.g.

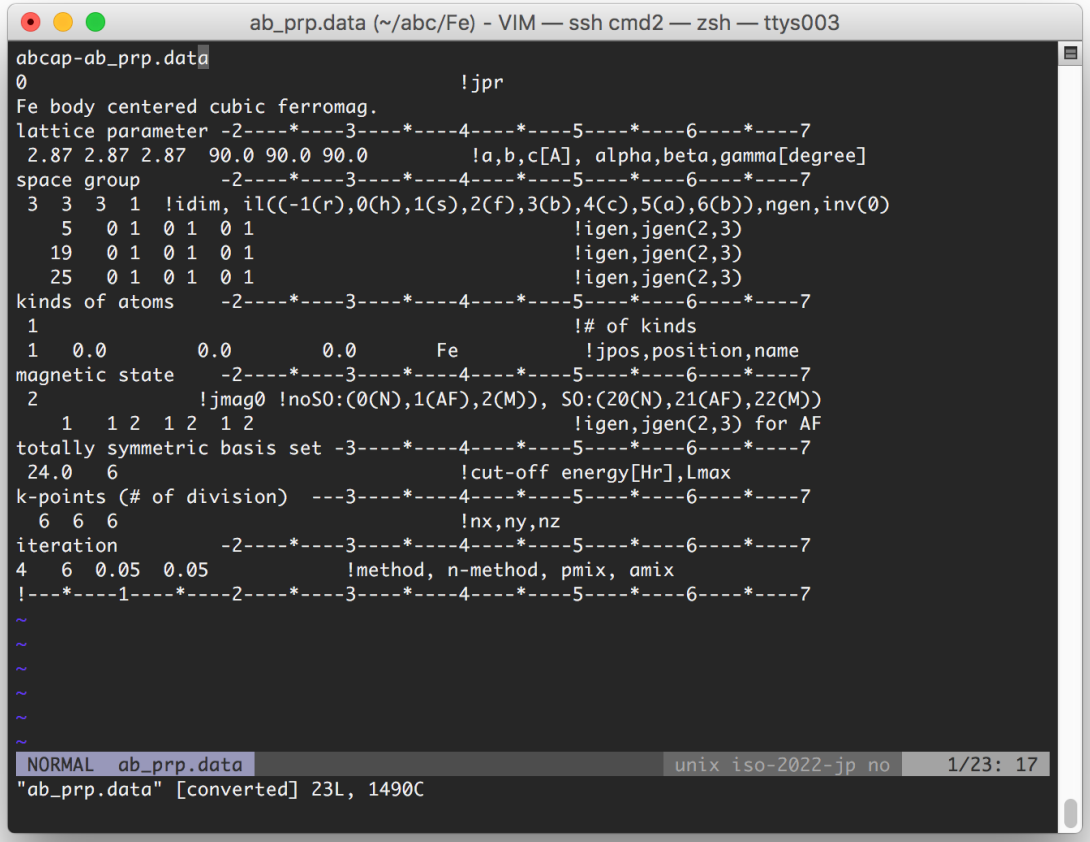
$$C_{2b} \cdot C_{2x} = C_{4z}^{-}$$

(14) (2) (24)

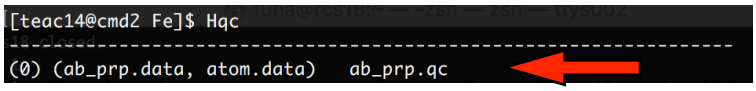
group multiplication table(including space inversion)

	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
1	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
2	26	25	28	27	32	31	30	29	34	33	36	35	48	45	44	42	47	40	46	39	38	43	41	37
3	27	28	25	26	30	29	32	31	35	36	33	34	45	48	41	46	39	43	42	47	37	40	44	38
4	28	27	26	25	31	32	29	30	36	35	34	33	38	37	47	43	44	46	40	41	48	42	39	45
5	29	30	31	32	33	36	34	35	25	27	28	26	47	41	46	48	42	38	37	40	39	45	43	44
6	30	29	32	31	35	34	36	33	27	25	26	28	44	39	40	38	43	48	45	46	41	37	42	47
7	31	32	29	30	36	33	35	34	28	26	25	27	39	44	42	45	46	37	38	43	47	48	40	41
8	32	31	30	29	34	35	33	36	26	28	27	25	41	47	43	37	40	45	48	42	44	38	46	39
9	33	36	34	35	25	26	27	28	29	31	32	30	43	42	45	44	38	41	47	48	46	39	37	40
10	34	35	33	36	26	25	28	27	32	30	29	31	46	40	38	39	45	47	41	37	43	44	48	42
11	35	34	36	33	27	28	25	26	30	32	31	29	42	43	37	47	48	39	44	38	40	41	45	46
12	36	33	35	34	28	27	26	25	31	29	30	32	40	46	48	41	37	44	39	45	42	47	38	43
13	37	45	48	38	46	43	42	40	44	47	39	41	25	28	35	32	36	31	30	33	26	29	34	27
14	38	48	45	37	42	40	46	43	41	39	47	44	28	25	34	30	33	29	32	36	27	31	35	26
15	39	47	41	44	48	38	37	45	43	40	42	46	31	30	25	34	27	35	33	28	32	36	26	29
16	40	42	43	46	47	39	44	41	45	38	48	37	36	34	30	25	32	26	27	31	33	28	29	35
17	41	44	39	47	38	48	45	37	42	46	43	40	32	29	27	36	25	33	35	26	31	34	28	30
18	42	40	46	43	41	44	39	47	38	45	37	48	35	33	31	26	29	25	28	30	34	27	32	36
19	43	46	40	42	39	47	41	44	48	37	45	38	33	35	32	28	30	27	26	29	36	25	31	34
20	44	41	47	39	37	45	48	38	46	42	40	43	30	31	26	33	28	36	34	27	29	35	25	32
21	45	37	38	48	40	42	43	46	47	44	41	39	27	26	33	31	34	32	29	35	28	30	36	25
22	46	43	42	40	44	41	47	39	37	48	38	45	34	36	29	27	31	28	25	32	35	26	30	33
23	47	39	44	41	45	37	38	48	40	43	46	42	29	32	28	35	26	34	36	25	30	33	27	31
24	48	38	37	45	43	46	40	42	39	41	44	47	26	27	36	29	35	30	31	34	25	32	33	28

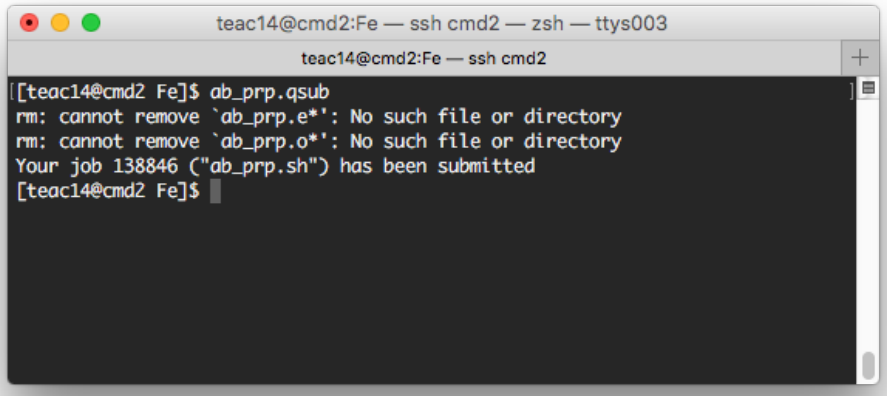
ab_prp.data for bcc ferromagnetic Iron



1. Crystal Structure



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.

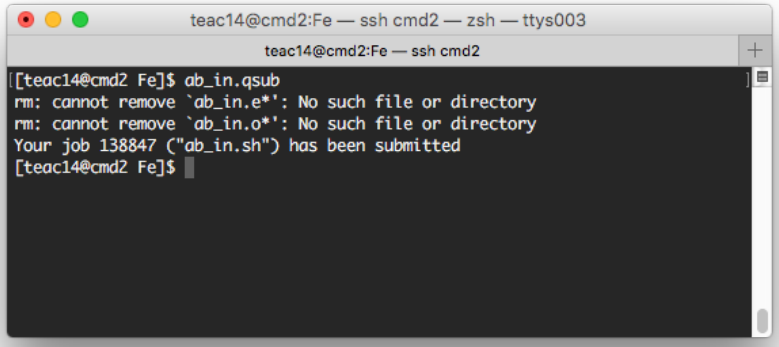


The file, ***ab_input.data***, is made from the informations of ***ab_prp.data*** and ***atom.data***.
The ***atom.data*** file is a data base for atoms from H(hydrogen) to U(uranium).

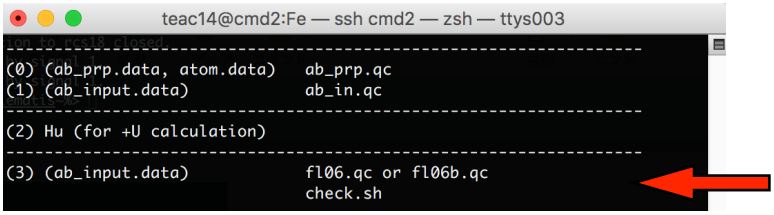
2. initial charge density, potential and etc…

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)

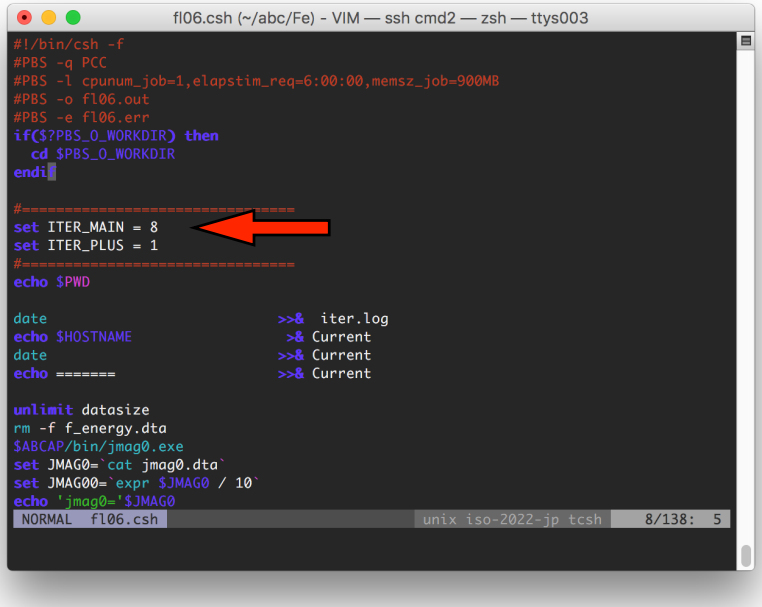


3. Self-Consistent Field(SCF) Calculation



Iteration for the self-consistent calculation. Edit ***fl06.sh*** and set the number of iteration at the parameter, ***ITER_MAIN***.

contents of ***"fl06.sh"***

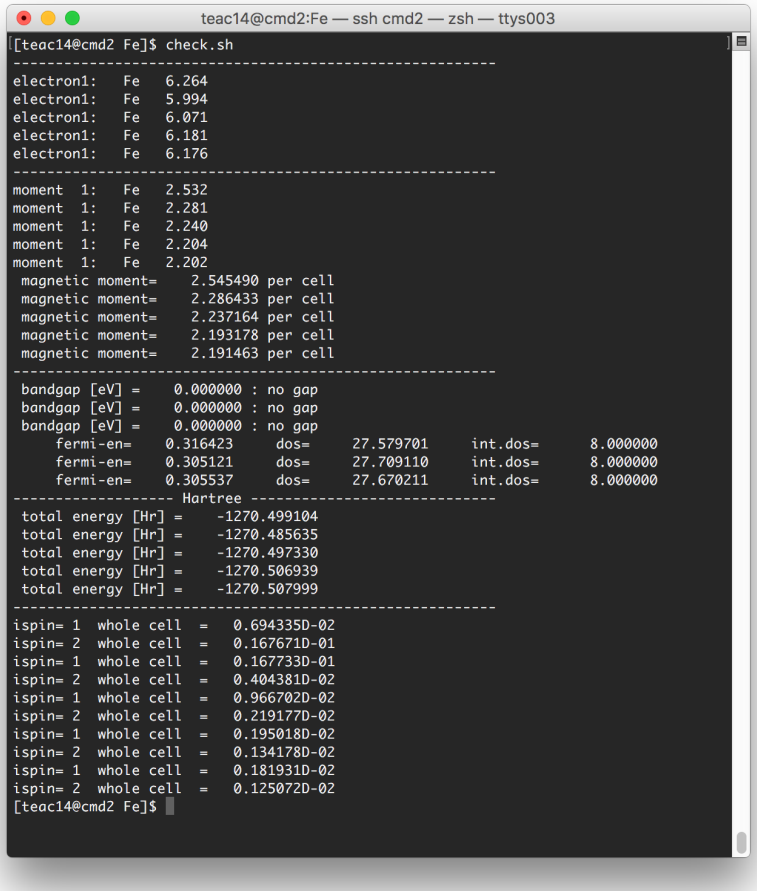


In ***fl06.qsub***, the following programs run:

- ***fl_pot.exe***: makes the potential from the charge density.
- ***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 density 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.

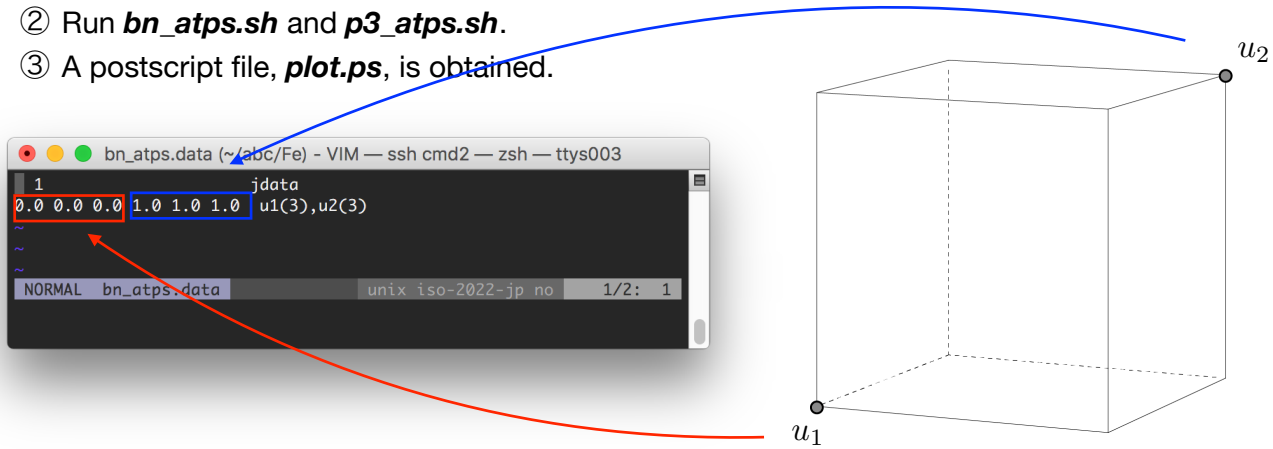
Here, ***fl_ptuj.exe*** works only with lda+u> 0.

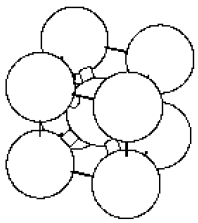
A summary on each cycle of the iterative calculation is written in the file, ***iter.log***. The summary is shown on the display by the command, ***check.sh***



4-1. Drawing the Crystal Structure

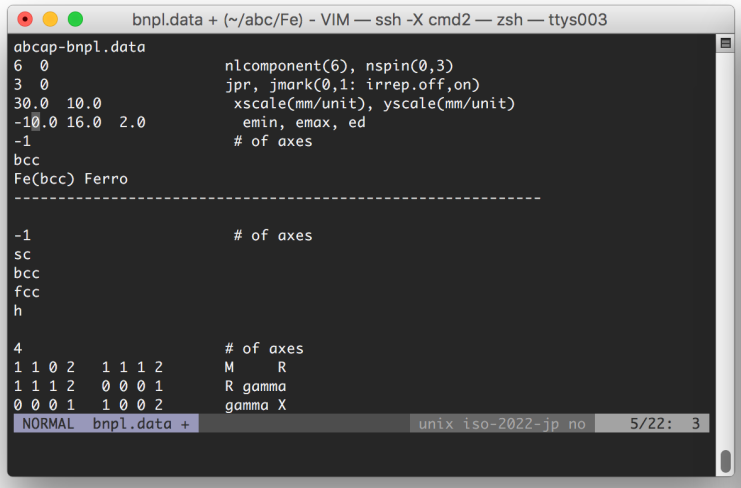
① Edit ***bn_atps.data***. Give the region of drawing in the file.
② Run ***bn_atps.sh*** and ***p3_atps.sh***.
③ A postscript file, ***plot.ps***, is obtained.

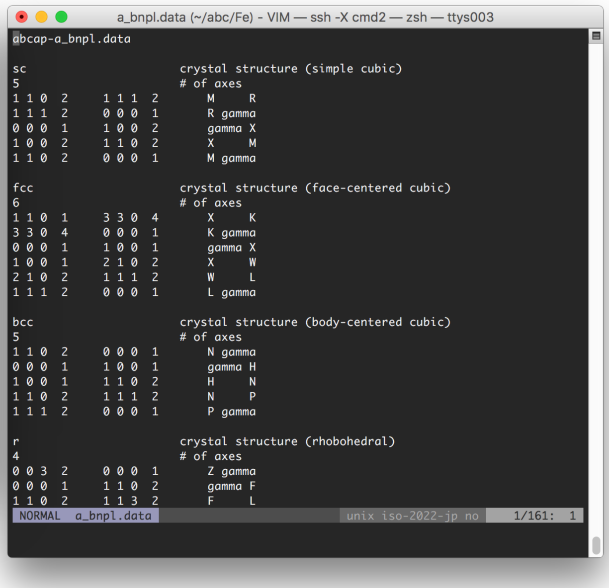


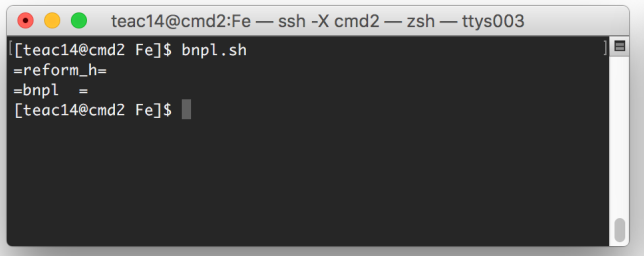


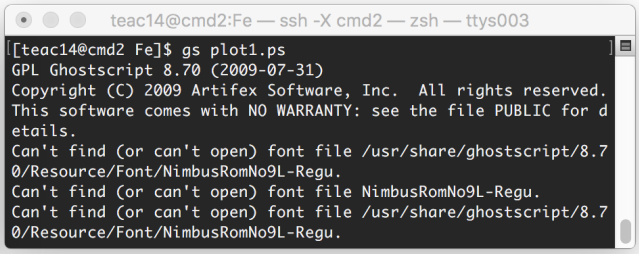
4-1. Drawing the band structure (e-k curve)

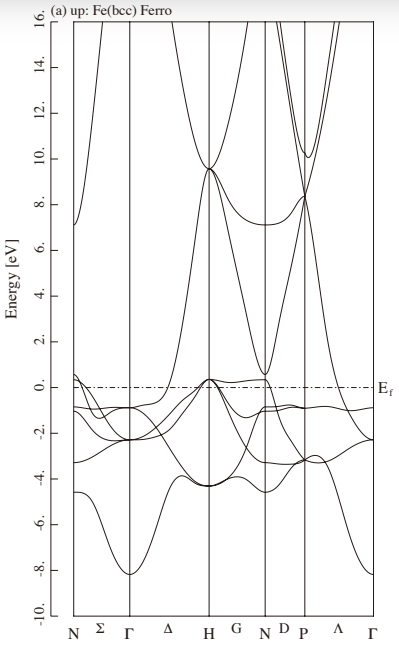
① Edit ***bnpl.data*** and ***a_bnpl.data*** . Give paths in the k-space to be drawn.
② Run ***bnpl.sh***.
③ ***plot.ps*** is obtained for the nonmagnetic case (jmag=0) or the antiferromagnetic case (jmag=1); ***plot1.ps*** and ***plot2.ps*** are obtained for the magnetic case (jmag=2).

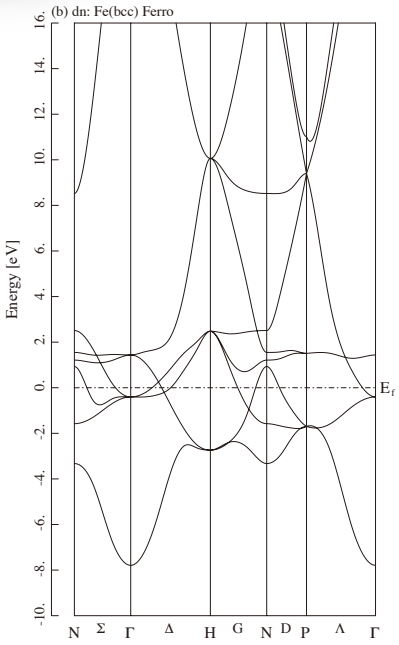








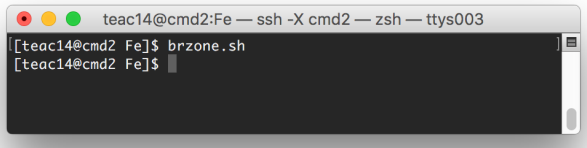


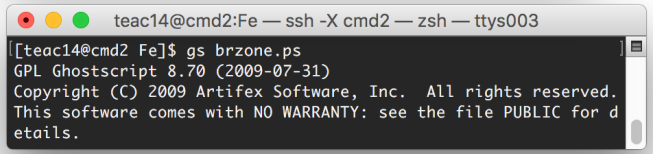


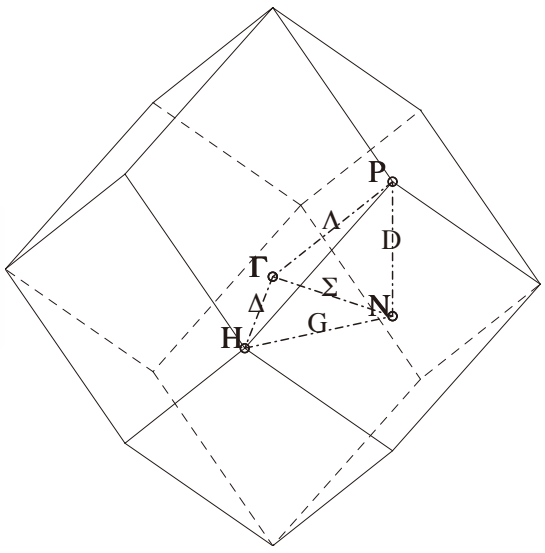
4-2. Drawing the k-space path and BZ

① Run ***brzone.sh***.

② ***brzone.ps*** is obtained, which shows the k-space path in the e-k curve.







4-2. Drawing the Density of States(DOS)

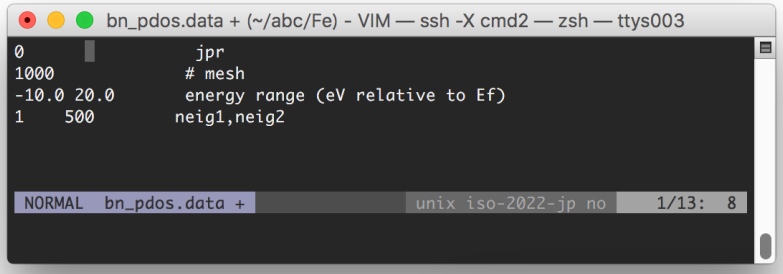
① Edit ***bn_pdos.data***. Give the energy region to be drawn.

② Run ***bn_pdos.sh***.

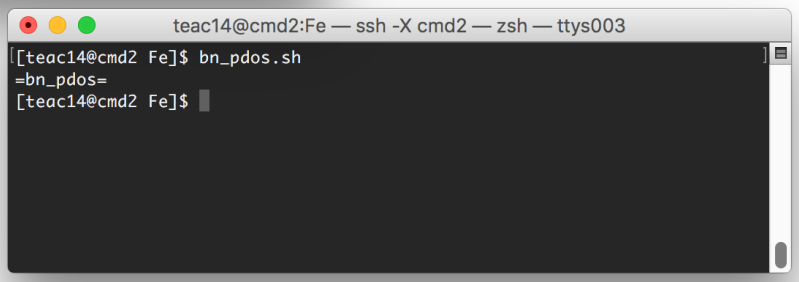
③ Edit ***p2_dos.data***. Select the total DOS, the s, p, d, and f partial DOS.

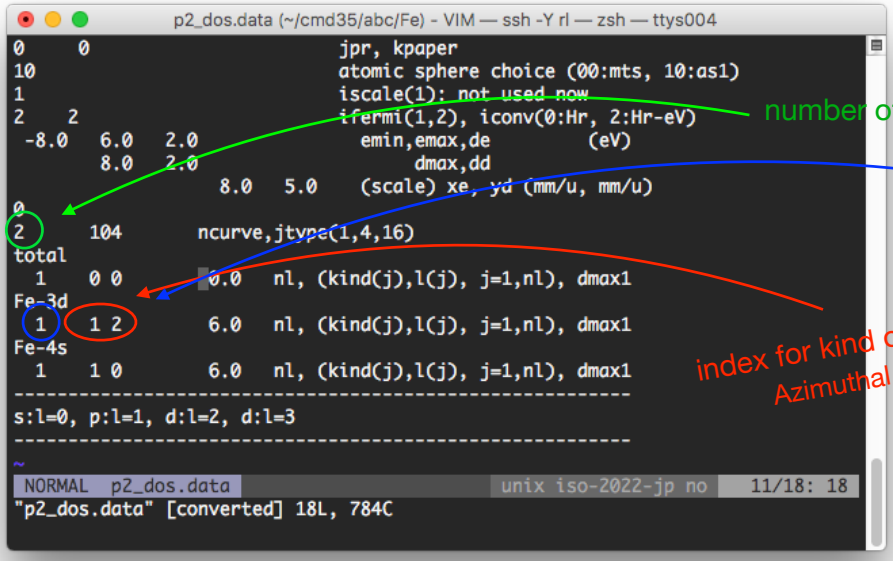
④ Run ***p2_dos.sh***

⑤ ***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).



calculate DOS





number of curves

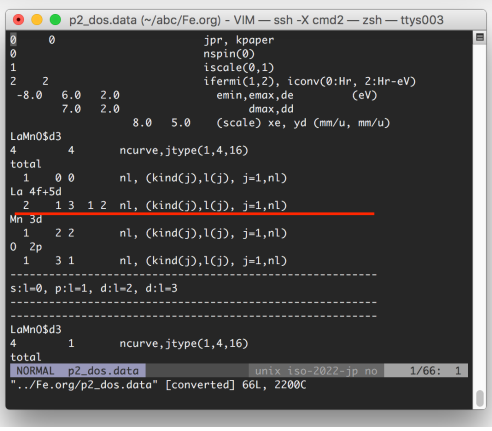
number of components

index for kind of atom

Azimuthal quantum number

$$\begin{cases} l=0 & (s) \\ l=1 & (p) \\ l=2 & (d) \\ l=3 & (f) \end{cases}$$

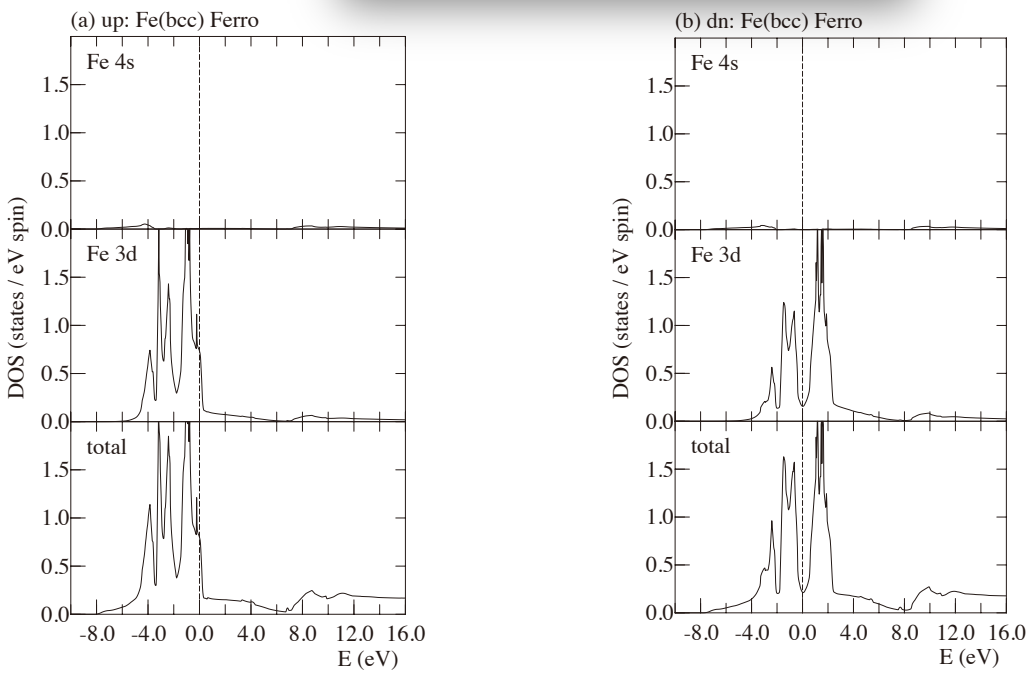
ref.)



drawing DOS curves

```
teac14@cmd2:Fe — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 Fe]$ p2_dos.sh
=p2_dos=
[teac14@cmd2 Fe]$
```

```
teac14@cmd2:Fe — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 Fe]$ gs plot1.ps
GPL Ghostscript 8.70 (2009-07-31)
Copyright (C) 2009 Artifex Software, Inc.  All rights reserved.
This software comes with NO WARRANTY: see the file PUBLIC for details
.
Can't find (or can't open) font file /usr/share/ghostscript/8.70/Reso
urce/Font/NimbusRomNo9L-Regu.
```



4. The *k* group

1. irreducible representation for *k* group

(1) Edit ***ab_irep.data***: Give k points to be calculated.

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

ab_irep.data

numerator

"0 0 0 1" means $\left(\frac{0}{1}, \frac{0}{1}, \frac{0}{1}\right)$

common denominator

(2) Run ***ab_irep.sh***.

```
teac14@cmd2:Fe — ssh cmd2 — zsh — ttys003
[teac14@cmd2 Fe]$ ./ab_irep.sh
=ab_irep=
[teac14@cmd2 Fe]$
```

(3) ***ab_irep.log***.

```
--- characters in (x,y,z) representation ---
jr3=  3 -1 -1 -1  0  0  0  0  0  0  0  0 -1 -1 -1 -1 -1 -1  1  1  1  1  1  1
     -3  1  1  1  0  0  0  0  0  0  0  0  1  1  1  1  1  1 -1 -1 -1 -1 -1 -1
order of the Gamma-point group = 48
no. of irreps=10  : dimension of irrep=  1  1  1  1  3  3  3  3  2  2
--- irredusible decomposition of Jones faithful rep.---
irrep= 6 :  ndim= 3
-----------------------------------------
```

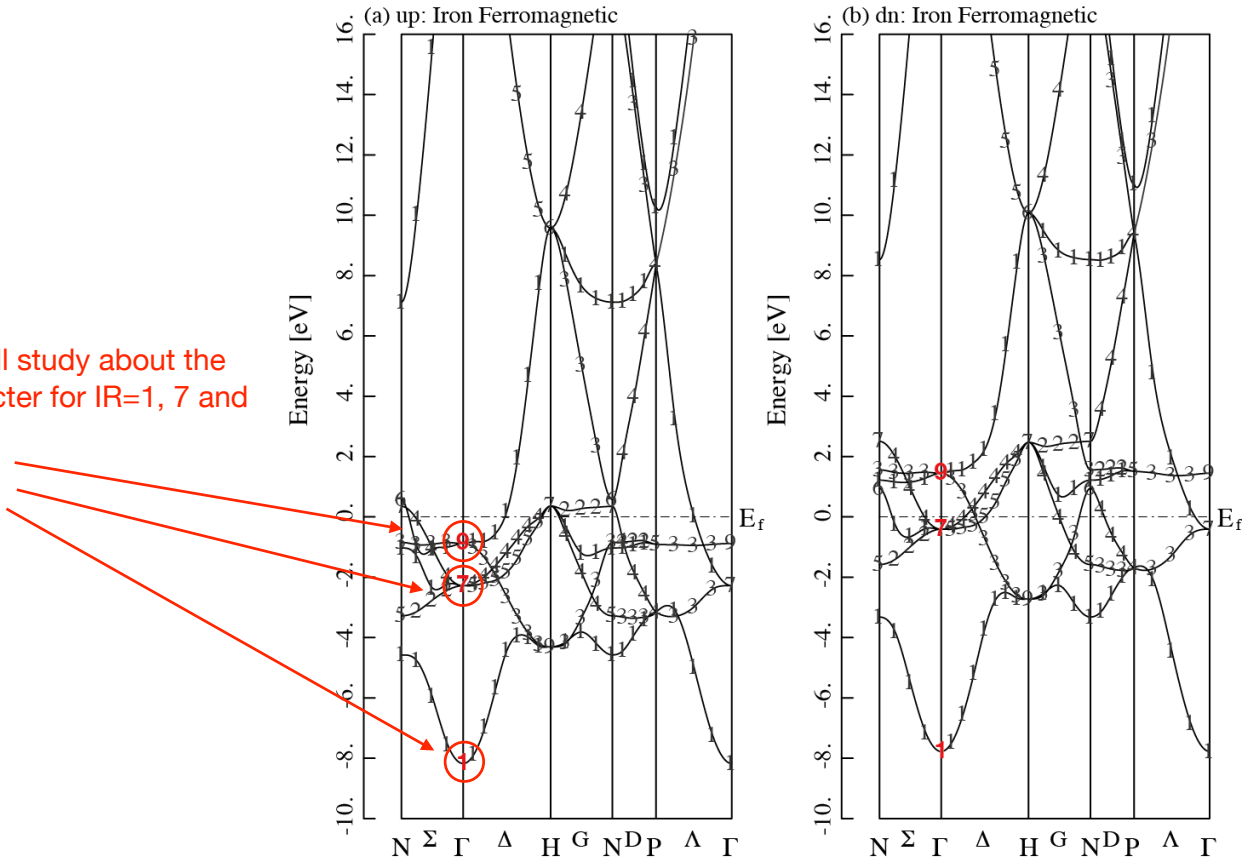
character of irreducible representation (case:Fe)

point group of k(case:Fe)

```
--- k = (    0    0    0 ) /    1  ---
   elements of pk-group k=  0  0  0/  1
```

1	1	e	x	y	z	0/1	0/1	0/1	0	0	0		25	25	ie	-x	-y	-z	0/1	0/1	0/1	0	0	0
2	2	c2x	x	-y	-z	0/1	0/1	0/1	0	0	0		26	26	ic2x	-x	y	z	0/1	0/1	0/1	0	0	0
3	3	c2y	-x	y	-z	0/1	0/1	0/1	0	0	0		27	27	ic2y	x	-y	z	0/1	0/1	0/1	0	0	0
4	4	c2z	-x	-y	z	0/1	0/1	0/1	0	0	0		28	28	ic2z	x	y	-z	0/1	0/1	0/1	0	0	0
5	5	c31+	z	x	y	0/1	0/1	0/1	0	0	0		29	29	ic31+	-z	-x	-y	0/1	0/1	0/1	0	0	0
6	6	c32+	-z	x	-y	0/1	0/1	0/1	0	0	0		30	30	ic32+	z	-x	y	0/1	0/1	0/1	0	0	0
7	7	c33+	-z	-x	y	0/1	0/1	0/1	0	0	0		31	31	ic33+	z	x	-y	0/1	0/1	0/1	0	0	0
8	8	c34+	z	-x	-y	0/1	0/1	0/1	0	0	0		32	32	ic34+	-z	x	y	0/1	0/1	0/1	0	0	0
9	9	c31-	y	z	x	0/1	0/1	0/1	0	0	0		33	33	ic31-	-y	-z	-x	0/1	0/1	0/1	0	0	0
10	10	c32-	y	-z	-x	0/1	0/1	0/1	0	0	0		34	34	ic32-	-y	z	x	0/1	0/1	0/1	0	0	0
11	11	c33-	-y	z	-x	0/1	0/1	0/1	0	0	0		35	35	ic33-	y	-z	x	0/1	0/1	0/1	0	0	0
12	12	c34-	-y	-z	x	0/1	0/1	0/1	0	0	0		36	36	ic34-	y	z	-x	0/1	0/1	0/1	0	0	0
13	13	c2a	y	x	-z	0/1	0/1	0/1	0	0	0		37	37	ic2a	-y	-x	z	0/1	0/1	0/1	0	0	0
14	14	c2b	-y	-x	-z	0/1	0/1	0/1	0	0	0		38	38	ic2b	y	x	z	0/1	0/1	0/1	0	0	0
15	15	c2c	z	-y	x	0/1	0/1	0/1	0	0	0		39	39	ic2c	-z	y	-x	0/1	0/1	0/1	0	0	0
16	16	c2d	-x	z	y	0/1	0/1	0/1	0	0	0		40	40	ic2d	x	-z	-y	0/1	0/1	0/1	0	0	0
17	17	c2e	-z	-y	-x	0/1	0/1	0/1	0	0	0		41	41	ic2e	z	y	x	0/1	0/1	0/1	0	0	0
18	18	c2f	-x	-z	-y	0/1	0/1	0/1	0	0	0		42	42	ic2f	x	z	y	0/1	0/1	0/1	0	0	0
19	19	c4x+	x	-z	y	0/1	0/1	0/1	0	0	0		43	43	ic4x+	-x	z	-y	0/1	0/1	0/1	0	0	0
20	20	c4y+	z	y	-x	0/1	0/1	0/1	0	0	0		44	44	ic4y+	-z	-y	x	0/1	0/1	0/1	0	0	0
21	21	c4z+	-y	x	z	0/1	0/1	0/1	0	0	0		45	45	ic4z+	y	-x	-z	0/1	0/1	0/1	0	0	0
22	22	c4x-	x	z	-y	0/1	0/1	0/1	0	0	0		46	46	ic4x-	-x	-z	y	0/1	0/1	0/1	0	0	0
23	23	c4y-	-z	y	x	0/1	0/1	0/1	0	0	0		47	47	ic4y-	z	-y	-x	0/1	0/1	0/1	0	0	0
24	24	c4z-	y	-x	z	0/1	0/1	0/1	0	0	0		48	48	ic4z-	-y	x	-z	0/1	0/1	0/1	0	0	0

We will study about the character for IR=1, 7 and 9 at Γ



Irreducible representation at Γ(case:Fe)

1

```
IMR NO  1  DIMENSION=  1
MATRIX REPRESENTATION
    1 2 3 4 5 6 7 8 9101112131415161718192021222324252627282930313233343536373839404142434445464748
1 1 + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
```

7

```
IMR NO  7  DIMENSION=  3
MATRIX REPRESENTATION
    1 2 3 4 5 6 7 8 9101112131415161718192021222324252627282930313233343536373839404142434445464748
1 1 + + - - 0 0 0 0 0 0 0 0 0 0 0 + 0 + - 0 0 - 0 0 + + - - 0 0 0 0 0 0 0 0 0 0 0 + 0 + - 0 0 - 0 0
1 2 0 0 0 0 0 0 0 0 + + - - - + 0 0 0 0 0 0 + 0 0 - 0 0 0 0 0 0 0 0 + + - - - + 0 0 0 0 0 0 + 0 0 -
1 3 0 0 0 0 + - - + 0 0 0 0 0 0 - 0 + 0 0 - 0 0 + 0 0 0 0 0 0 + - - + 0 0 0 0 0 0 - 0 + 0 0 - 0 0 + 0
2 1 0 0 0 0 + + - - 0 0 0 0 - + 0 0 0 0 0 0 - 0 0 + 0 0 0 0 + + - - 0 0 0 0 - + 0 0 0 0 0 0 - 0 0 +
2 2 + - + - 0 0 0 0 0 0 0 0 0 0 + 0 + 0 0 - 0 0 - 0 + - + - 0 0 0 0 0 0 0 0 0 0 + 0 + 0 0 - 0 0 - 0
2 3 0 0 0 0 0 0 0 0 0 + - + - 0 0 0 - 0 + + 0 0 - 0 0 0 0 0 0 0 0 0 0 + - + - 0 0 0 - 0 + + 0 0 - 0 0
3 1 0 0 0 0 0 0 0 0 + - - + 0 0 - 0 + 0 0 + 0 0 - 0 0 0 0 0 0 0 0 0 + - - + 0 0 - 0 + 0 0 + 0 0 - 0
3 2 0 0 0 0 + - + - 0 0 0 0 0 0 0 - 0 + - 0 0 + 0 0 0 0 0 0 + - + - 0 0 0 0 0 0 0 - 0 + - 0 0 + 0 0
3 3 + - - + 0 0 0 0 0 0 0 0 + + 0 0 0 0 0 0 - 0 0 - + - - + 0 0 0 0 0 0 0 0 0 + + 0 0 0 0 0 0 - 0 0 -
```

9

```
IMR NO  9  DIMENSION=  2
MATRIX REPRESENTATION
    1 2 3 4 5 6 7 8 9101112131415161718192021222324252627282930313233343536373839404142434445464748
1 1 + + + + V V V V W W W W 0 0 0 0 0 0 0 0 0 0 0 0 + + + + V V V V W W W W 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 2 0 0 0 0 0 0 0 0 0 0 0 0 + + V W V W W V + W V + 0 0 0 0 0 0 0 0 0 0 0 0 + + V W V W W V + W V +
2 1 0 0 0 0 0 0 0 0 0 0 0 0 + + W V W V V W + V W + 0 0 0 0 0 0 0 0 0 0 0 0 + + W V W V V W + V W +
2 2 + + + + W W W W V V V V 0 0 0 0 0 0 0 0 0 0 0 0 + + + + W W W W V V V V 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

"+" indicates "1", "-" indicates "-1"

"V" indicates "$\exp\left(\frac{2\pi}{3}i\right)$"

"W" indicates "$\exp\left(\frac{4\pi}{3}i\right)$" respectively.

Example: IR=9, symmetry operation index = 20

$$\begin{bmatrix} 0 & V \\ W & 0 \end{bmatrix} = \begin{bmatrix} 0 & \exp(2\pi i/3) \\ \exp(4\pi i/3) & 0 \end{bmatrix}$$

character table of Irreducible representation at Γ

```
1 : ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)

7 : ( 3.00 0.00) (-1.00 0.00) (-1.00 0.00) (-1.00 0.00) ( 0.00 0.00)
    ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00)
    ( 0.00 0.00) ( 0.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) (-1.00 0.00) (-1.00 0.00)
    (-1.00 0.00) (-1.00 0.00) (-1.00 0.00) (-1.00 0.00) ( 3.00 0.00)
    (-1.00 0.00) (-1.00 0.00) (-1.00 0.00) ( 0.00 0.00) ( 0.00 0.00)
    ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00)
    ( 0.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00) ( 1.00 0.00)
    ( 1.00 0.00) ( 1.00 0.00) (-1.00 0.00) (-1.00 0.00) (-1.00 0.00)
    (-1.00 0.00) (-1.00 0.00) (-1.00 0.00)

9 : ( 2.00 0.00) ( 2.00 0.00) ( 2.00 0.00) ( 2.00 0.00) (-1.00 0.00)
    (-1.00 0.00) (-1.00 0.00) (-1.00 0.00) (-1.00 0.00) (-1.00 0.00)
    (-1.00 0.00) (-1.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00)
    ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00)
    ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 2.00 0.00)
    ( 2.00 0.00) ( 2.00 0.00) ( 2.00 0.00) (-1.00 0.00) (-1.00 0.00)
    (-1.00 0.00) (-1.00 0.00) (-1.00 0.00) (-1.00 0.00) (-1.00 0.00)
    (-1.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00)
    ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00)
    ( 0.00 0.00) ( 0.00 0.00) ( 0.00 0.00)
```

1.　立方晶系の点群

O_h	E	$6C_4$	$3C_4^2$	$6C_2'$	$8C_3$	I	$6IC_4$	$3\sigma_h$	$6\sigma_d$	$8IC_3$	Γ, R, H	
A_{1g} Γ_1^+	1	1	1	1	1	1	1	1	1	1	Γ_1	1
A_{2g} Γ_2^+	1	−1	1	−1	1	1	−1	1	−1	1	Γ_2	
E_g Γ_3^+	2	0	2	0	−1	2	0	2	0	−1	Γ_{12}	9
T_{1g} Γ_4^+	3	1	−1	−1	0	3	1	−1	−1	0	Γ_{15}'	
T_{2g} Γ_5^+	3	−1	−1	1	0	3	−1	−1	1	0	Γ_{25}'	7
A_{1u} Γ_1^-	1	1	1	1	1	−1	−1	−1	−1	−1	Γ_1'	
A_{2u} Γ_2^-	1	−1	1	−1	1	−1	1	−1	1	−1	Γ_2'	
E_u Γ_3^-	2	0	2	0	−1	−2	0	−2	0	1	Γ_{12}'	
T_{1u} Γ_4^-	3	1	−1	−1	0	−3	−1	1	1	0	Γ_{15}	
T_{2u} Γ_5^-	3	−1	−1	1	0	−3	1	1	−1	0	Γ_{25}	
$E_{1/2g}$ Γ_6^+	2 −2	$\sqrt{2}$ $-\sqrt{2}$	0	0	1 −1	2 −2	$\sqrt{2}$ $-\sqrt{2}$	0	0	1 −1	Γ_6^+	
$E_{5/2g}$ Γ_7^+	2 −2	$-\sqrt{2}$ $\sqrt{2}$	0	0	1 −1	2 −2	$-\sqrt{2}$ $\sqrt{2}$	0	0	1 −1	Γ_7^+	
$G_{3/2g}$ Γ_8^+	4 −4	0 0	0	0	−1 1	4 −4	0 0	0	0	−1 1	Γ_8^+	
$E_{1/2u}$ Γ_6^-	2 −2	$\sqrt{2}$ $-\sqrt{2}$	0	0	1 −1	−2 2	$-\sqrt{2}$ $\sqrt{2}$	0	0	−1 1	Γ_6^-	
$E_{5/2u}$ Γ_7^-	2 −2	$-\sqrt{2}$ $\sqrt{2}$	0	0	1 −1	−2 2	$\sqrt{2}$ $-\sqrt{2}$	0	0	−1 1	Γ_7^-	
$G_{3/2u}$ Γ_8^-	4 −4	0 0	0	0	−1 1	−4 4	0 0	0	0	1 −1	Γ_8^-	

A_{1g}: $r^2,\ x^4+y^4+z^4-\frac{3}{5}r^4$ 1

A_{2g}: $x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)$

9 E_g : $\{u, v\},\ u\equiv 2z^2-x^2-y^2,\ v\equiv\sqrt{3}(x^2-y^2)$

T_{1g}: $\{yz(y^2-z^2),\ zx(z^2-x^2),\ xy(x^2-y^2)\}$

T_{2g}: $\{yz, zx, xy\}$ 7

Γ_6^+: $\{\alpha, \beta\}$

Γ_7^+: $\{xy\alpha+(yz+izx)\beta,\ -xy\beta+(yz-izx)\alpha\}$

Γ_8^+: $\{v\beta, -u\alpha, u\beta, -v\alpha\}$, $\{(zx+iyz)\alpha+2ixy\beta,\ -\sqrt{3}(zx+iyz)\beta,\ -\sqrt{3}(zx-iyz)\alpha,\ (zx-iyz)\beta+2ixy\alpha\}$

Γ_6^-: $\{z\alpha+(x+iy)\beta,\ -z\beta+(x-iy)\alpha\}$

Γ_7^-: $\{xyz\alpha,\ xyz\beta\}$

A_{1u}: $(A_{2g})\times xyz$

A_{2u}: xyz

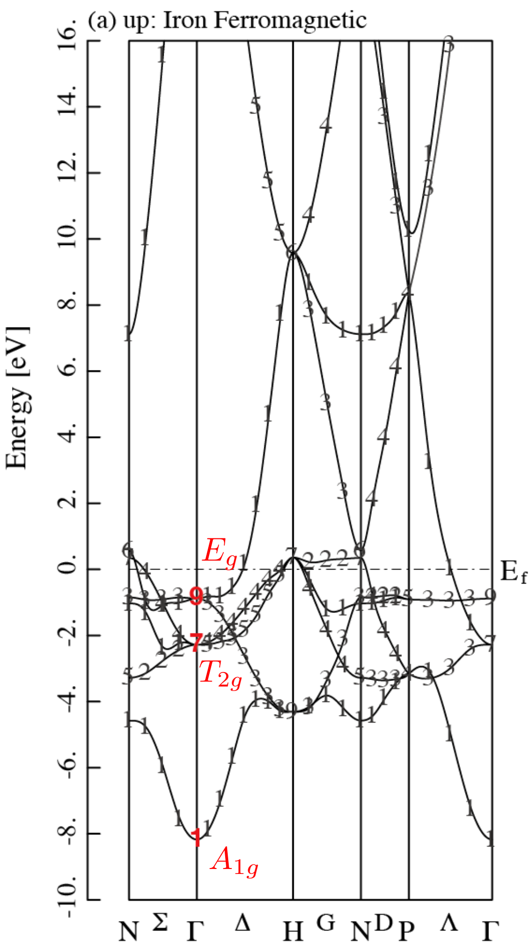
E_u : $\{xyzv, -xyzu\}$

T_{1u}: $\{x, y, z\}$

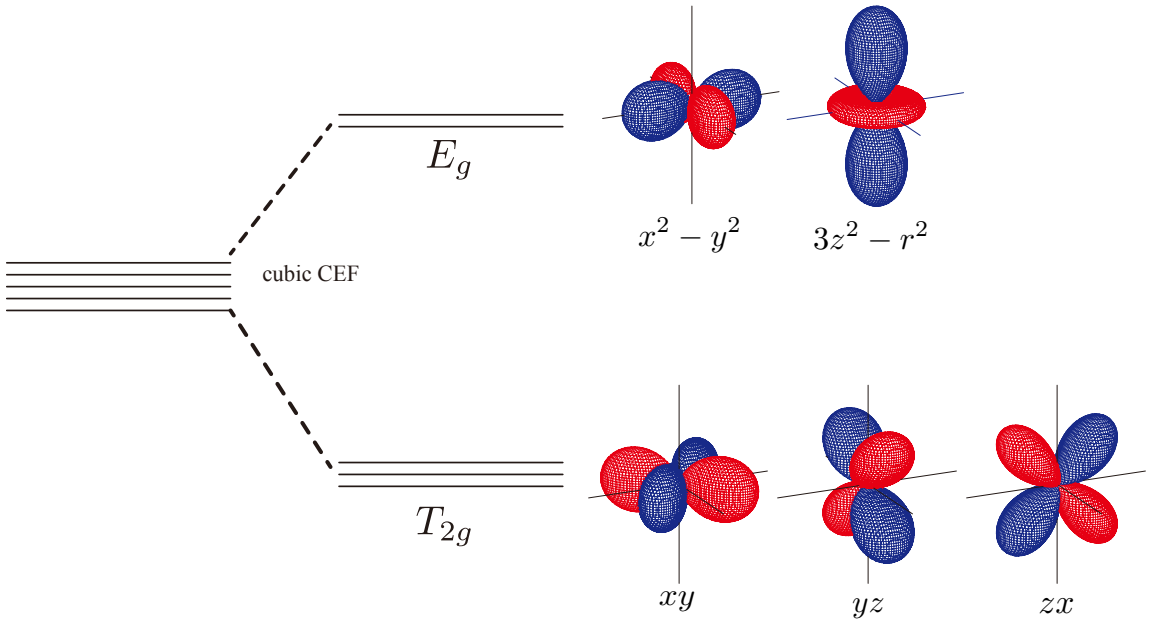
T_{2u}: $\{x(y^2-z^2),\ y(z^2-x^2),\ z(x^2-y^2)\}$

Because there are redundant degrees of freedom of unitary transformation about representation matrix, we use the trace of representation matrix (character).

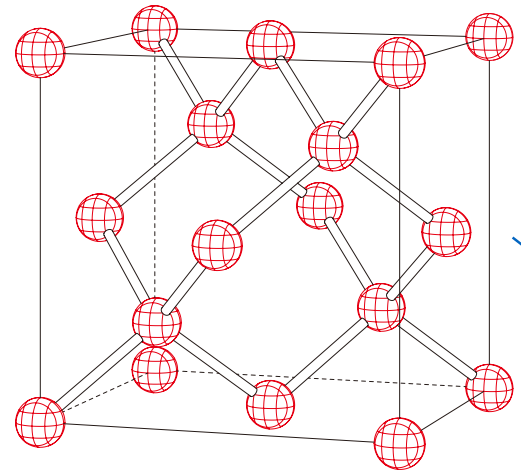
$$\begin{cases} E_g : d\gamma(x^2-y^2, 3z^2-r^2) \\ T_{2g} : d\varepsilon(xy, yz, zx) \\ A_{1g} : s \end{cases}$$



Cubic Crystal Electric Field(CEF) for 3d



2-2. Si



Si(0.0, 0.0, 0.0)

Diamond Structure

$\mathrm{Fd\bar{3}m}(\mathrm{O_h}^7, \#227)$

Lattice Type

Point group O_h has full cubic symmetry.

3-fold rotation

```
>>>>>>>>> ab_prp.data >>>>>>>>>>>
Si (227, Oh7, Fd-3m)
  a=5.4296 A
  face-centered (il=2)
  generators    5  (0/1, 0/1, 0/1)   C3
               19  (1/4, 1/4, 1/4)   C4
               25  (1/4, 1/4, 1/4)   Ci
  atomic position (0.0, 0.0, 0.0)
  nonmagnetic (jmag=0)
>>>>>>>>> ab_prp.data >>>>>>>>>>>
```

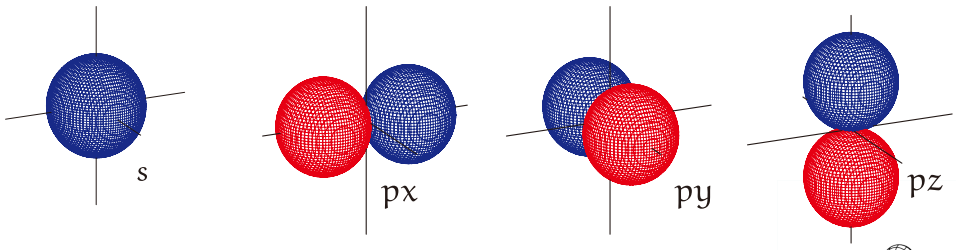
Symmetry operation for Si

```
                 ----- group elements --------
 1   ( 1)    e      ( x, y, z)  ( 0 / 1,  0/ 1,  0 / 1 )
 2   ( 2)    c2x    ( x,-y,-z)  ( 0 / 1,  1/ 4,  1 / 4 )
 3   ( 3)    c2y    (-x, y,-z)  ( 1 / 4,  0/ 1,  1 / 4 )
 4   ( 4)    c2z    (-x,-y, z)  ( 1 / 4,  1/ 4,  0 / 1 )
 5   ( 5)    c31+   ( z, x, y)  ( 0 / 1,  0/ 1,  0 / 1 )
 6   ( 6)    c32+   (-z, x,-y)  ( 1 / 4,  0/ 1,  1 / 4 )
 7   ( 7)    c33+   (-z,-x, y)  ( 1 / 4,  1/ 4,  0 / 1 )
 8   ( 8)    c34+   ( z,-x,-y)  ( 0 / 1,  1/ 4,  1 / 4 )
 9   ( 9)    c31-   ( y, z, x)  ( 0 / 1,  0/ 1,  0 / 1 )
10   (10)    c32-   ( y,-z,-x)  ( 0 / 1,  1/ 4,  1 / 4 )
11   (11)    c33-   (-y, z,-x)  ( 1 / 4,  0/ 1,  1 / 4 )
12   (12)    c34-   (-y,-z, x)  ( 1 / 4,  1/ 4,  0 / 1 )
13   (13)    c2a    ( y, x,-z)  ( 1 / 4,  1/ 4,  0 / 1 )
14   (14)    c2b    (-y,-x, z)  ( 0 / 1,  0/ 1,  0 / 1 )
15   (15)    c2c    ( z,-y, x)  ( 1 / 4,  0/ 1,  1 / 4 )
16   (16)    c2d    (-x, z, y)  ( 0 / 1,  1/ 4,  1 / 4 )
17   (17)    c2e    (-z,-y,-x)  ( 0 / 1,  0/ 1,  0 / 1 )
18   (18)    c2f    (-x,-z,-y)  ( 0 / 1,  0/ 1,  0 / 1 )
19   (19)    c4x+   ( x,-z, y)  ( 1 / 4,  0/ 1,  1 / 4 )
20   (20)    c4y+   ( z, y,-x)  ( 1 / 4,  1/ 4,  0 / 1 )
21   (21)    c4z+   (-y, x, z)  ( 0 / 1,  1/ 4,  1 / 4 )
22   (22)    c4x-   ( x, z,-y)  ( 1 / 4,  1/ 4,  0 / 1 )
23   (23)    c4y-   (-z, y, x)  ( 0 / 1,  1/ 4,  1 / 4 )
24   (24)    c4z-   ( y,-x, z)  ( 1 / 4,  0/ 1,  1 / 4 )
25   (25)    ie     (-x,-y,-z)  ( 0 / 1,  0/ 1,  0 / 1 )
26   (26)    ic2x   (-x, y, z)  ( 0 / 1,  1/ 4,  1 / 4 )
27   (27)    ic2y   ( x,-y, z)  ( 1 / 4,  0/ 1,  1 / 4 )
28   (28)    ic2z   ( x, y,-z)  ( 1 / 4,  1/ 4,  0 / 1 )
29   (29)    ic31+  (-z,-x,-y)  ( 0 / 1,  0/ 1,  0 / 1 )
30   (30)    ic32+  ( z,-x, y)  ( 1 / 4,  0/ 1,  1 / 4 )
31   (31)    ic33+  ( z, x,-y)  ( 1 / 4,  1/ 4,  0 / 1 )
32   (32)    ic34+  (-z, x, y)  ( 0 / 1,  1/ 4,  1 / 4 )
33   (33)    ic31-  (-y,-z,-x)  ( 0 / 1,  0/ 1,  0 / 1 )
34   (34)    ic32-  (-y, z, x)  ( 0 / 1,  1/ 4,  1 / 4 )
35   (35)    ic33-  ( y,-z, x)  ( 1 / 4,  0/ 1,  1 / 4 )
36   (36)    ic34-  ( y, z,-x)  ( 1 / 4,  1/ 4,  0 / 1 )
37   (37)    ic2a   (-y,-x, z)  ( 1 / 4,  1/ 4,  0 / 1 )
38   (38)    ic2b   ( y, x, z)  ( 0 / 1,  0/ 1,  0 / 1 )
39   (39)    ic2c   (-z, y,-x)  ( 1 / 4,  0/ 1,  1 / 4 )
40   (40)    ic2d   ( x,-z,-y)  ( 0 / 1,  1/ 4,  1 / 4 )
41   (41)    ic2e   ( z, y, x)  ( 0 / 1,  0/ 1,  0 / 1 )
42   (42)    ic2f   ( x, z, y)  ( 0 / 1,  0/ 1,  0 / 1 )
43   (43)    ic4x+  (-x, z,-y)  ( 1 / 4,  0/ 1,  1 / 4 )
44   (44)    ic4y+  (-z,-y, x)  ( 1 / 4,  1/ 4,  0 / 1 )
45   (45)    ic4z+  ( y,-x,-z)  ( 0 / 1,  1/ 4,  1 / 4 )
46   (46)    ic4x-  (-x,-z, y)  ( 1 / 4,  1/ 4,  0 / 1 )
47   (47)    ic4y-  ( z,-y,-x)  ( 0 / 1,  1/ 4,  1 / 4 )
48   (48)    ic4z-  (-y, x,-z)  ( 1 / 4,  0/ 1,  1 / 4 )
```

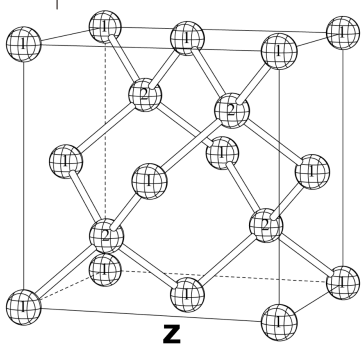
rotation translation

result of "*ab_in.log*"

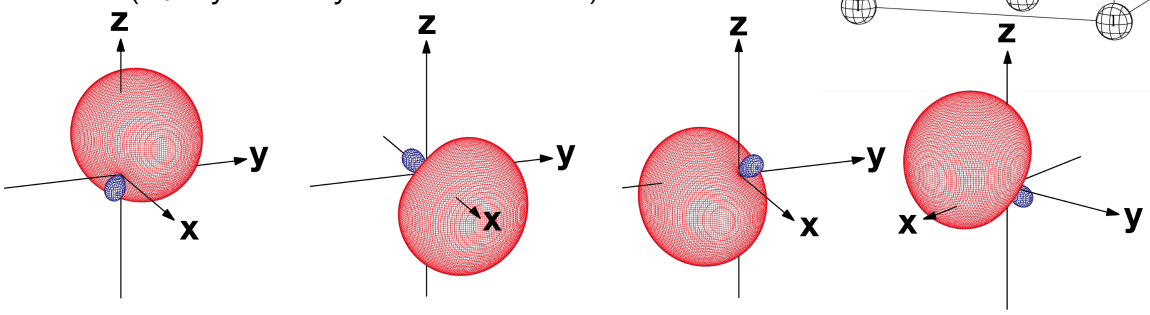
sp^3 basis function



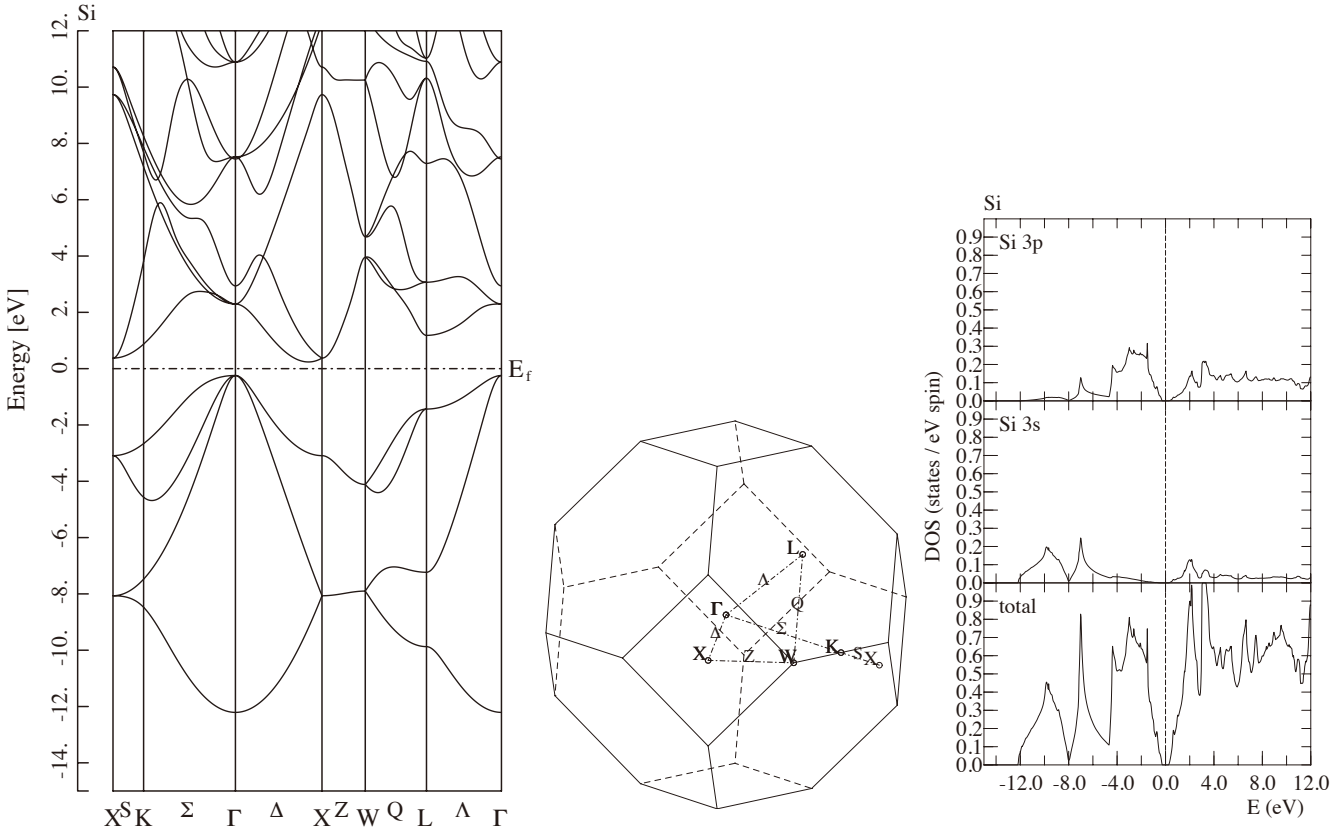
$$\begin{cases} |h_1\rangle = \frac{1}{2}\{|s\rangle + |p_x\rangle + |p_y\rangle + |p_z\rangle\} & [111] \\ |h_2\rangle = \frac{1}{2}\{|s\rangle + |p_x\rangle - |p_y\rangle - |p_z\rangle\} & [1\bar{1}\bar{1}] \\ |h_3\rangle = \frac{1}{2}\{|s\rangle - |p_x\rangle + |p_y\rangle - |p_z\rangle\} & [\bar{1}1\bar{1}] \\ |h_4\rangle = \frac{1}{2}\{|s\rangle - |p_x\rangle - |p_y\rangle + |p_z\rangle\} & [\bar{1}\bar{1}1] \end{cases}$$



(T_d-Symmetry basis function)



Electronic structure of Silicon

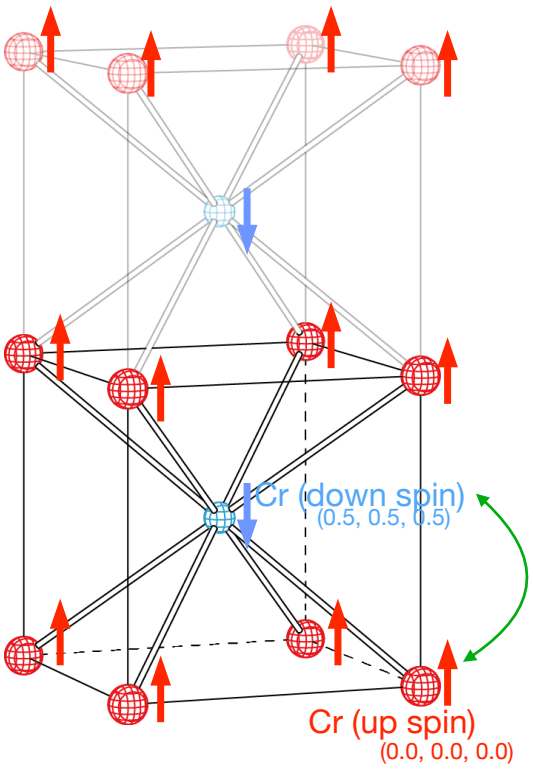


Magnetic states and LDA +*U*

- Anti-Ferromagnetic Cr
- Nonmagnetic NiO
- Ferromagnetic NiO
- Anti-Ferromagnetic NiO Type1
- Anti-Ferromagnetic NiO Type2

3-1. Anti-ferromagnetic Cr

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
Cr antiferromagnetic (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)
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```



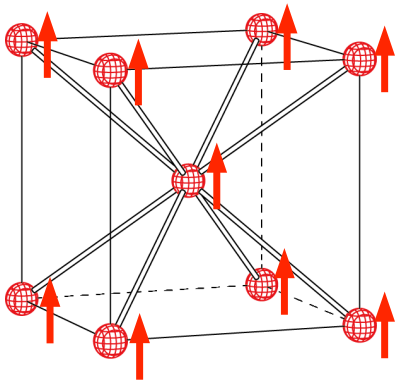
anti-ferromagnetic
(simple lattice)

relationship between up spin atom and down spin atom is

identical rotation

+

$\begin{bmatrix}1/2\\1/2\\1/2\end{bmatrix}$ translation



ferromagnetic
(body centered lattice)

LDA+*U* method

$$E_{\mathrm{LDA}+U}[n^\sigma(\boldsymbol{r}),\{n_m^\sigma\}] = E_{\mathrm{LDA}}[n^\sigma(\boldsymbol{r})] + E_U(\{n_m^\sigma\}) - E_{dc}(\{n_m^\sigma\})$$

total energy of scf calculation using LDA

effective interaction within Hartree-Fock approximation

double counting term

$(\sigma = \uparrow, \downarrow)$

$(m = 1, 2, \cdots, 2l+1)$

where we defined the Hartree-Fock approximation term for localized orbitals as

$$E_U(\{n_m^\sigma\}) = \frac{1}{2}U\sum_\sigma\sum_{m,m'} n_m^\sigma n_{m'}^{-\sigma} + \frac{1}{2}(U-J)\sum_\sigma\sum_{m\neq m'} n_m^\sigma n_{m'}^\sigma$$

U: effective Coulomb integration
J: effective exchange integration

we use the relationship about the number of localized electrons

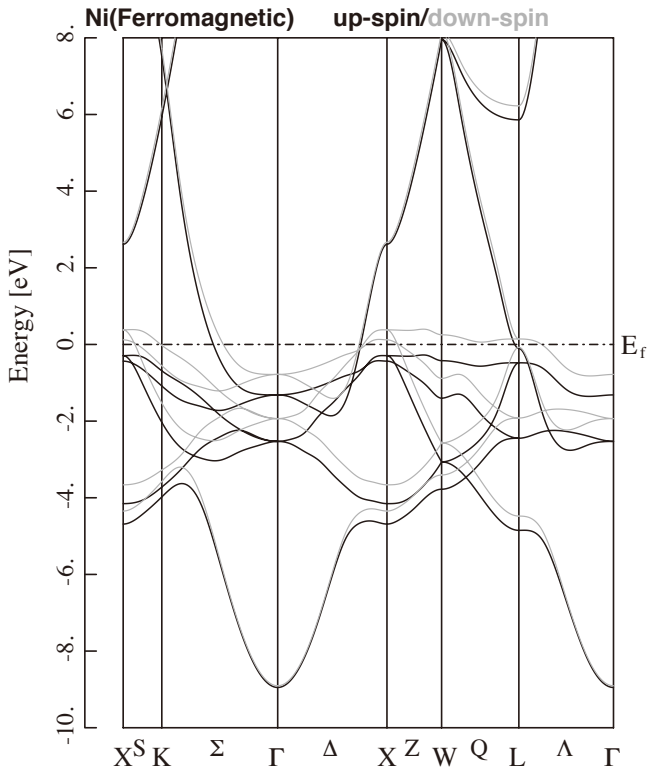
$$\begin{cases} N^\sigma = \sum_m n_m^\sigma \\ N = N^\uparrow + N^\downarrow \end{cases}$$

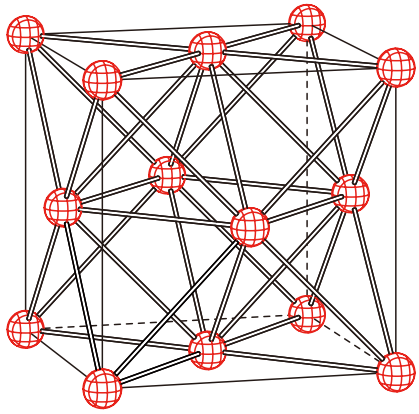
effective interaction in atomic limit,

$$E_U(\{n_m^\sigma\}) = \frac{1}{2}UN(N-1) - \frac{1}{2}J\sum_\sigma N^\sigma(N^\sigma-1) + \frac{1}{2}(U-J)\left[N - \sum_\sigma\sum_m (n_m^\sigma)^2\right]$$

$$E_{dc}(\{n_m^\sigma\}) = \frac{1}{2}UN(N-1) - \frac{1}{2}J\sum_\sigma N^\sigma(N^\sigma-1)$$

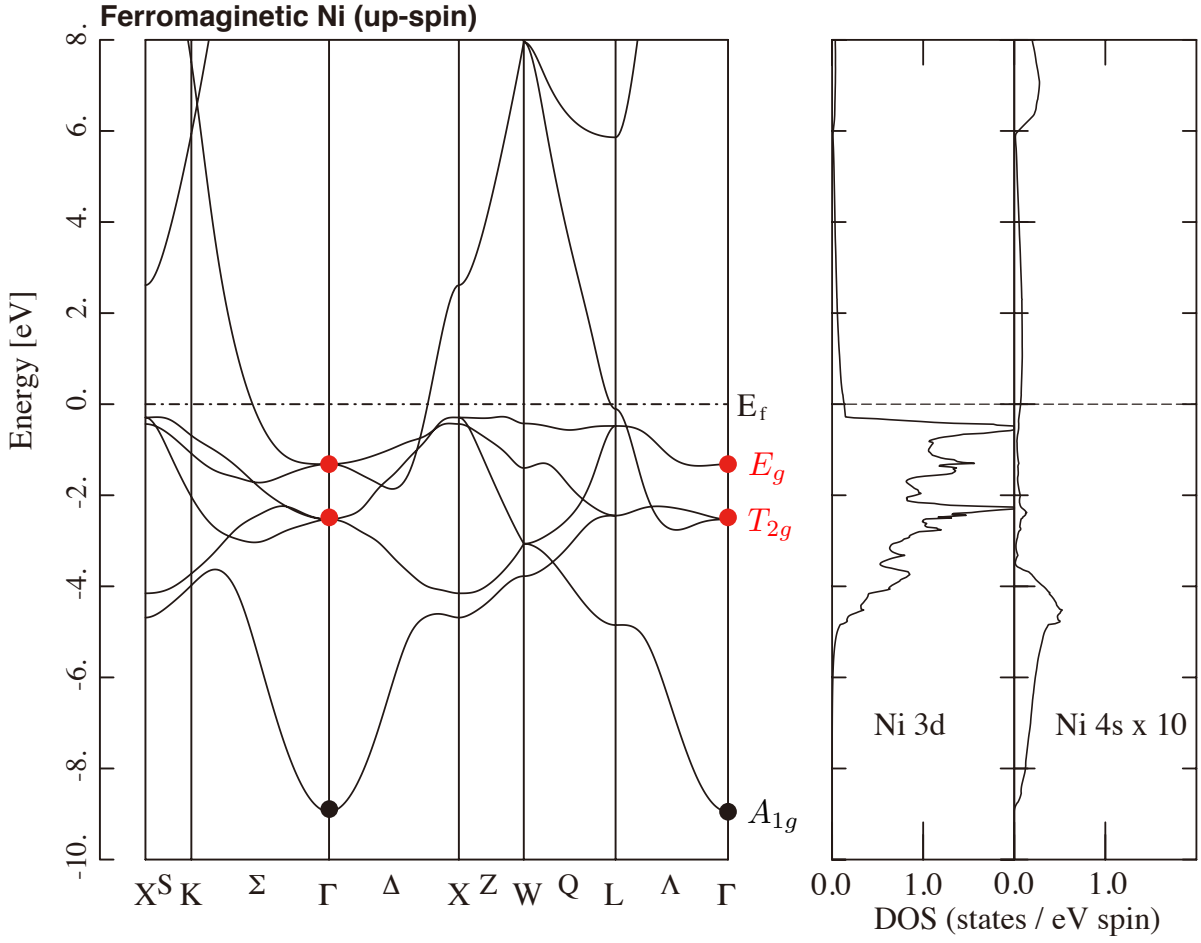
Ref: Ni



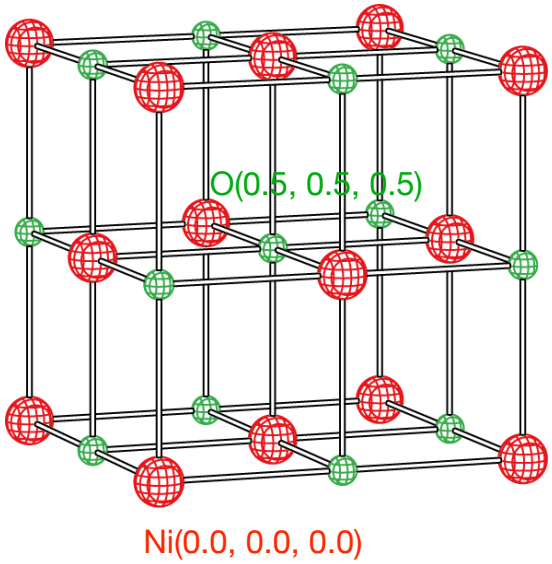


$\mathrm{Fm\bar{3}m}(O_h{}^5, \#225)$

```
>>>>>>>>> ab_prp.data >>>>>>>>>>>
Ni (225, Oh5, Fm-3m) fcc
  a=3.499 A
  face-centered (il=2)
  generators
     5  (0, 0, 0)
    19  (0, 0, 0)
    25  (0, 0, 0)
  atomic position
      (0.0, 0.0, 0.0)
 ferromagnetic (jmag=1)
>>>>>>>>> ab_prp.data >>>>>>>>>>>
```



3-2-1. Nonmagnetic and ferromagnetic NiO



Rock-Solt Structure

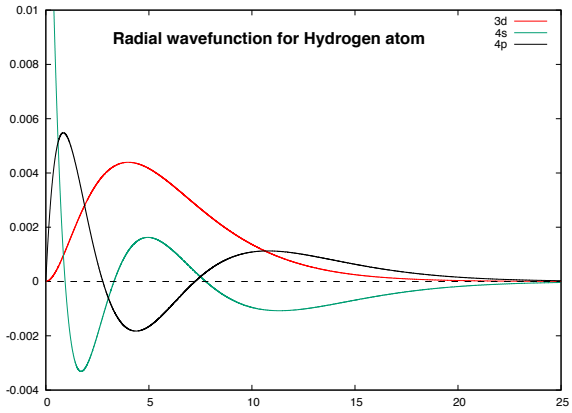
```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
NiO
  a=4.17A,   NaCl structure
  face-centered (il=2) cubic lattice
  generators
     5  (0, 0, 0)
    19  (0, 0, 0)
    25  (0, 0, 0)
  atomic positions
    (0.0, 0.0, 0.0) Ni
    (0.5, 0.5, 0.5) O
  nonmagnetic   (jmag=0)
  ferromagnetic (jmag=2)
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>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

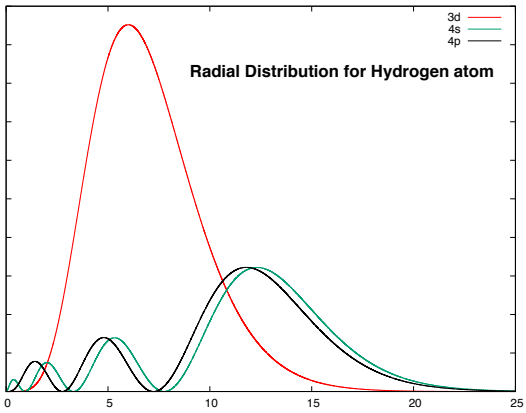
“*ab_prp.data*” for NiO-Ferromagnetic case

For nonmagnetic case,
`jmag0 = 0`

ab_prp.data (~/abc/NiO-ferro) - VIM — ssh -X cmd2 — zsh — ttys003

```
abcap-ab_prp.data
0                                   !jpr
NiO Ferromagnetic
lattice parameter -2----*----3----*----4----*----5----*----6----*----7
 4.17 4.17 4.17  90.0 90.0 90.0         !a,b,c[A], alpha,beta,gamma[degree]
space group       -2----*----3----*----4----*----5----*----6----*----7
 3  2  3  0  !idim, il((-1(r),0(h),1(s),2(f),3(b),4(c),5(a),6(b)),ngen,inv(0)
    5   0 1  0 1  0 1                          !igen,jgen(2,3)
   19   0 1  0 1  0 1                          !igen,jgen(2,3)
   25   0 1  0 1  0 1                          !igen,jgen(2,3)
kinds of atoms    -2----*----3----*----4----*----5----*----6----*----7
 2                                             !# of kinds
 1   0.0        0.0        0.0       Ni        !jpos,position,name
 1   0.5        0.5        0.5       O         !jpos,position,name
magnetic state    -2----*----3----*----4----*----5----*----6----*----7
 2              !jmag0 !noSO:(0(N),1(AF),2(M)), SO:(20(N),21(AF),22(M))
   1   1 2  1 2  1 2                           !igen,jgen(2,3) for AF
totally symmetric basis set -3----*----4----*----5----*----6----*----7
 24.0   6                                     !cut-off energy[Hr],Lmax
k-points (# of division)  ---3----*----4----*----5----*----6----*----7
  8  8  8                                     !nx,ny,nz
iteration         -2----*----3----*----4----*----5----*----6----*----7
4   6  0.05  0.05           !method, n-method, pmix, amix
!---*----1----*----2----*----3----*----4----*----5----*----6----*----7
~
~
~
 NORMAL  ab_prp.data                          unix iso-2022-jp no    2/24:  2
"ab_prp.data" [converted] 24L, 1543C
```





Hybridization V vs Coulomb interaction U

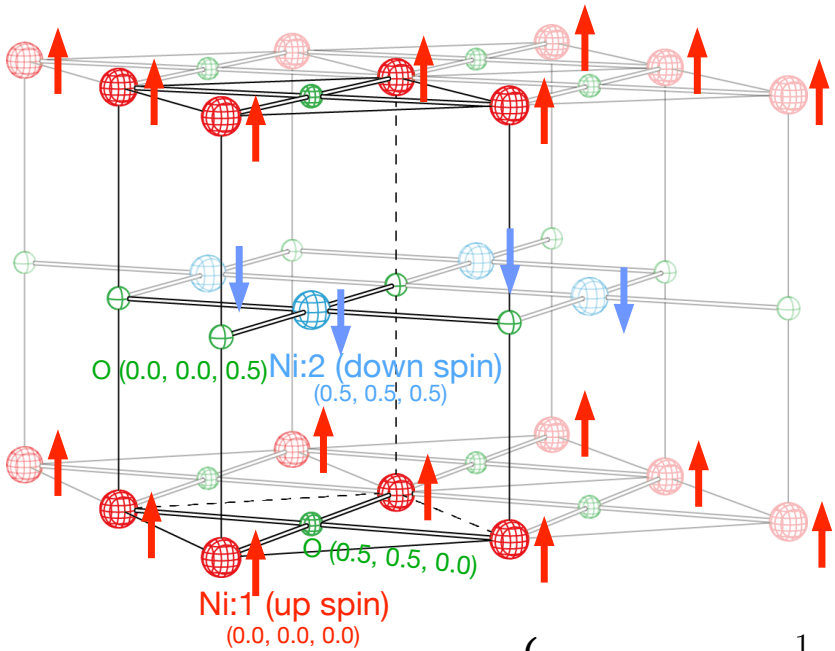
d-electron for transition metal(large V)

⇨ transition metal oxide has large U

3-2-2. Anti-ferromagnetic NiO

$$\mathrm{P4/mmm(D}_{4h}^{1}, \#123)$$

Type I AFM



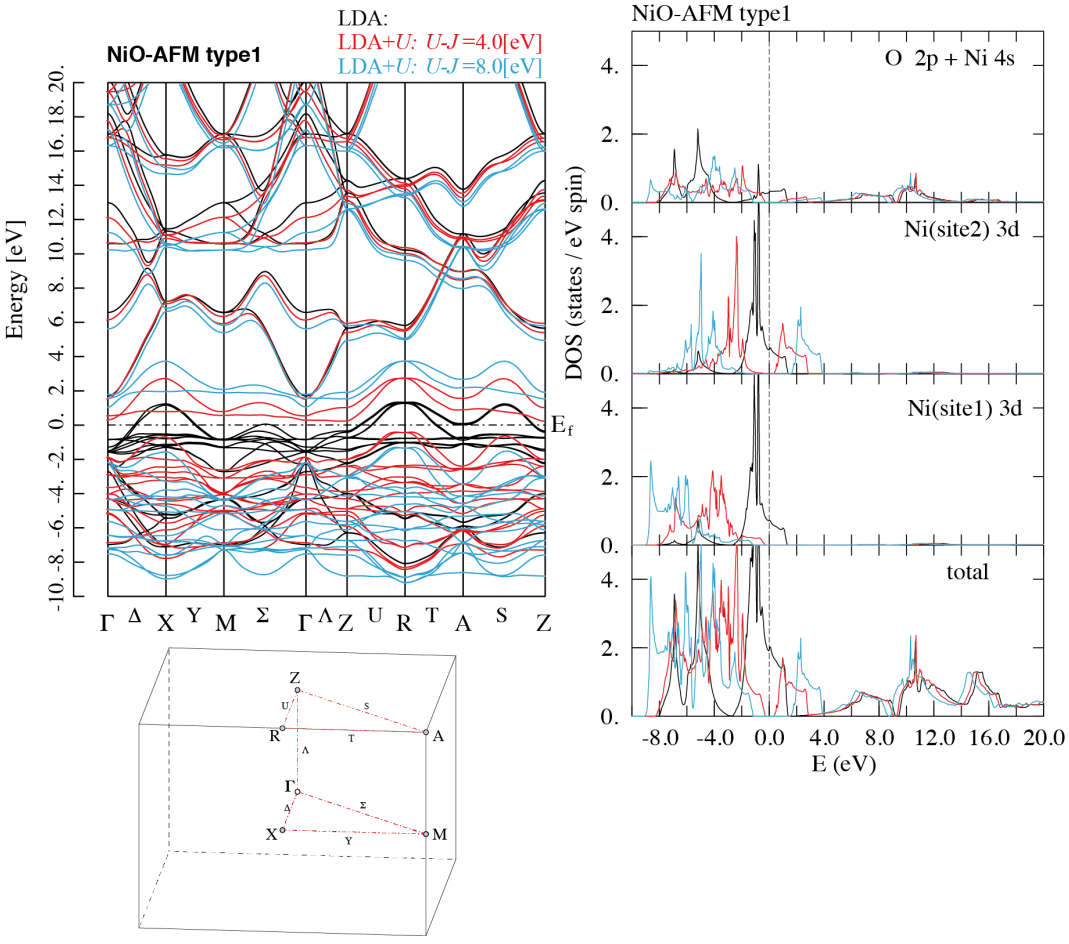

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
NiO [a(cubic)=4.17A]
  a=2.948635A, c=4.17A
  simple (il=1) tetragonal lattice
  generators
     2  (0, 0, 0)
    21  (0, 0, 0)
    25  (0, 0, 0)
atomic positions
    (0.0, 0.0, 0.0) Ni-up
    (0.5, 0.5, 0.5) Ni-down
    (0.5, 0.5, 0.0) O
    (0.0, 0.0, 0.5) O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

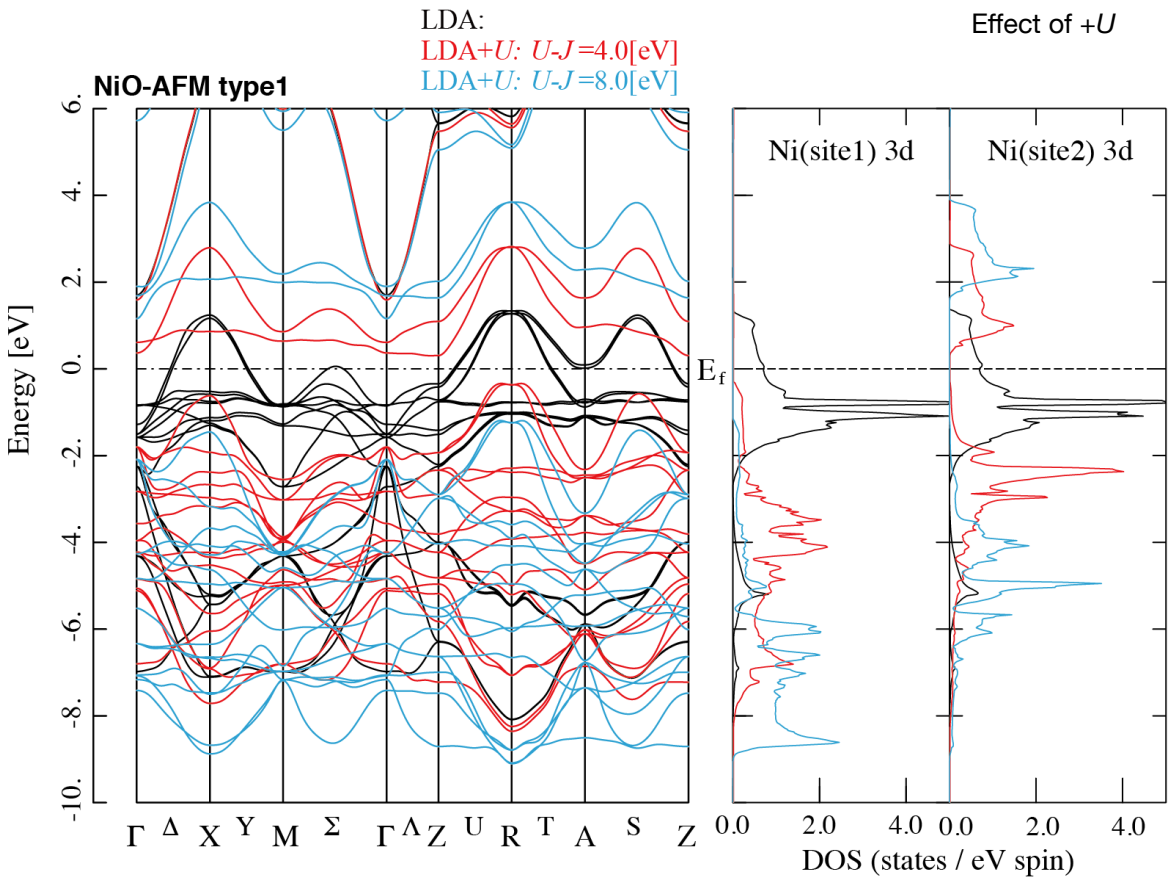
$$\begin{cases} a_{\mathrm{tetra}} = a_{\mathrm{cubic}} \times \dfrac{1}{\sqrt{2}} \\ c_{\mathrm{tetra}} = a_{\mathrm{cubic}} \end{cases}$$

“*ab_prp.data*” for NiO-AFM type1

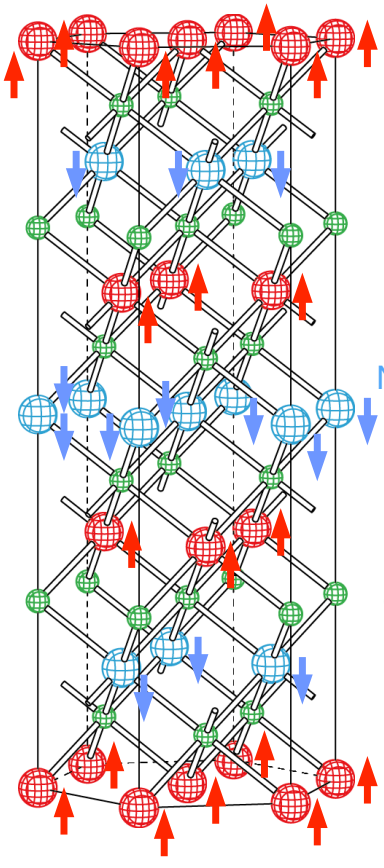
ab_prp.data (~/abc/NiO-antiferro-type1/u0) - VIM — ssh -X cmd2 — zsh — ttys003

```
abcap-ab_prp.data
0                                       !jpr
NiO-antiferro type1
lattice parameter -2----*----3----*----4----*----5----*----6----*----7
 2.948635 2.948635 4.17  90.0 90.0 90.0        !a,b,c[A], alpha,beta,gamma[degree]
space group       -2----*----3----*----4----*----5----*----6----*----7
 3  1  3  0  !idim, il((-1(r),0(h),1(s),2(f),3(b),4(c),5(a),6(b)),ngen,inv(0)
    2   0 1  0 1  0 1                       !igen,jgen(2,3)
   21   0 1  0 1  0 1                       !igen,jgen(2,3)
   25   0 1  0 1  0 1                       !igen,jgen(2,3)
kinds of atoms    -2----*----3----*----4----*----5----*----6----*----7
 4                                          !# of kinds
 1   0.0        0.0        0.0       Ni     ! Ni up-spin
 1   0.5        0.5        0.5       Ni     ! Ni down-spin
 1   0.5        0.5        0.0       O      !
 1   0.0        0.0        0.5       O      !
magnetic state    -2----*----3----*----4----*----5----*----6----*----7
 1             !jmag0 !noSO:(0(N),1(AF),2(M)), SO:(20(N),21(AF),22(M))
    1   1 2  1 2  1 2                       !igen,jgen(2,3) for AF
totally symmetric basis set -3----*----4----*----5----*----6----*----7
 24.0   6                              !cut-off energy[Hr],Lmax
k-points (# of division)  ---3----*----4----*----5----*----6----*----7
 12  12  8                              !nx,ny,nz
iteration         -2----*----3----*----4----*----5----*----6----*----7
4   6  0.05  0.05           !method, n-method, pmix, amix
!---*----1----*----2----*----3----*----4----*----5----*----6----*----7
~
NORMAL  ab_prp.data                    unix iso-2022-jp no    5/26: 19
```





Type II AFM



Ni:2 (down spin)
(0.0, 0.0, 0.5)

O (0.0, 0.0, 0.25)

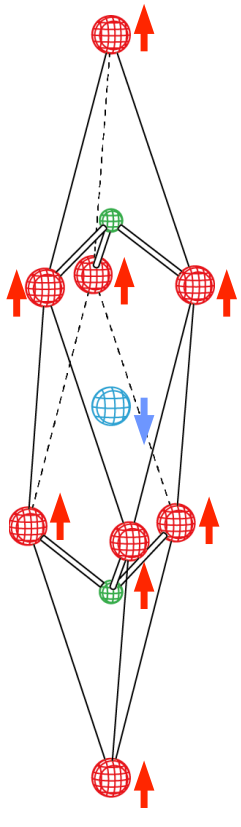
Ni:1 (up spin)
(0.0, 0.0, 0.0)

Hexagonal axis

$$\mathrm{R\bar{3}m(D_{3d}^{5}, \#166)}$$

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
NiO [a(cubic)=4.17A]
  a=2.948635A, c=14.445304A
  Rhombohedral (il=-1) lattice
  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
    (0.0, 0.0, 0.25) O
  antiferromagnetic (jmag=1)
                1  (0, 0, 1/2)
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
```

$$\begin{cases} a_{\mathrm{hex}} = a_{\mathrm{cubic}} \times \dfrac{1}{\sqrt{2}} \\ c_{\mathrm{hex}} = a_{\mathrm{cubic}} \times 2\sqrt{3} \end{cases}$$



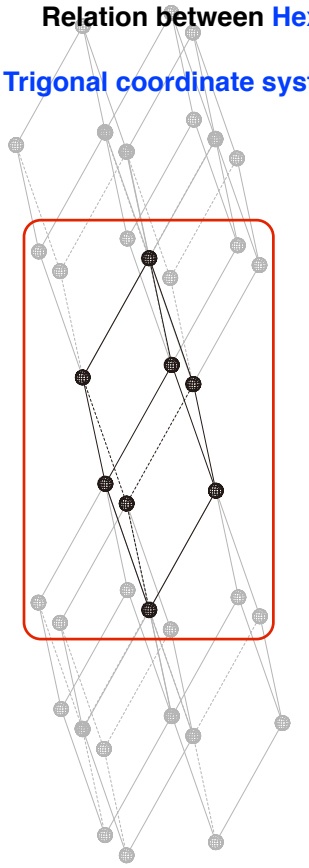
Trigonal axis

“*ab_prp.data*” for NiO-AFM type2

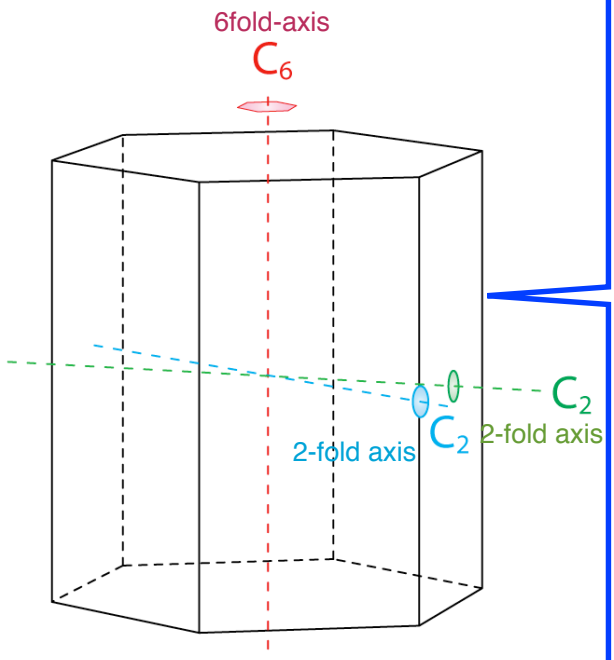
ab_prp.data (~/abc/NiO-antiferro-type2/u0) - VIM — ssh -X cmd2 — zsh — ttys003

```
abcap-ab_prp.data
0                                   !jpr
NiO anti-ferro type2
lattice parameter -2----*----3----*----4----*----5----*----6----*----7
 2.948635 2.948635 14.445304 90.0 90.0 120.0         !a,b,c[A], alpha,beta,gamma[degree]
space group       -2----*----3----*----4----*----5----*----6----*----7
 3 -1  3  0  !idim, il((-1(r),0(h),1(s),2(f),3(b),4(c),5(a),6(b)),ngen,inv(0)
    3   0 1  0 1  0 1                          !igen,jgen(2,3)
   10   0 1  0 1  0 1                          !igen,jgen(2,3)
   13   0 1  0 1  0 1                          !igen,jgen(2,3)
kinds of atoms    -2----*----3----*----4----*----5----*----6----*----7
 3                                             !# of kinds
 1   0.0        0.0        0.0       Ni        ! Ni up-spin
 1   0.0        0.0        0.5       Ni        ! Ni down-spin
 1   0.0        0.0        0.25      O         !
magnetic state    -2----*----3----*----4----*----5----*----6----*----7
 1             !jmag0 !noSO:(0(N),1(AF),2(M)), SO:(20(N),21(AF),22(M))
    1   0 1  0 1  1 2                          !igen,jgen(2,3) for AF
totally symmetric basis set -3----*----4----*----5----*----6----*----7
 24.0   6                                      !cut-off energy[Hr],Lmax
k-points (# of division)  ---3----*----4----*----5----*----6----*----7
 12 12  6                                      !nx,ny,nz
iteration         -2----*----3----*----4----*----5----*----6----*----7
4   6  0.05  0.05           !method, n-method, pmix, amix
!---*----1----*----2----*----3----*----4----*----5----*----6----*----7
~
~
 NORMAL  ab_prp.data                    unix iso-2022-jp no    18/25: 20
"ab_prp.data" [converted] 25L, 1598C
```

Relation between Hexagonal coordinate system
and
Trigonal coordinate system in Rhombohedral Crystal



Point Group: D_{6h}



Hexagonal Symmetry D_{6h}

$E \cdots\cdots 1$	identity operation
$C_6 \cdots\cdots 2$	$\pm\pi/3$
$C_6^2 \cdots\cdots 2$	$\pm 2\pi/3$
$C_6^3 \cdots\cdots 1$	$\pm\pi$
$C_2' \cdots\cdots 3$	$\pm\pi$
$C_2'' \cdots\cdots 3$	$\pm\pi$

12 rotational operation

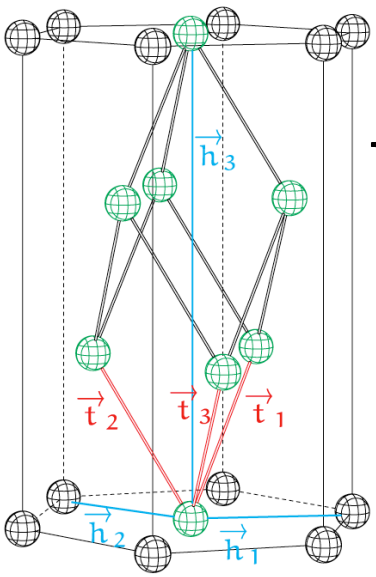
+ inversion, rotation inversion, reflection and rotational reflection

24 symmetry operation

subgroup of D_{6h}

Rhombohedral $D_{3d}, C_{3v}, C_3, \cdots$

Relation between Hexagonal coordinate system and Trigonal coordinate system in Rhombohedral Crystal

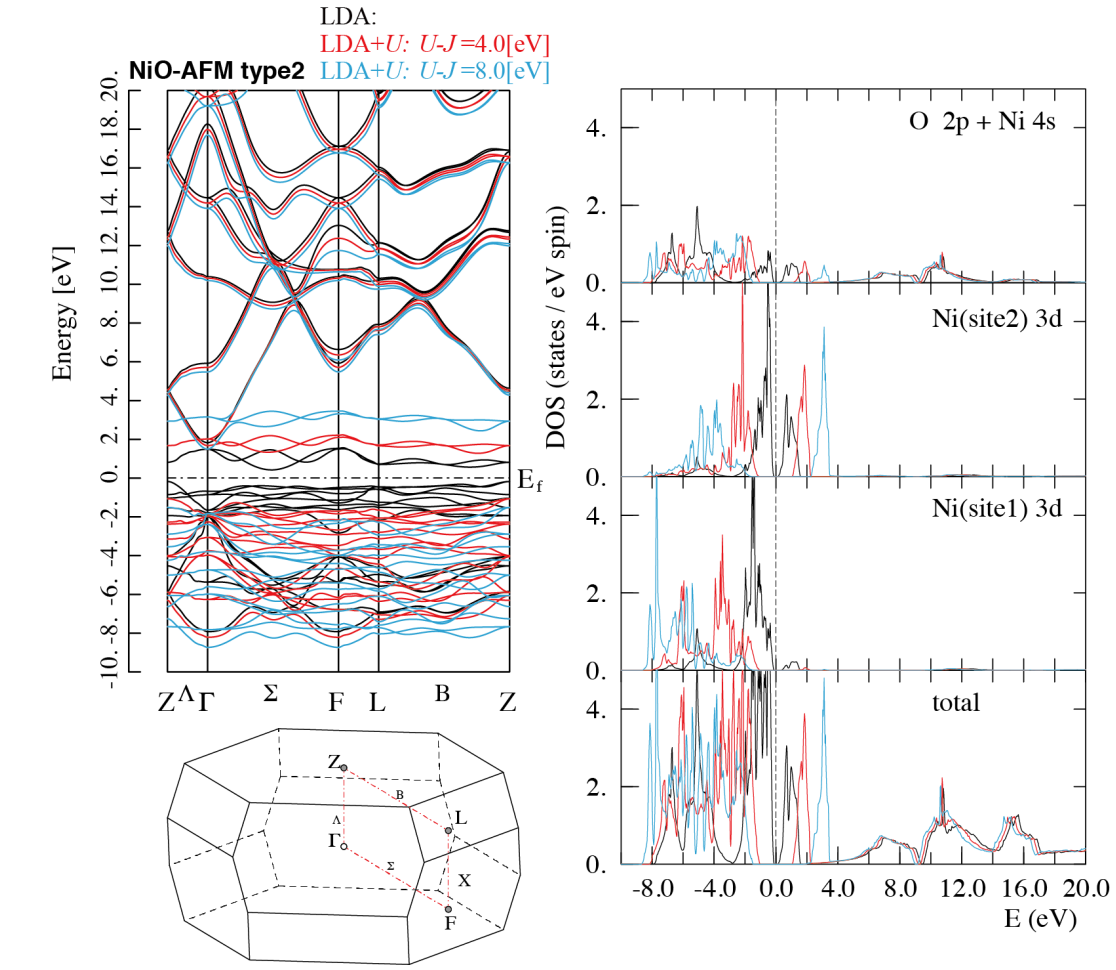


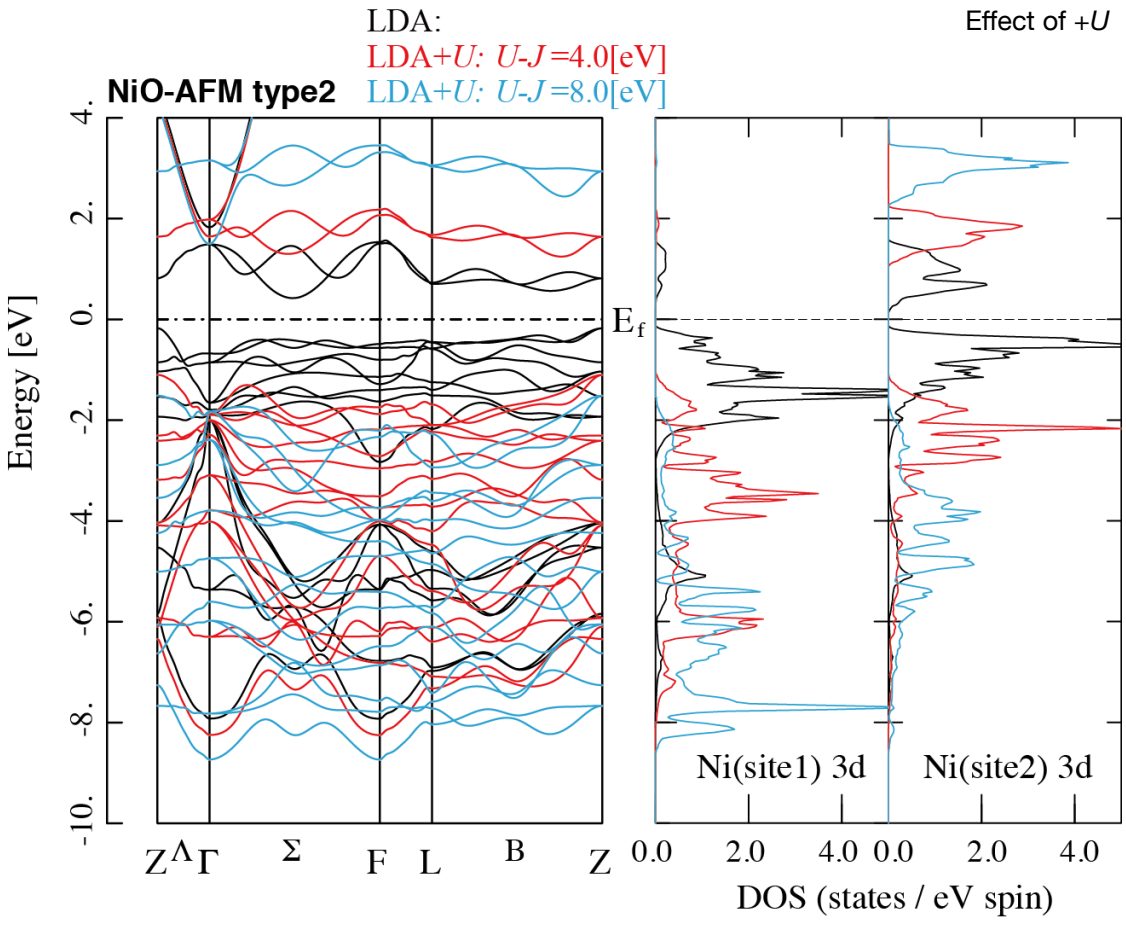
transformation basis

$$\vec{t}_1 = \frac{2}{3}\vec{h}_1 + \frac{1}{3}\vec{h}_2 + \frac{1}{3}\vec{h}_3$$
$$\vec{t}_2 = -\frac{1}{3}\vec{h}_1 + \frac{1}{3}\vec{h}_2 + \frac{1}{3}\vec{h}_3$$
$$\vec{t}_3 = -\frac{1}{3}\vec{h}_1 - \frac{2}{3}\vec{h}_2 + \frac{1}{3}\vec{h}_3$$

$$\vec{h}_1 = \vec{t}_1 - \vec{t}_2$$
$$\vec{h}_2 = \vec{t}_2 - \vec{t}_3$$
$$\vec{h}_3 = \vec{t}_1 + \vec{t}_2 + \vec{t}_3$$

primitive trigonal lattice + add lattice point → Hexagonal Lattice


LDA:
LDA+U: U-J=4.0[eV]
LDA+U: U-J=8.0[eV]
NiO-AFM type2
Energy [eV]
E_f
Z Λ Γ Σ F L B Z
DOS (states / eV spin)
O 2p + Ni 4s
Ni(site2) 3d
Ni(site1) 3d
total
E (eV)
Z
B
L
Λ
Γ
Σ
X
F


LDA:
LDA+U: U-J=4.0[eV]
LDA+U: U-J=8.0[eV]
Effect of +U
NiO-AFM type2
Energy [eV]
E_f
Z Λ Γ Σ F L B Z
Ni(site1) 3d
Ni(site2) 3d
DOS (states / eV spin)

Optical property for semiconductor and metal

- AlP (semiconductor)
- Al(metal)

Optical property

$$\frac{\epsilon_{ij}(\omega)}{\epsilon_0} = \delta_{ij} + \frac{e^2}{\epsilon_0 m\omega^2}\left\{\frac{1}{m}\chi_{ij}(\omega) - n\right\}$$

$$\chi_{ij}(\omega) = 2\sum_{cv}\left\{\chi_{ij}^{cv}(\omega + i\eta) + \chi_{ij}^{cv}(-\omega + i\eta)^*\right\}$$

$$\chi_{ij}^{cv}(z) = -\frac{1}{N}\sum_{\boldsymbol{k}}\frac{f_{\boldsymbol{k}v}\left(1 - f_{\boldsymbol{k}c}\right)\langle v\,|\,p_i\,|\,c\rangle\langle c\,|\,p_j\,|\,v\rangle}{z - \left(\varepsilon_{\boldsymbol{k}c} - \varepsilon_{\boldsymbol{k}v}\right)}$$

For metallic case, we add *the Drude term*,

$$\frac{i}{\omega}\frac{\sigma_{ij}(0)}{1 - i\omega\tau} = \frac{-1}{\omega}\frac{\sigma_{ij}(0)/\tau}{\omega + i/\tau}$$

$$\sigma_{ij}(0)/\tau = \frac{e^2}{\epsilon_0}\langle v_i v_j\rangle_F D\left(\varepsilon_F\right)$$

Where v is the velocity and defined using the wave function $\psi_{\boldsymbol{k},n}$ which is obtained from DFT calculation,

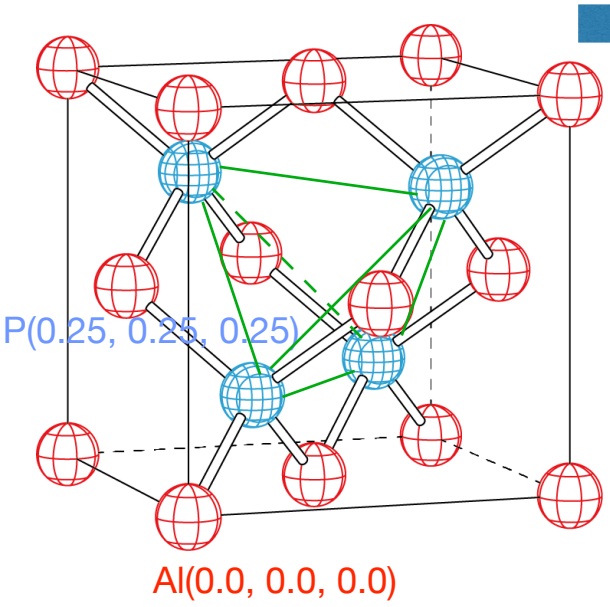
$$v_{\boldsymbol{k},n} = \left\langle \psi_{\boldsymbol{k},n} \middle| \frac{\boldsymbol{p}}{m} \middle| \psi_{\boldsymbol{k},n} \right\rangle$$

Where $\boldsymbol{p}$ is the momentum, m is mass of the electron, $\boldsymbol{k}$ is the crystal wave number, and n is the band index, respectively.

4-1. AlP

Zincblende Structure

$$\mathrm{F}\bar{4}3m(T_d{}^2, \#216)$$



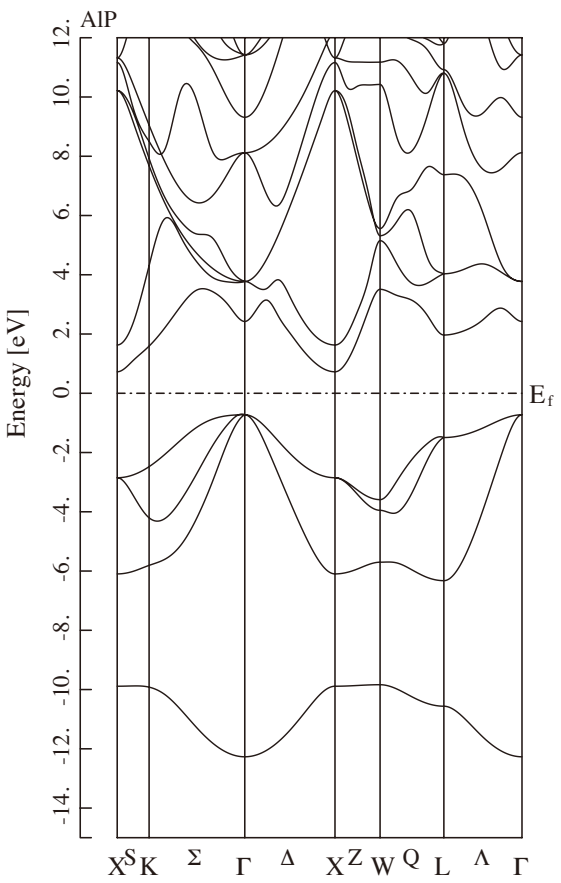
Point group T_d has full tetrahedral symmetry.

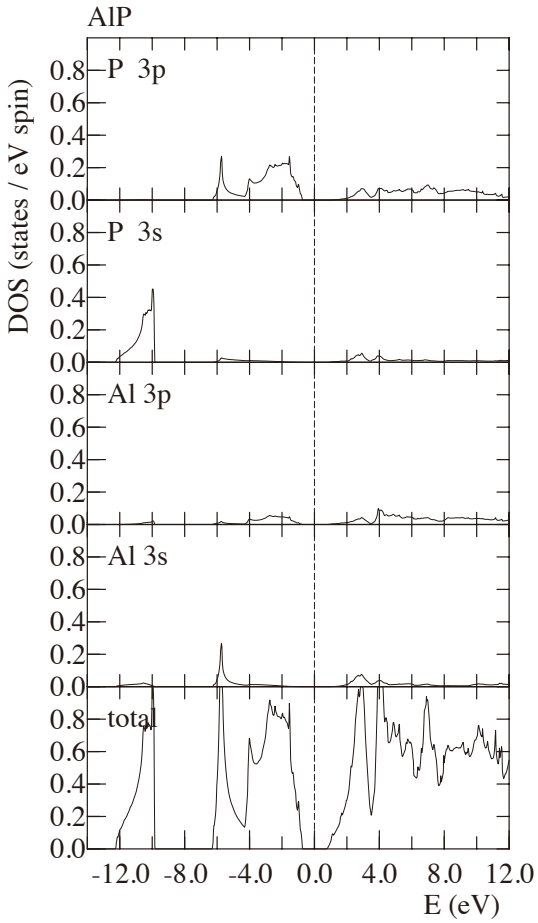
```
>>>>>>>>> ab_prp.data >>>>>>>>>>>
AlP (216, Td2, F-43m) zinc blende
  a=5.45 A
  face-centered (il=2)
  generators    5  (0, 0, 0)
               43  (0, 0, 0)
  atomic positions
           (0.0,  0.0,  0.0 )  Al
           (0.25, 0.25, 0.25)  P
  nonmagnetic (jmag=0)
>>>>>>>>> ab_prp.data >>>>>>>>>>>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

“*ab_prp.data*” for AlP

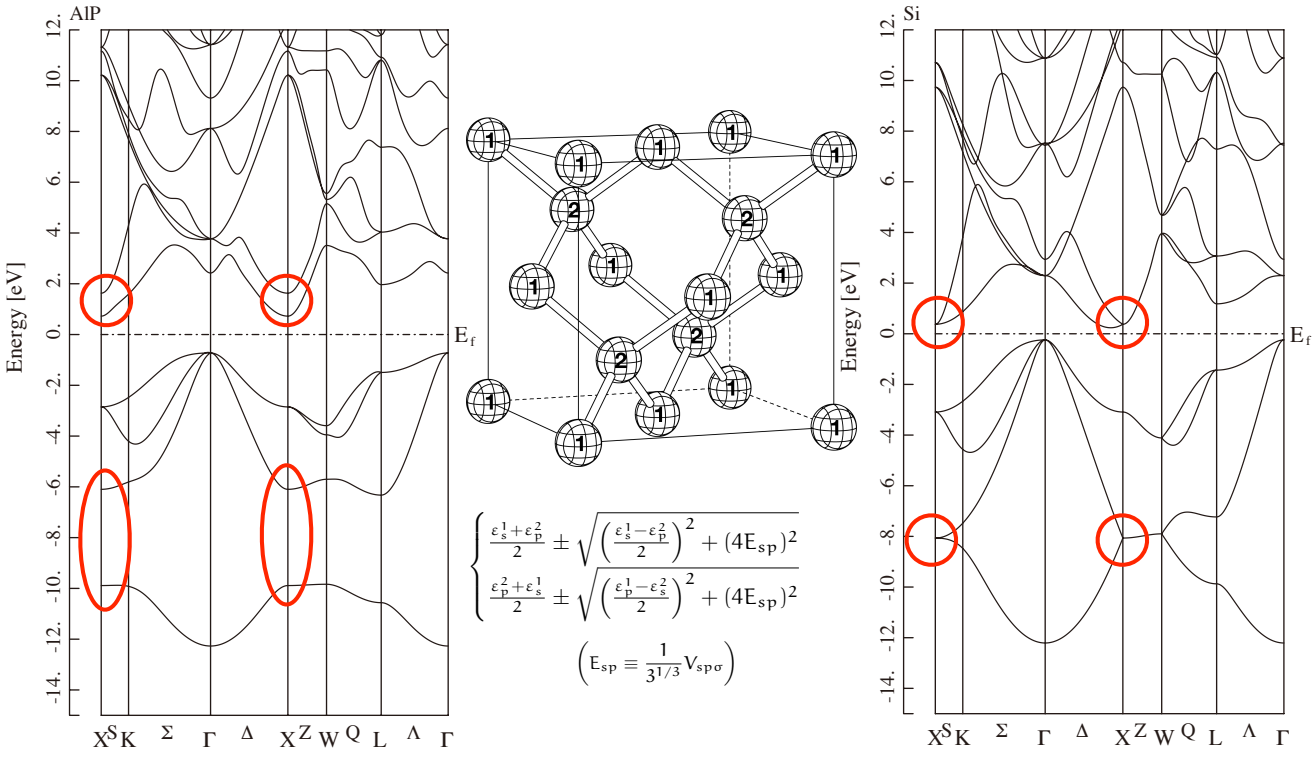
ab_prp.data (~/abc/AlP) - VIM — ssh -X cmd2 — zsh — ttys003

```
abcap-ab_prp.data
0                                   !jpr
AlN
lattice parameter -2----*----3----*----4----*----5----*----6----*----7
 5.45 5.45 5.45  90.0 90.0 90.0         !a,b,c[A], alpha,beta,gamma[degree]
space group       -2----*----3----*----4----*----5----*----6----*----7
 3  2  2  0  !idim, il((-1(r),0(h),1(s),2(f),3(b),4(c),5(a),6(b)),ngen,inv(0)
    5   0 1  0 1  0 1                  !igen,jgen(2,3)
   43   0 1  0 1  0 1                  !igen,jgen(2,3)
kinds of atoms    -2----*----3----*----4----*----5----*----6----*----7
 2                                     !# of kinds
 1   0.0        0.0        0.0        Al          !jpos,position,name
 1   0.25       0.25       0.25       P           !jpos,position,name
magnetic state    -2----*----3----*----4----*----5----*----6----*----7
 0              !jmag0 !noSO:(0(N),1(AF),2(M)), SO:(20(N),21(AF),22(M))
    1   1 2  1 2  1 2                  !igen,jgen(2,3) for AF
totally symmetric basis set -3----*----4----*----5----*----6----*----7
 24.0   6                              !cut-off energy[Hr],Lmax
k-points (# of division)  ---3----*----4----*----5----*----6----*----7
  8  8  8                             !nx,ny,nz
iteration         -2----*----3----*----4----*----5----*----6----*----7
4   6  0.05  0.05           !method, n-method, pmix, amix
!---*----1----*----2----*----3----*----4----*----5----*----6----*----7
~
~
 NORMAL  ab_prp.data                    unix iso-2022-jp no    13/23: 38
"ab_prp.data" [converted] 23L, 1464C
```

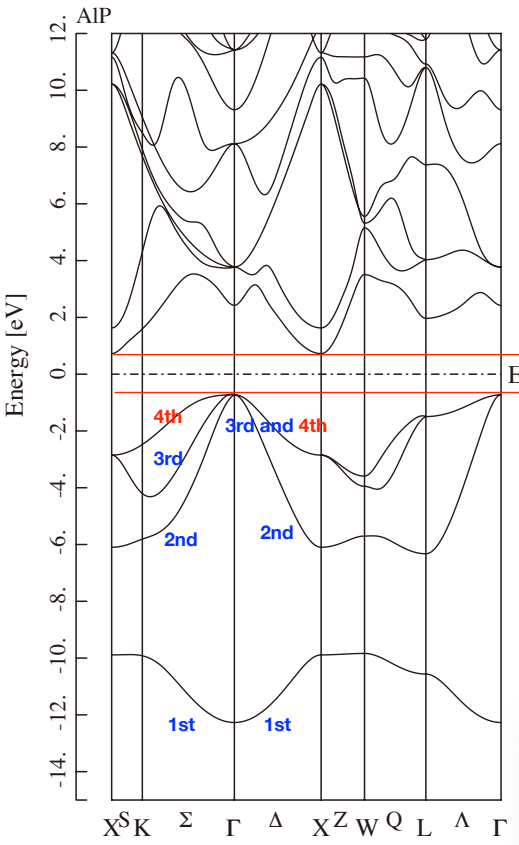


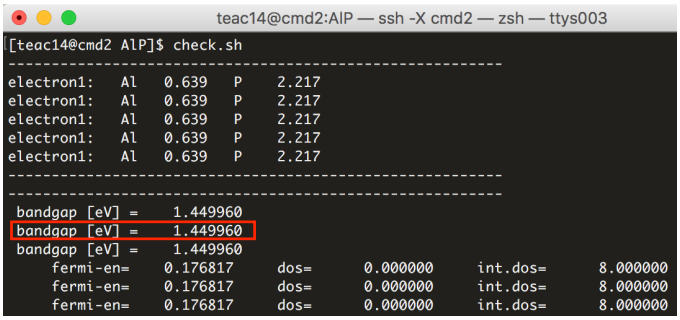


Comparison between E-k curves
(Zincblende and Diamond Structure)



result of "***check.sh***"





1.449960[ev] (indirect)

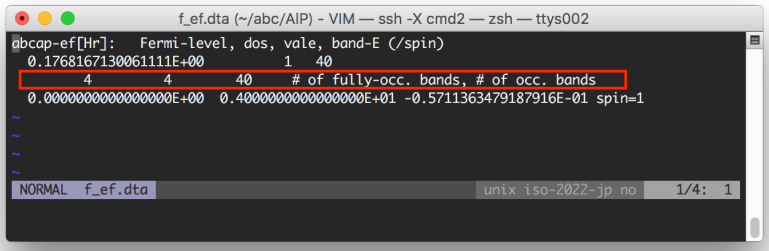
underestimated bandgap

experimental data:
2.45[ev](indirect)

L. I. Berger, *"Semiconductor Materials"* (1996). CRC Press.

information about fermi level:

result of "***f_ef.dta***"

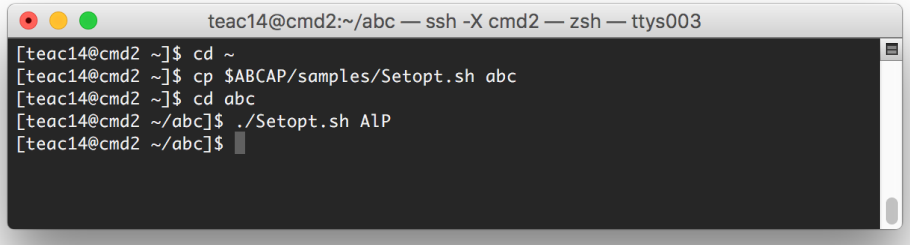


preparation to calculation for optical properties

Make a directory for the calculation for optical properties for AlP.

Use a shell-script file, ***Setopt.sh***, as follows:

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



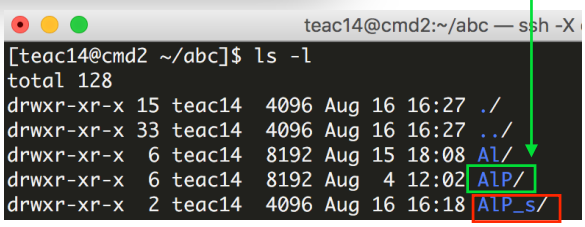
working directory for SCF calc.

The shell-script file ***"Setopt.csh"*** is used on starting a new calculation optical properties:

① script makes working directory for the calculation for optical properties *"AlP_s"*.

② results for SCF calculation for "AlP" is copied from "AlP" to "AlP_s"

③ files needed for the optical calculation are copied from the directories, ***$ABCAP/samples/ZnO_5_s0/*** .



working directory for the calculation for optical properties (script makes).

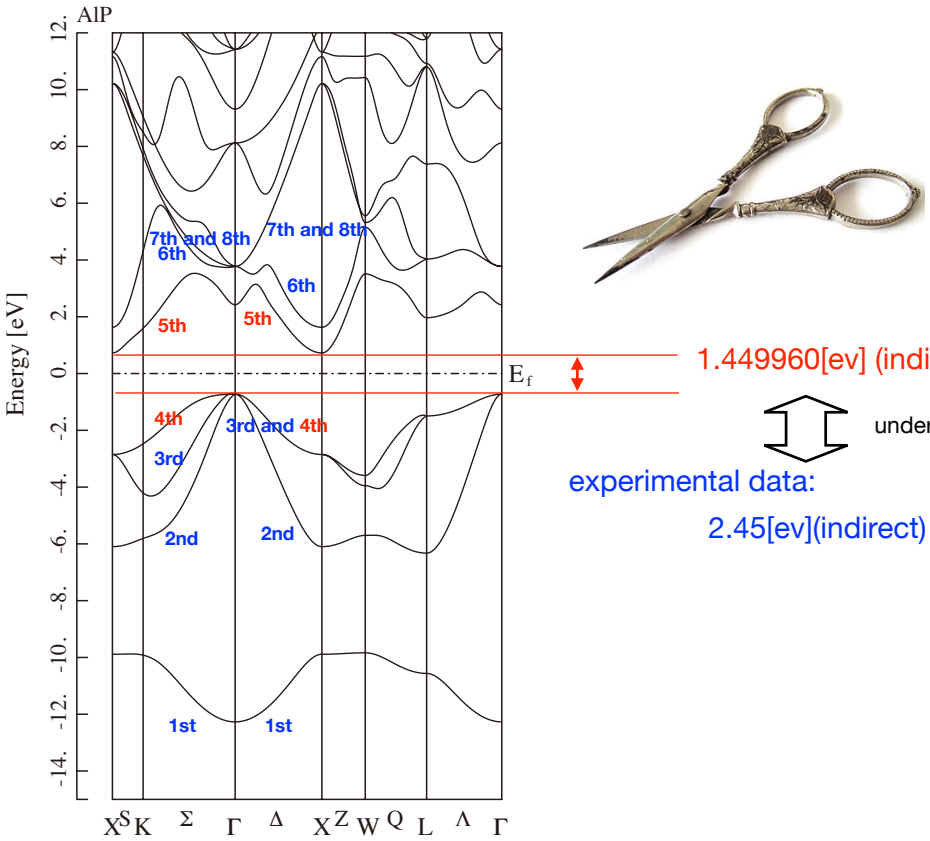
Firstly, we enter the working directory, *"AlP_s"*

```
teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys002
[teac14@cmd2 ~/abc]$ cd AlP_s
[teac14@cmd2 AlP_s]$
```

Enter a command, ***H***, which shows procedures of the calculation.

```
teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys002
[teac14@cmd2 AlP_s]$ H
-------------------------------------------------
(0) (bn_scis.data)  bn_scis.sh  (do this just once)
                    bngap.sh    !optical gap
-------------------------------------------------
(1) (bn_dope.data)  bn_dope.sh  !bands at the fermi energy
    (bnpl.data)     bnpl.sh     !E-k curve
(2) (df01.data)     df01.sh     !dielectric function (interband epsilon(omega))
(3) (wpw.data)      wpw.sh      !<w|p|w>
                    bn_efp2.sh  !Fermi velocity <v_i*v_j>
    (df_total.data) df_total.sh !dielectric function (+Drude term)
-------------------------------------------------
(4) (p2_dielec.data)  p2_dielec.sh  !total dielectric function (epsilon)
    (p2_optnk.data)   p2_optnk.sh   !n, k
    (p2_absorb.data)  p2_absorb.sh  !abcorption coefficient (alpha)
(5) (optra.data)      optra.sh      !T, R, A : no ps-file
    (p2_optra.data)   p2_optra.sh   !T, R, A
------------------------------------------------- (plot.ps) -----

[teac14@cmd2 AlP_s]$
```

correct to optical band gap (Scissors Operator)



1.449960[ev] (indirect)

underestimated band gap(~1.0eV)

experimental data:

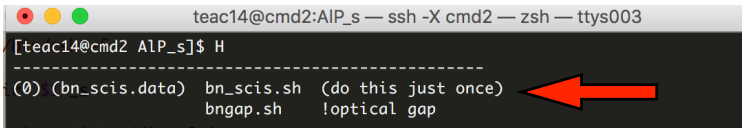
2.45[ev](indirect)

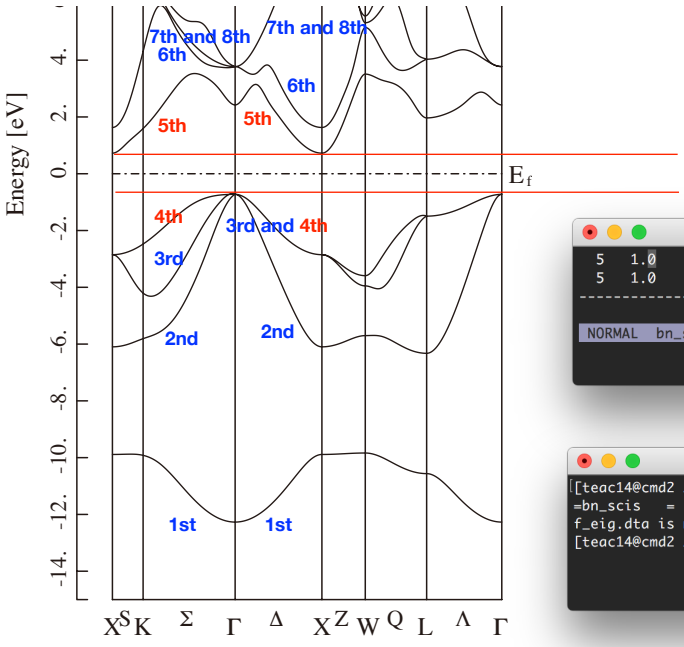
L. I. Berger, *"Semiconductor Materials"* (1996). CRC Press.

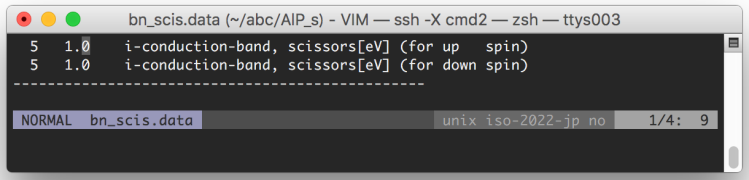
① Edit ***bn_scis.data*** Set band indexes which Scissors operator operate.

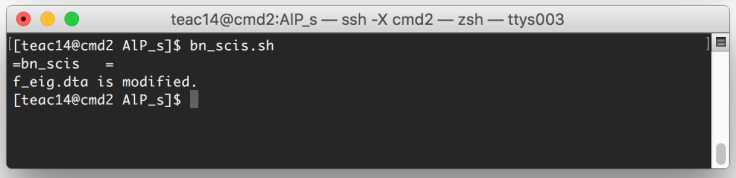
② Run ***bn_scis.sh***.

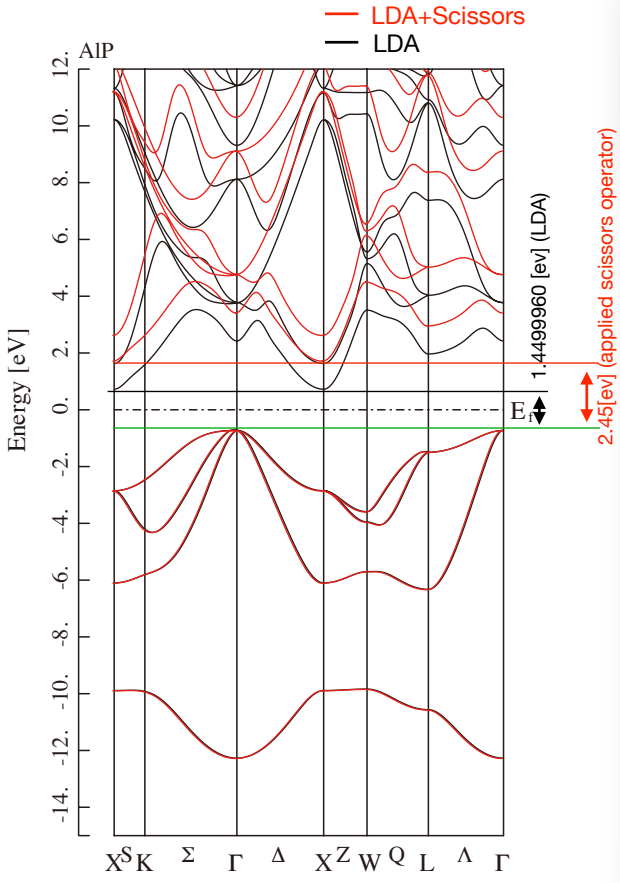
③ ***bngap.sh*** show the information about optical band gap

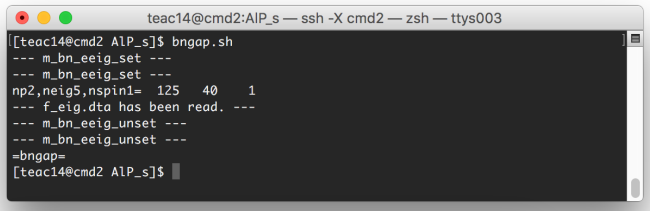


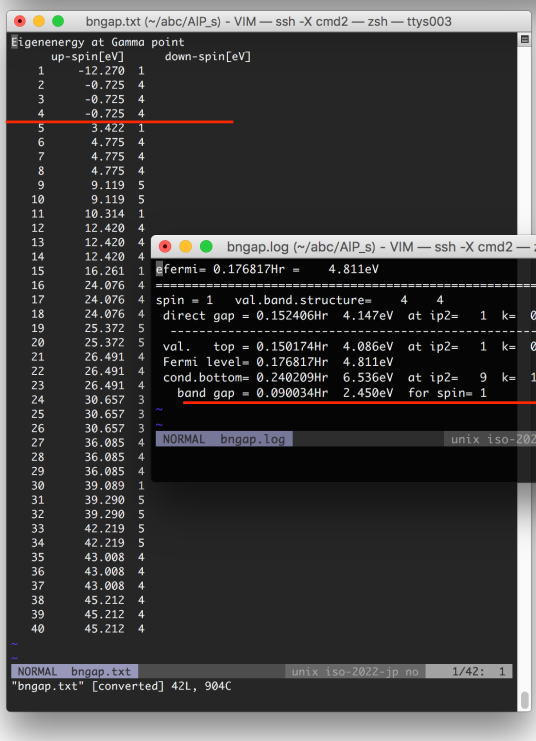


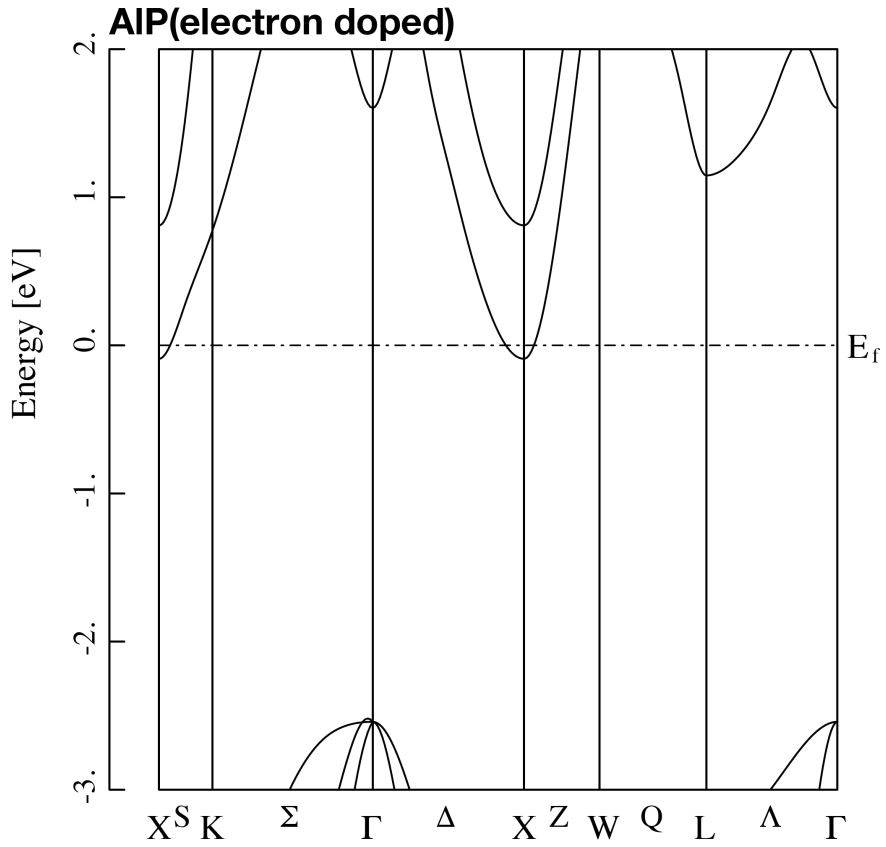












Calculation for $\epsilon_{ij}(\omega)$

$$\frac{\epsilon_{ij}(\omega)}{\epsilon_0} = \delta_{ij} + \frac{e^2}{\epsilon_0 m\omega^2}\left\{\frac{1}{m}\chi_{ij}(\omega) - n\right\}$$

$$\chi_{ij}(\omega) = 2\sum_{cv}\left\{\chi^{cv}_{ij}(\omega + i\eta) + \chi^{cv}_{ij}(-\omega + i\eta)^*\right\}$$

$$\chi^{cv}_{ij}(z) = -\frac{1}{N}\sum_{\boldsymbol{k}}\frac{f_{\boldsymbol{k}v}\left(1 - f_{\boldsymbol{k}c}\right)\langle v\,|\,p_i\,|\,c\rangle\langle c\,|\,p_j\,|\,v\rangle}{z - \left(\varepsilon_{\boldsymbol{k}c} - \varepsilon_{\boldsymbol{k}v}\right)}$$

df01.data (~/abc/AlP_s) - VIM — ssh -X cmd2 — zsh — ttys008

```
0               jpr
200              ne  # mesh
0.0  10.0        emin,emax [eV]
0.000005 1 0     eshift[Hr],ipath,matopt
2   4           nv1,nv2  : valence bands
5   8           nw1,nw2  : conduction bands
=====================================
 3 18    3 16    nv1,nv2(up), nv1,nv2(down) : valence bands
19 26   17 25    nw1,nw2(up), nw1,nw2(down) : conduction bands
=====================================
10   18          nv1,nv2  : valence bands
17   25          nw1,nw2  : conduction bands
=====================================
0               jpr
1000             ne  # mesh
0.0  10.0        emin,emax [eV]
0.000005 1 0     esift,ipath,matopt
 1   18          nv1,nv2
19   48          nw1,nw2
c-------------------------------------------------------------------
c     jpr    i4 (O) : print option
c     ne     i4 (O) : number of mesh for complex energy parameter z
c     emin   r8 (O) : min. value of Re(z)   ( when ipath=1 )
c                     min. value of Im(z)   ( when ipath=2 )
c     emax   r8 (O) : max. value of Re(z)   ( when ipath=1 )
c                     max. value of Im(z)   ( when ipath=2 )
c     esift  r8 (O) : imaginary part of z   ( when ipath=1 )
c                     real      part of z   ( when ipath=2 )
c     ipath  i4 (O) : integral path index
c                    =1 : along real axis
c                    =2 : along imaginary axis
c     matopt i4 (O) : matrix element option
c                    = 0 : F(n'sigma'k,n sigma k)
c                    = 1 : 1.0
c     nv1    i4 (O) : min. band index for valence band
c     nv2    i4 (O) : max. band index for valence band
c     nw1    i4 (O) : min. band index for conduction band
c     nw2    i4 (O) : max. band index for conduction band

~
~
~
~
NORMAL  df01.data                                  unix iso-2022-jp no    6/39:  5
"df01.data" [converted] 39L, 1738C
```

teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys009

```
[teac14@cmd2 AlP_s]$ df01.qc
Your job 84216 ("df01.csh") has been submitted
[teac14@cmd2 AlP_s]$
```

Calculation for the velocity

wpw.data (~/abc/AlP_s) - VIM — ssh -X cmd2 — zsh — ttys008

```
-3  4       bnbgn+, bnend+  (spin up)
-3  4       bnbgn+, bnend+  (spin down)
~
~
NORMAL  wpw.data                          unix iso-2022-jp no     2/2:  5
"wpw.data" [converted] 2L, 76C
```

teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys008

```
[teac14@cmd2 AlP_s]$ wpw.sh
=wpw    =
[teac14@cmd2 AlP_s]$
```

wpw.log + (~/abc/AlP_s) - VIM — ssh -X cmd2 — zsh — ttys000

```
npw9=   189     neig9=    40
npw9=   180     neig9=    40

 ispin = 1
   2  band                <px>                    <py>                    <pz>
    1          0.000000000000          -0.000000000000          0.000000000000
    2          -0.310694881987          -0.000000000000          0.000000000000
    3          -0.416184783701          0.000000000000          0.000000000000
    4          -0.436564647111          0.000000000000          -0.000000000000
    5          -0.428526895962          -0.000000000000          0.000000000000
    6          -0.399840889706          0.000000000000          0.000000000000
    7          -0.337197468719          0.000000000000          0.000000000000
    8          -0.209523773776          0.000000000000          -0.000000000000
    9          -0.000000000000          0.000000000000          -0.000000000000
   10          -0.319525616057          -0.319525616057          -0.000000000000
   11          -0.369644936101          -0.302128644337          -0.000000000000
   12          -0.381029828053          -0.244773922385          0.000000000000
   13          -0.377409671605          -0.168290632212          0.000000000000
   14          -0.358474769104          -0.089767639685          0.000000000000
   15          -0.307159302117          -0.022727481425          -0.000000000000
   16          -0.192146329511          0.024495544411          0.000000000000
   17          -0.000000000000          0.042569280745          -0.000000000000
   18          -0.331146689585          -0.331146689585          -0.000000000000
NORMAL  wpw.log +                          unix iso-2022-jp no   839/1724:  5
  117          0.126067430781          -0.133909906667          -0.133909906667
  118          0.227806047680          -0.186462818440          -0.186462818440
  119          0.063818681539          0.063818681539          -0.121408303448
  120          0.258601091511          0.000000000037          -0.258601091535
  121          0.186462818438          0.186462818438          -0.227806047679
  122          -0.133909906667          -0.126067430781          -0.133909906667
  123          0.063818681539          -0.063818681539          -0.121408303448
  124          -0.040577521040          0.040577521040          -0.040577521040
  125          -0.000000000000          -0.000000000000          -0.000000000000
    8  band                <px>                    <py>                    <pz>
    1          0.000000000000          0.000000000000          -0.000000000000
    2          0.202692821443          0.000000000000          0.000000000000
    3          0.343306505478          -0.000000000000          -0.000000000000
    4          0.425387619533          0.000000000000          0.000000000000
    5          0.474367219485          0.000000000000          0.000000000000
    6          0.504470227333          -0.000000000000          -0.000000000000
    7          0.525264031176          0.000000000000          0.000000000000
    8          0.514307213681          -0.000000000000          -0.000000000000
    9          0.000000000000          -0.000000000000          -0.000000000000
   10          0.242404580245          0.242404580245          0.000000000000
   11          0.237687358120          0.206289993908          0.000000000000
   12          0.438579602866          -0.097011318680          -0.000000000000
NORMAL  wpw.log +                          unix iso-2022-jp no  1588/1724:  1
```

v is the velocity and defined using the wave function $\psi_{\boldsymbol{k},n}$ which is obtained from DFT calculation,

$$v_{\boldsymbol{k},n} = \left\langle \psi_{\boldsymbol{k},n} \left| \frac{\boldsymbol{p}}{m} \right| \psi_{\boldsymbol{k},n} \right\rangle$$

Where $\boldsymbol{p}$ is the momentum, m is mass of the electron, $\boldsymbol{k}$ is the crystal wave number, and n is the band index, respectively.

teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys001

```
[teac14@cmd2 AlP_s]$ bn_efp2.sh
=bn_efp2 =
[teac14@cmd2 AlP_s]$
```

bn_efp2.log (~/hamada/CMD/29/local/AlP_s16) - VIM — vim bn_efp2.log — zsh — ttys004

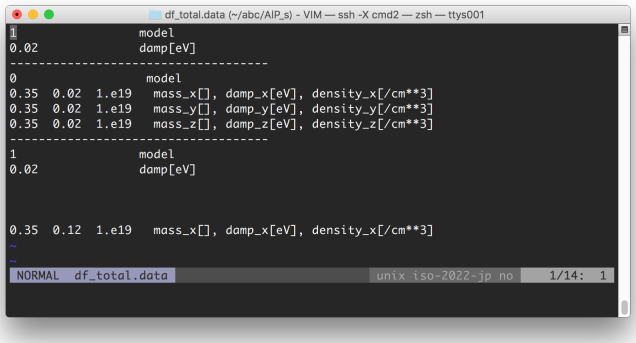
```
isp,ibn,ieig=    1    6    7
isp,ibn,ieig=    1    7    8

 --- p**2 (atomic unit) --- (each band)

 --- p**2 (anisotropy) --- (each band)

 --- DOS[/Hr], v [m/s] (SI unit) --- (each band)

 --- p**2 (atomic unit) --- (each spin)
    1    0.001820  0.000496  0.000000 -0.000000  0.000496  0.000000  0.000496
 --- DOS[/Hr], v [m/s] (SI unit) --- (each spin)
    1    0.001820    48703.    48703.    48703.

--- DOS,  xx,  yx,yy,  zx,zy,zz --- =(whole bands)=
 DOS[/Hr]=    0.003640
 --- p**2 (atomic unit) ---
  0.000496
  0.000000  0.000496
 -0.000000  0.000000  0.000496
 --- v [m/s] (SI unit) ---
    48703.    48703.    48703.
                           --- p**2 (anisotropy) ---
                                (vxx+vyy)/2*vzz =    1.000000
                           --- v    (anisotropy) ---
                           sqrt((vxx+vyy)/2*vzz)=    1.000000



--------- Conductivity ----------------------
delta= 0.020000eV,    tau=  3.291061E-14 s
mean free path=  1.602846E+01  1.602846E+01  1.602846E+01 A
conductivity=  7.451791E+00  7.451791E+00  7.451791E+00 [/(Ohm*m)]
conductivity=  7.451791E-02  7.451791E-02  7.451791E-02 [/(Ohm*cm)]
-----------------------------------------



--- m_bn_eeig_unset ---
--- m_bn_kp_unset ---
--- end m_input_unset ---
NORMAL  bn_efp2.log                        unix iso-2022-jp no  14873/14873:  1
```

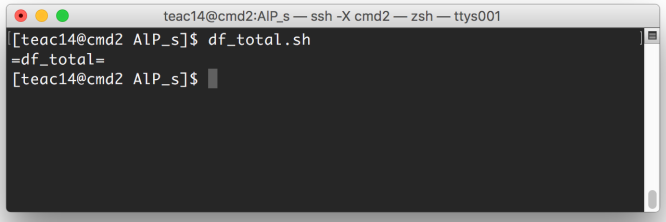
Calculation for the Drude term and total dielectric function

For metallic case, we add *the Drude term*,

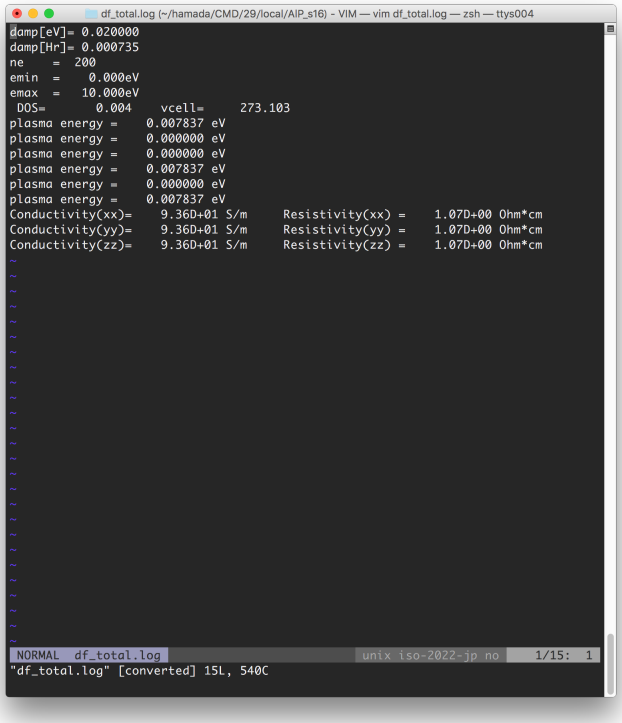
$$\frac{i}{\omega}\frac{\sigma_{ij}(0)}{1-i\omega\tau} = \frac{-1}{\omega}\frac{\sigma_{ij}(0)/\tau}{\omega + i/\tau}$$

$$\sigma_{ij}(0)/\tau = \frac{e^2}{\epsilon_0}\left\langle v_i v_j \right\rangle_F D\left(\varepsilon_F\right)$$





result for total dielectric function



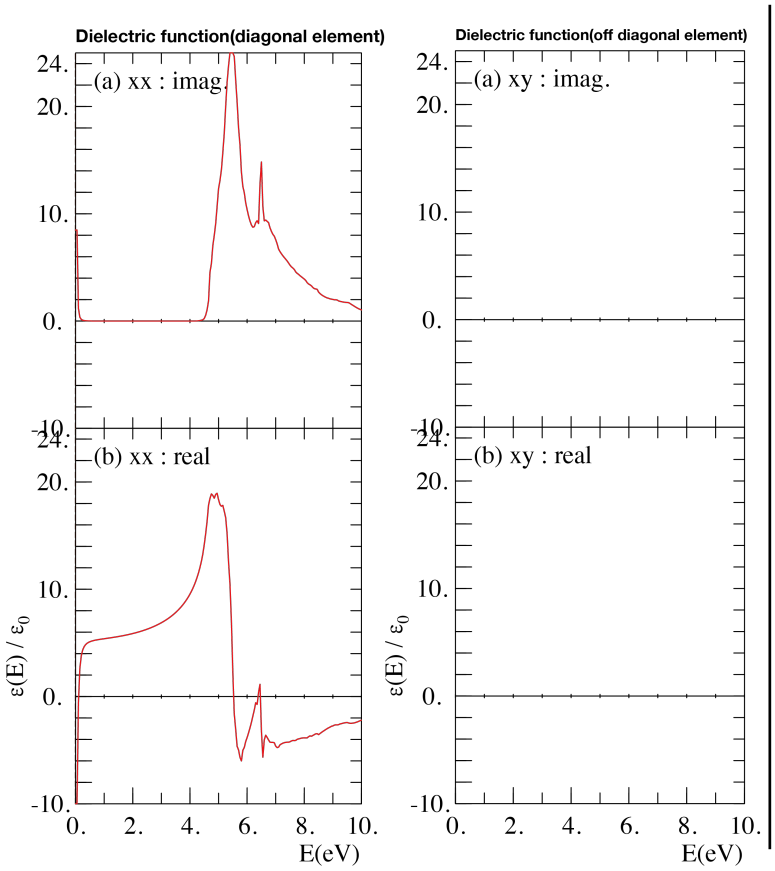
Index of the component for the dielectric function

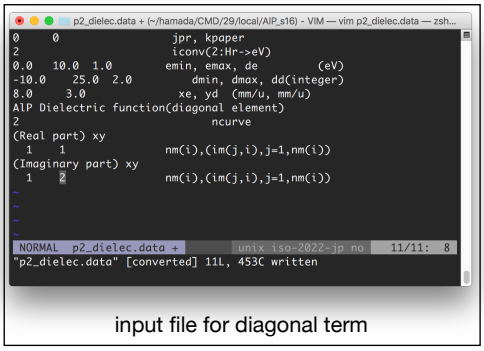
$$\epsilon = \begin{bmatrix} \underset{(1)}{\mathrm{Re}(\epsilon_{xx})} & \underset{(2)}{\mathrm{Im}(\epsilon_{xx})} & \underset{(3)}{\mathrm{Re}(\epsilon_{xy})} & \underset{(4)}{\mathrm{Im}(\epsilon_{xy})} & \underset{(5)}{\mathrm{Re}(\epsilon_{xz})} & \underset{(6)}{\mathrm{Im}(\epsilon_{xz})} \\ \mathrm{Re}(\epsilon_{yx}) & \mathrm{Im}(\epsilon_{yx}) & \underset{(7)}{\mathrm{Re}(\epsilon_{yy})} & \underset{(8)}{\mathrm{Im}(\epsilon_{yy})} & \underset{(9)}{\mathrm{Re}(\epsilon_{yz})} & \underset{(10)}{\mathrm{Im}(\epsilon_{yz})} \\ \mathrm{Re}(\epsilon_{zx}) & \mathrm{Im}(\epsilon_{zx}) & \mathrm{Re}(\epsilon_{zy}) & \mathrm{Im}(\epsilon_{zy}) & \underset{(11)}{\mathrm{Re}(\epsilon_{zz})} & \underset{(12)}{\mathrm{Im}(\epsilon_{zz})} \end{bmatrix}$$

In this case, this crystal has a cubic symmetry,

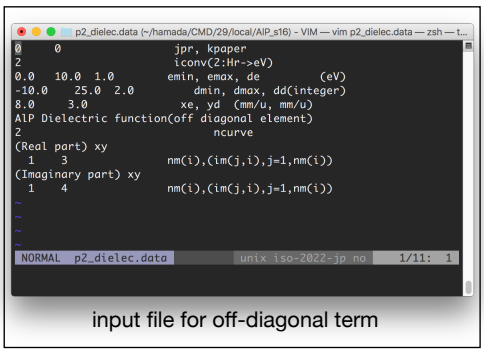
$$\begin{cases} \epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz} & \text{diagonal element} \\ \epsilon_{xy} = \epsilon_{yz} = \epsilon_{zx} & \text{off-diagonal element} \end{cases}$$

diagonal and off diagonal element of dielectric function tensor

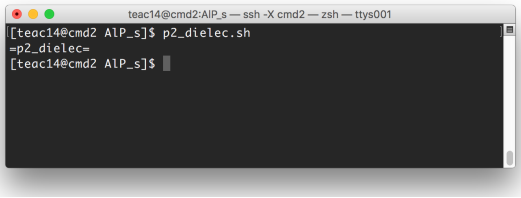




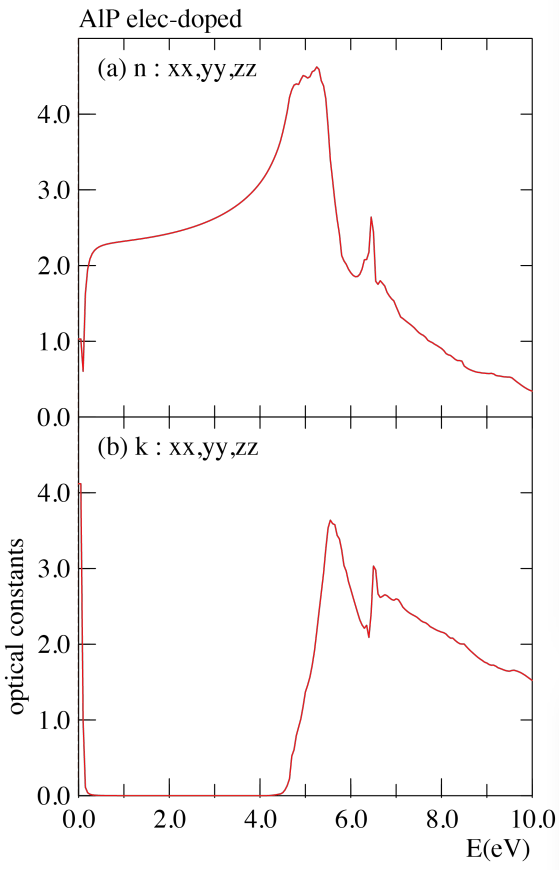
input file for diagonal term

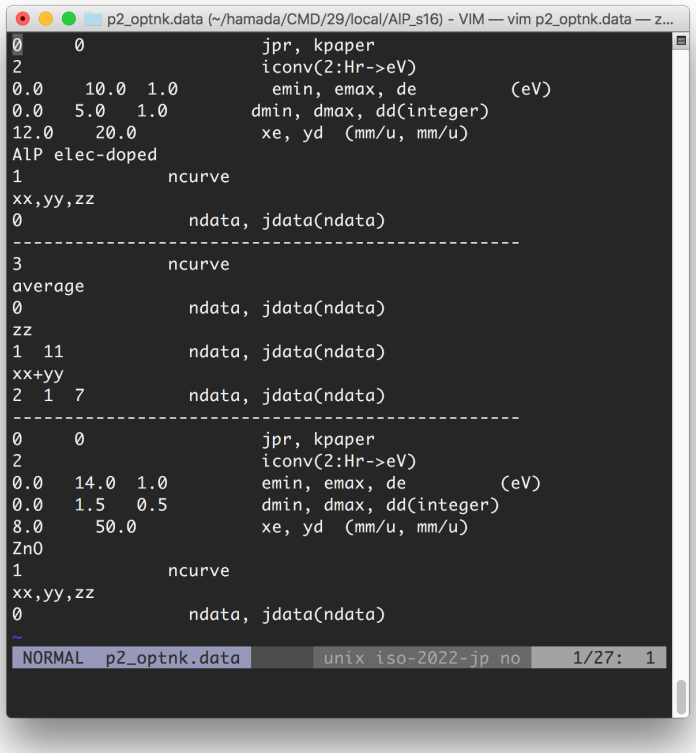


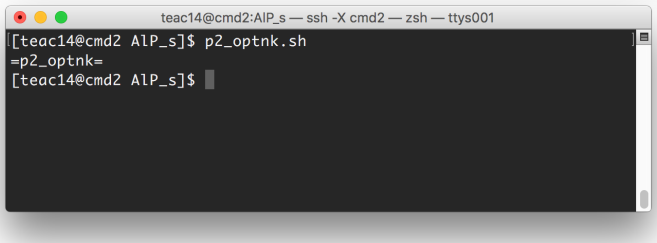
input file for off-diagonal term



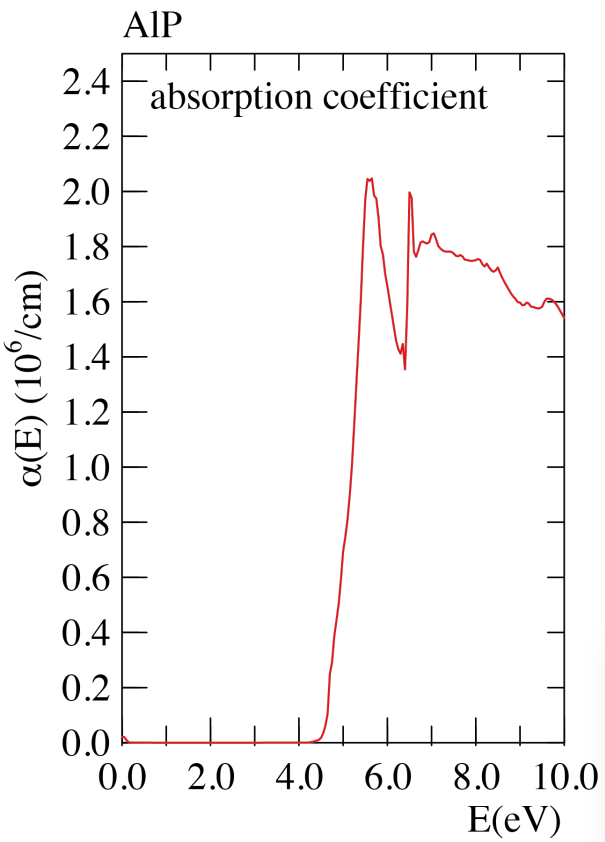
optical constant







absorb constant



p2_absorb.data (~/hamada/CMD/29/local/AlP_s16) - VIM — vim p2_absorb.data —...

```
0     0                jpr, kpaper
2                      iconv(2:Hr->eV)
0.0   10.0  1.0        emin, emax, de          (eV)
0.0   2.5   0.2        dmin, dmax, dd(integer)
8.0     50.0           xe, yd  (mm/u, mm/u)
AlP
1              ncurve
xx,yy,zz
0                ndata, jdata(ndata)
-------------------------------------------------
3              ncurve
average
0                ndata, jdata(ndata)
zz
1  11            ndata, jdata(ndata)
xx+yy
2  1  7          ndata, jdata(ndata)
-------------------------------------------------
~
~
~
~
~
~
~
~
~
~
 NORMAL  p2_absorb.data      unix iso-2022-jp no      1/18:  1
"p2_absorb.data" [converted] 18L, 561C
```

teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys001

```
[teac14@cmd2 AlP_s]$ p2_absorb.sh
=p2_absorb=
[teac14@cmd2 AlP_s]$
```

optra.data (~/hamada/CMD/29/local/AlP_s16) - VIM — vim optra.data — zsh — tty...

```
  1                          ij_epsilon(1:xx,4:yy,6:zz)
  200.0                      ddd [nm]
  1.0d0    1.53d0            n-incident, n-substrate
-------------------------------------------------------
  ij_epsilon: tensor component of the dielectric constant
              (direction of the incident beam)
  ddd  : thickness of the material [nm]
  n-incident  : refractive index in front of the material
  n-substrate : refractive index of substrate


  1.0d0    1.53d0            n-incident, n-substrate
  1.0d0    1.46d0            n-incident, n-substrate
~
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~
 NORMAL  optra.data          unix iso-2022-jp no      1/13:  1
"optra.data" [converted] 13L, 572C
```
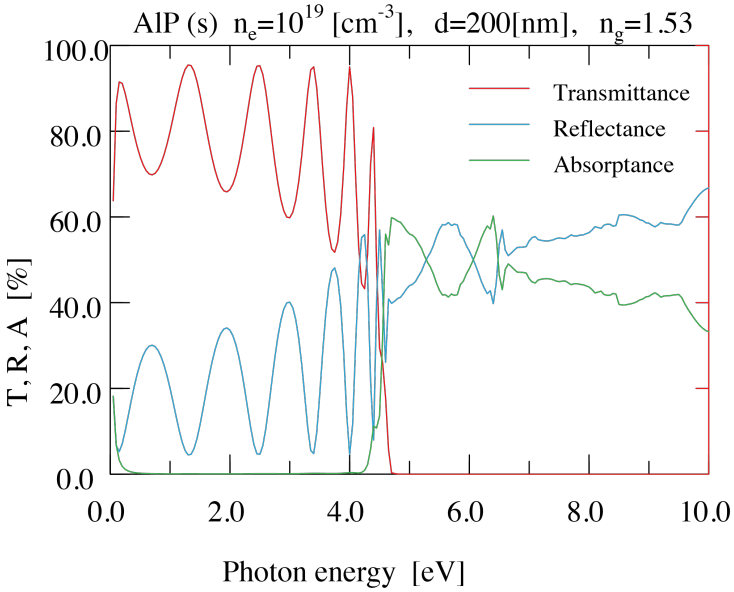
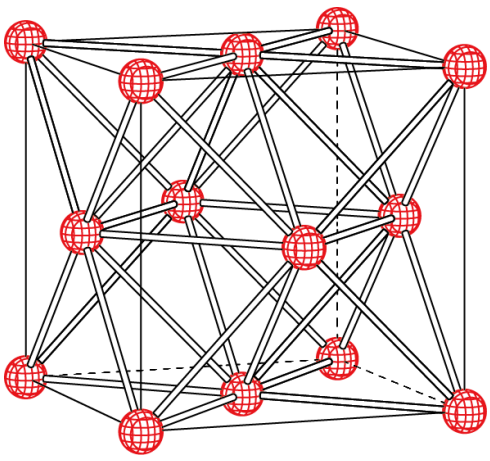

teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys001

```
[teac14@cmd2 AlP_s]$ optra.sh
=optra =
[teac14@cmd2 AlP_s]$
```



4-2. Al



Al(0.0, 0.0, 0.0)

$$\mathrm{Fm\bar{3}m}(O_h{}^5, \#225)$$

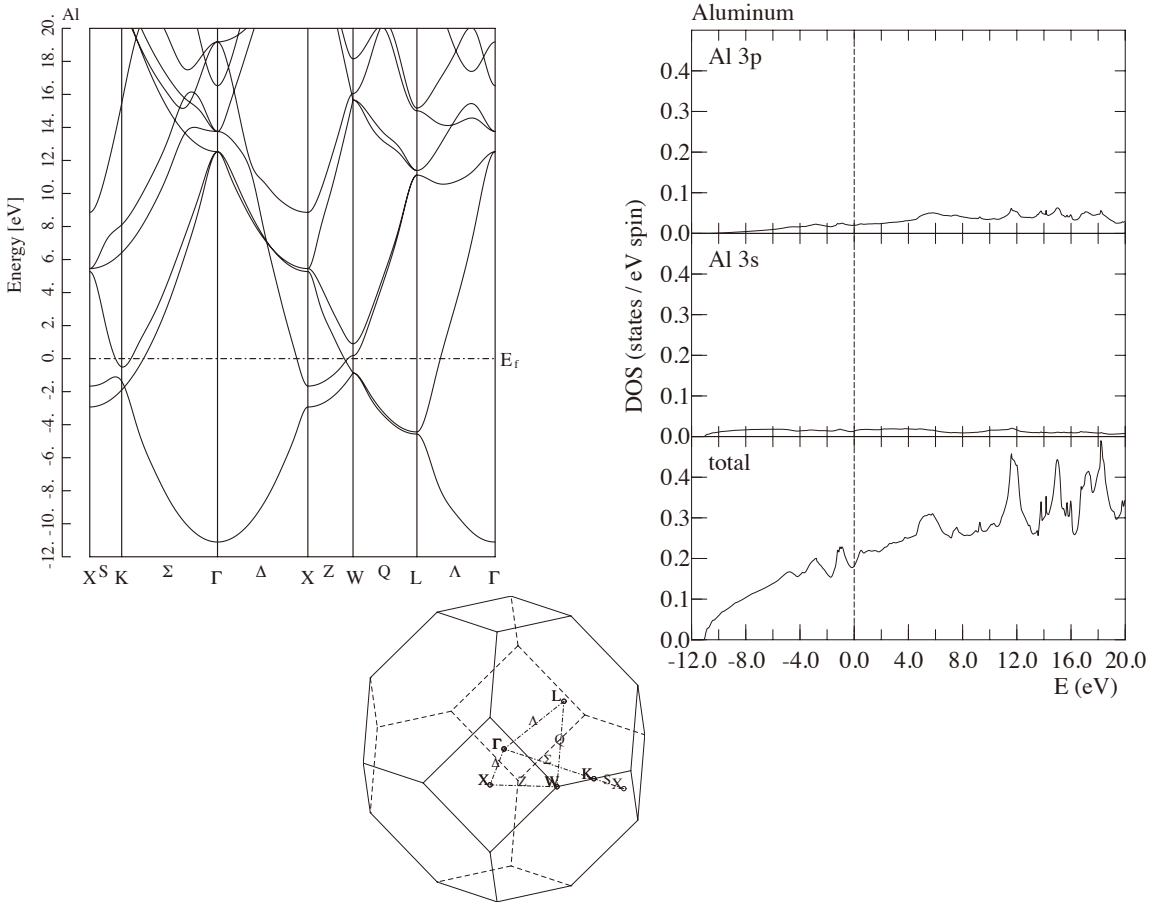
```
>>>>>>>>>> ab_prp.data >>>>>>>>>>>
Al (225, Oh5, Fm-3m) fcc
  a=4.05 A
  face-centered (il=2)
  generators
     5  (0, 0, 0)
    19  (0, 0, 0)
    25  (0, 0, 0)
  atomic position
       (0.0, 0.0, 0.0)
 nonmagnetic (jmag=0)
>>>>>>>>>> ab_prp.data >>>>>>>>>>>
```

“*ab_prp.data*” for Aluminum

ab_prp.data (~/abc/Al) - VIM — ssh -X cmd2 — zsh — ttys003

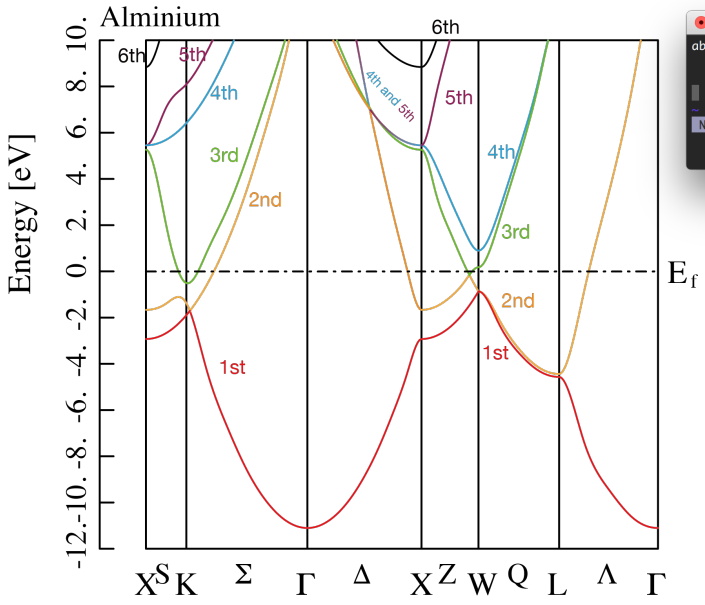
```
abcap-ab_prp.data
0                                       !jpr
aluminum
lattice parameter -2----*----3----*----4----*----5----*----6----*----7
 4.05 4.05 4.05  90.0 90.0 90.0         !a,b,c[A], alpha,beta,gamma[degree]
space group       -2----*----3----*----4----*----5----*----6----*----7
 3  2  3  0  !idim, il((-1(r),0(h),1(s),2(f),3(b),4(c),5(a),6(b)),ngen,inv(0)
    5   0 1  0 1  0 1                      !igen,jgen(2,3)
   19   0 1  0 1  0 1                      !igen,jgen(2,3)
   25   0 1  0 1  0 1                      !igen,jgen(2,3)
kinds of atoms    -2----*----3----*----4----*----5----*----6----*----7
 1                                         !# of kinds
 1   0.0        0.0        0.0       Al    !jpos,position,name
magnetic state    -2----*----3----*----4----*----5----*----6----*----7
 0             !jmag0 !noSO:(0(N),1(AF),2(M)), SO:(20(N),21(AF),22(M))
    1   1 2  1 2  1 2                      !igen,jgen(2,3) for AF
totally symmetric basis set -3----*----4----*----5----*----6----*----7
 24.0   6                                  !cut-off energy[Hr],Lmax
k-points (# of division)  ---3----*----4----*----5----*----6----*----7
  8  8  8                                 !nx,ny,nz
iteration         -2----*----3----*----4----*----5----*----6----*----7
4   6  0.05  0.05           !method, n-method, pmix, amix
!---*----1----*----2----*----3----*----4----*----5----*----6----*----7
~
~
 NORMAL  ab_prp.data                    unix iso-2022-jp no    1/23:  1
"ab_prp.data" [converted] 23L, 1465C
```

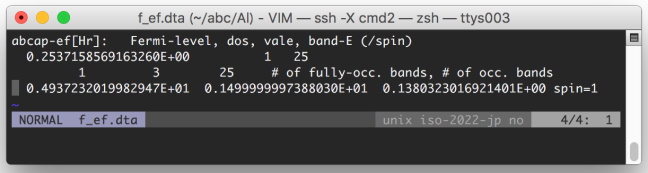
Electronic structure of Aluminum



information about fermi level:

result of "***f_ef.dta***"





1st band… full-occupied

2nd and 3rd band… partially occupied

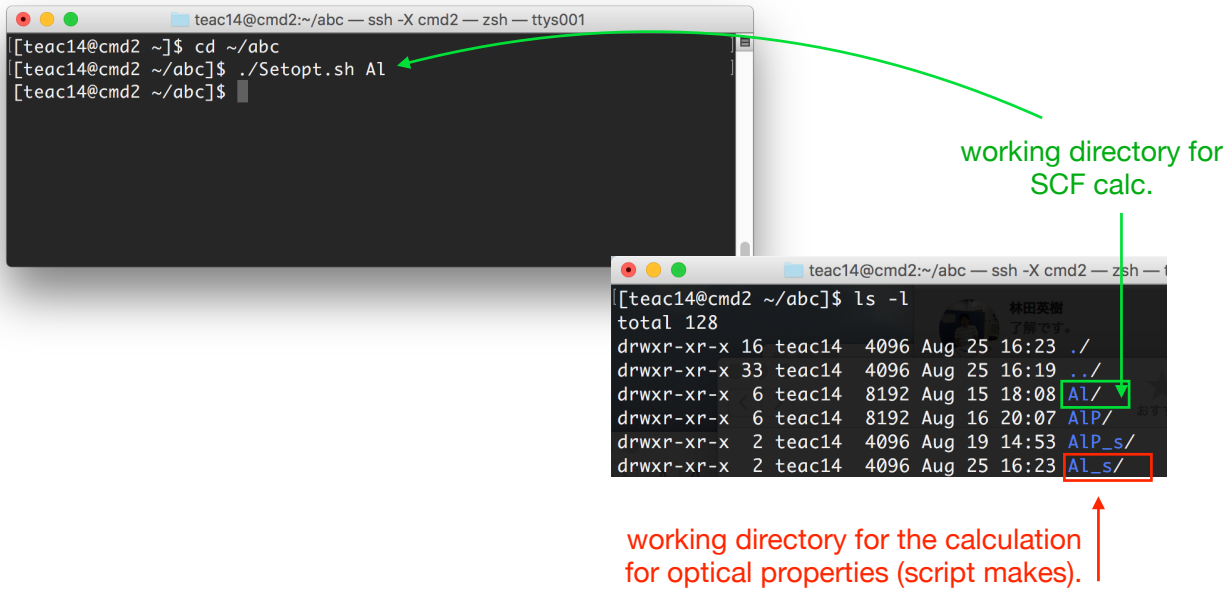
Energy of visible light: 1.6-3.3[eV]

preparation to calculation for optical properties

Make a directory for the calculation for optical properties for Al.

Use a shell-script file, ***Setopt.sh***, as follows:

```
cd ~/abc
./Setopt.sh Al
```



Firstly, we enter the working directory, *“Al_s”*

```
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys001
[teac14@cmd2 ~]$ cd ~/abc/Al_s
[teac14@cmd2 Al_s]$
```

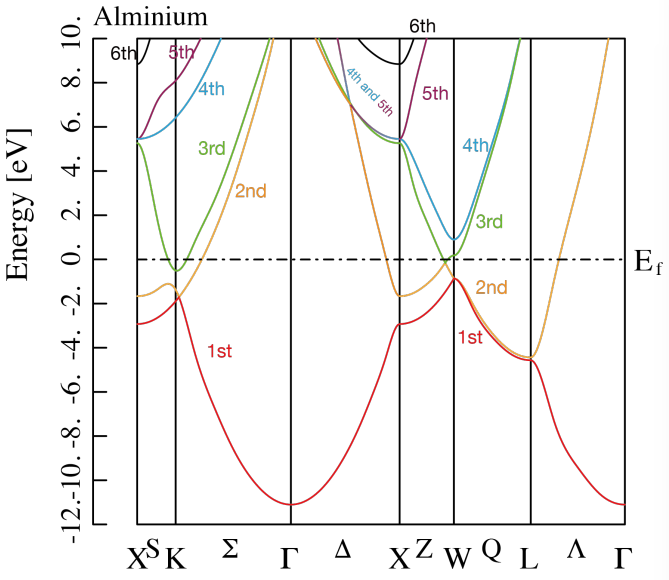
Enter a command, ***H***, which shows a procedure of the calculation.

```
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys001
[teac14@cmd2 Al_s]$ H
-------------------------------------------------
(0) (bn_scis.data)  bn_scis.sh  (do this just once)
                    bngap.sh    !optical gap
-------------------------------------------------
(1) (bn_dope.data)  bn_dope.sh  !bands at the fermi energy
    (bnpl.data)     bnpl.sh     !E-k curve
(2) (df01.data)     df01.sh     !dielectric function (interband epsilo
n(omega))
(3) (wpw.data)      wpw.sh      !<w|p|w>
                    bn_efp2.sh  !Fermi velocity <v_i*v_j>
    (df_total.data) df_total.sh !dielectric function (+Drude term)
-------------------------------------------------
(4) (p2_dielec.data)  p2_dielec.sh  !total dielectric function (epsilo
n)
    (p2_optnk.data)   p2_optnk.sh   !n, k
    (p2_absorb.data)  p2_absorb.sh  !abcorption coefficient (alpha)
(5) (optra.data)      optra.sh      !T, R, A : no ps-file
    (p2_optra.data)   p2_optra.sh   !T, R, A
------------------------------------------------- (plot.ps) -----

[teac14@cmd2 Al_s]$
```

In this case, we skip these process

Because aluminum is not insulator/ semiconductor but metal, thus we don’t need to operate “Scissors operator”(bn_scis.sh) and dope carriers(bn_dope.sh).

Calculation for $\epsilon_{ij}(\omega)$




```
df01.data + (~/abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys000
0                jpr
200              ne  # mesh
0.0  10.0        emin,emax [eV]
0.000005 1 0     eshift[Hr],ipath,matopt
1   3          nv1,nv2  : valence bands
2   6          nw1,nw2  : conduction bands
====================================
 3 18    3 16     nv1,nv2(up), nv1,nv2(down) : valence bands
19 26   17 25     nw1,nw2(up), nw1,nw2(down) : conduction bands
====================================
10   18          nv1,nv2  : valence bands
17   25          nw1,nw2  : conduction bands
====================================
0                jpr
1000             ne  # mesh
0.0  10.0        emin,emax [eV]
0.000005 1 0     esift,ipath,matopt
 1   18          nv1,nv2
19   48          nw1,nw2
c-------------------------------------------------------------------
c     jpr    i4 (0) : print option
c     ne     i4 (0) : number of mesh for complex energy parameter z
c     emin   r8 (0) : min. value of Re(z)   ( when ipath=1 )
c                     min. value of Im(z)   ( when ipath=2 )
c     emax   r8 (0) : max. value of Re(z)   ( when ipath=1 )
c                     max. value of Im(z)   ( when ipath=2 )
c     esift  r8 (0) : imaginary part of z   ( when ipath=1 )
c                     real      part of z   ( when ipath=2 )
c     ipath  i4 (0) : integral path index
c                     =1 : along real axis
c                     =2 : along imaginary axis
c     matopt i4 (0) : matrix element option
c                     = 0 : F(n'sigma'k,n sigma k)
c                     = 1 : 1.0
c     nv1    i4 (0) : min. band index for valence band
c     nv2    i4 (0) : max. band index for valence band
c     nw1    i4 (0) : min. band index for conduction band
c     nw2    i4 (0) : max. band index for conduction band
~
NORMAL  df01.data +                    unix iso-2022-jp no    6/39:  5
```

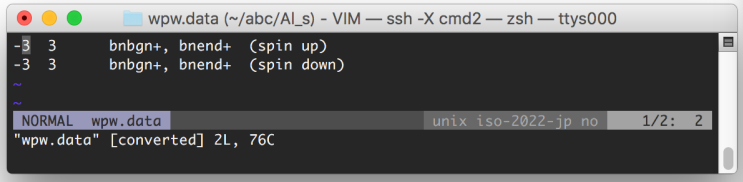
```
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys000
[teac14@cmd2 Al_s]$ ./df01.qc
Your job 84362 ("df01.csh") has been submitted
[teac14@cmd2 Al_s]$
```

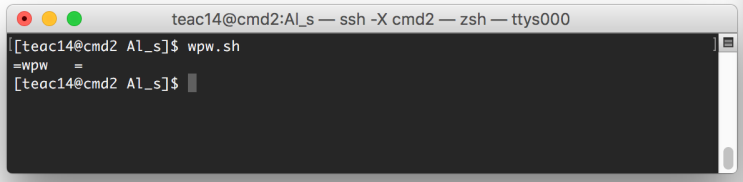
$$\frac{\epsilon_{ij}(\omega)}{\epsilon_0} = \delta_{ij} + \frac{e^2}{\epsilon_0 m\omega^2}\left\{\frac{1}{m}\chi_{ij}(\omega) - n\right\}$$

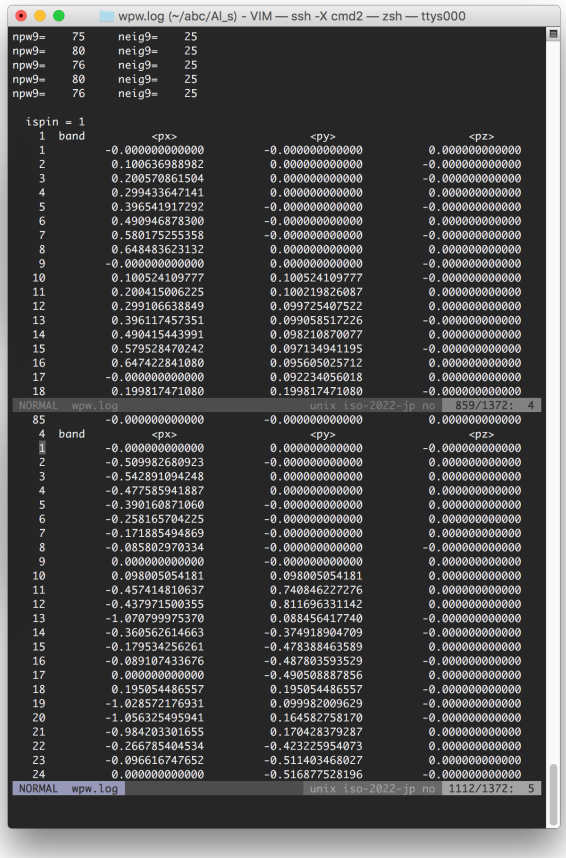
$$\chi_{ij}(\omega) = 2\sum_{cv}\left\{\chi_{ij}^{cv}(\omega + i\eta) + \chi_{ij}^{cv}(-\omega + i\eta)^*\right\}$$

$$\chi_{ij}^{cv}(z) = -\frac{1}{N}\sum_{\boldsymbol{k}}\frac{f_{\boldsymbol{k}_v}\left(1 - f_{\boldsymbol{k}_c}\right)\langle v\,|\,p_i\,|\,c\rangle\langle c\,|\,p_j\,|\,v\rangle}{z - \left(\varepsilon_{\boldsymbol{k}_c} - \varepsilon_{\boldsymbol{k}_v}\right)}$$

Calculation for the velocity



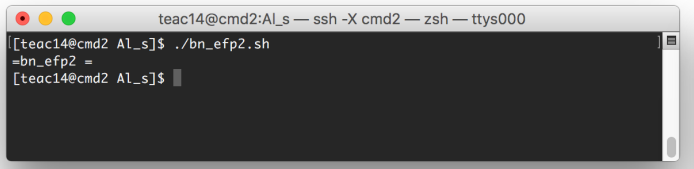


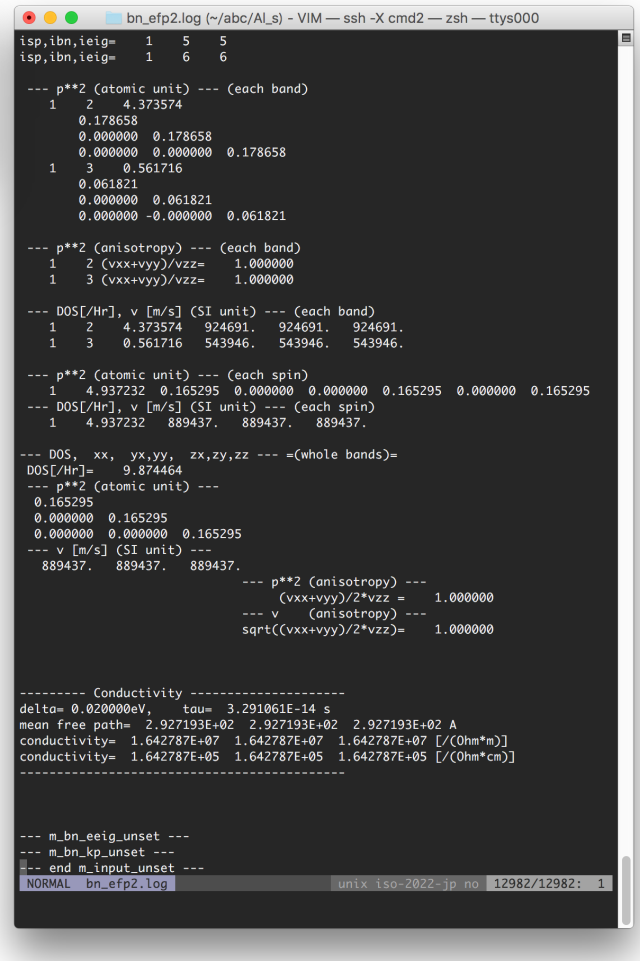


v is the velocity and defined using the wave function $\psi_{\boldsymbol{k},n}$ which is obtained from DFT calculation,

$$v_{\boldsymbol{k},n} = \left\langle \psi_{\boldsymbol{k},n} \left| \frac{\boldsymbol{p}}{m} \right| \psi_{\boldsymbol{k},n} \right\rangle$$

Where $\boldsymbol{p}$ is the momentum, m is mass of the electron, $\boldsymbol{k}$ is the crystal wave number, and n is the band index, respectively.





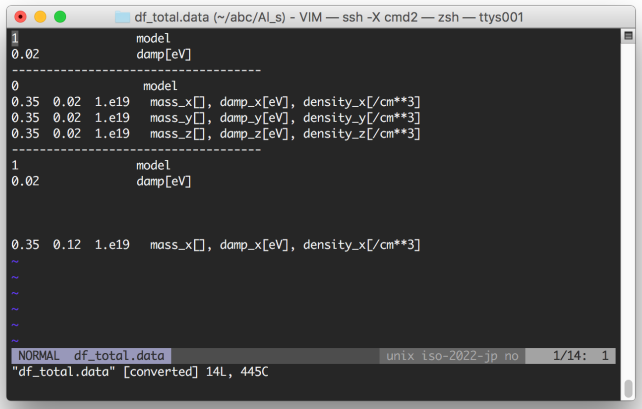
Calculation for the Drude term and total dielectric function

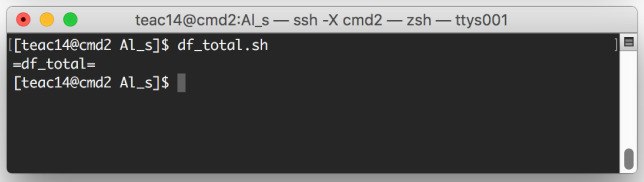
For metallic case, we add *the Drude term*,

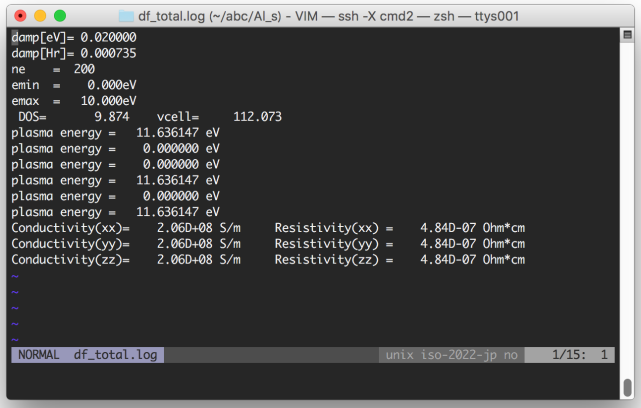
$$\frac{i}{\omega}\frac{\sigma_{ij}(0)}{1-i\omega\tau} = \frac{-1}{\omega}\frac{\sigma_{ij}(0)/\tau}{\omega + i/\tau}$$

$$\sigma_{ij}(0)/\tau = \frac{e^2}{\epsilon_0}\langle v_i v_j \rangle_F D(\varepsilon_F)$$

result for total dielectric function





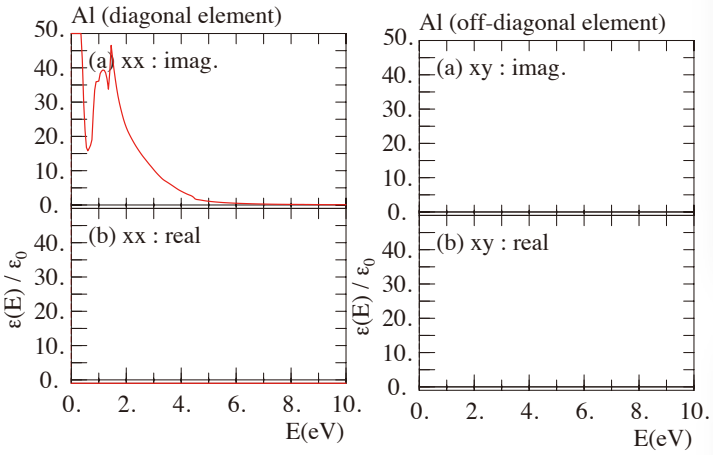


Index of the component for the dielectric function

$$\epsilon = \begin{bmatrix} \underset{(1)}{\mathrm{Re}(\epsilon_{xx})} & \underset{(2)}{\mathrm{Im}(\epsilon_{xx})} & \underset{(3)}{\mathrm{Re}(\epsilon_{xy})} & \underset{(4)}{\mathrm{Im}(\epsilon_{xy})} & \underset{(5)}{\mathrm{Re}(\epsilon_{xz})} & \underset{(6)}{\mathrm{Im}(\epsilon_{xz})} \\ \mathrm{Re}(\epsilon_{yx}) & \mathrm{Im}(\epsilon_{yx}) & \underset{(7)}{\mathrm{Re}(\epsilon_{yy})} & \underset{(8)}{\mathrm{Im}(\epsilon_{yy})} & \underset{(9)}{\mathrm{Re}(\epsilon_{yz})} & \underset{(10)}{\mathrm{Im}(\epsilon_{yz})} \\ \mathrm{Re}(\epsilon_{zx}) & \mathrm{Im}(\epsilon_{zx}) & \mathrm{Re}(\epsilon_{zy}) & \mathrm{Im}(\epsilon_{zy}) & \underset{(11)}{\mathrm{Re}(\epsilon_{zz})} & \underset{(12)}{\mathrm{Im}(\epsilon_{zz})} \end{bmatrix}$$

In this case, this crystal has a cubic symmetry,

$$\begin{cases} \epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz} & \text{diagonal element} \\ \epsilon_{xy} = \epsilon_{yz} = \epsilon_{zx} & \text{off-diagonal element} \end{cases}$$



p2_dielec.data (~/abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys001

```
0     0                jpr, kpaper
2                      iconv(2:Hr->eV)
0.0   10.0  1.0        emin, emax, de          (eV)
-1.0   50.0  5.0        dmin, dmax, dd(integer)
8.0     1.0            xe, yd  (mm/u, mm/u)
Al (diagonal element)
2                             ncurve
(real part) xx,yy,zz
  1    1                nm(i),(im(j,i),j=1,nm(i))
(imaginary part) xx,yy,zz
  1    2                nm(i),(im(j,i),j=1,nm(i))
~
~
~
~
 NORMAL  p2_dielec.data                 unix iso-2022-jp no     4/11:  14
"p2_dielec.data" [converted] 11L, 443C
```

input file for diagonal term

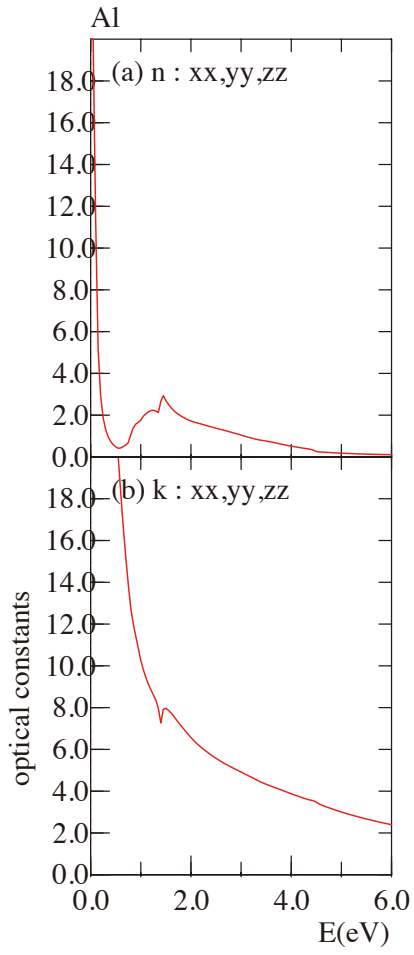
p2_dielec.data (~/abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys001

```
0     0                jpr, kpaper
2                      iconv(2:Hr->eV)
0.0   10.0  1.0        emin, emax, de          (eV)
-1.0   50.0  5.0        dmin, dmax, dd(integer)
8.0     1.0            xe, yd  (mm/u, mm/u)
Al (off-diagonal element)
2                             ncurve
(real part) xx,yy,zz
  1    3                nm(i),(im(j,i),j=1,nm(i))
(imaginary part) xx,yy,zz
  1    4                nm(i),(im(j,i),j=1,nm(i))
~
~
~
~
 NORMAL  p2_dielec.data                 unix iso-2022-jp no     6/11:  8
"p2_dielec.data" [converted] 11L, 447C written
```

input file for off-diagonal term

teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys001

```
[teac14@cmd2 Al_s]$ p2_dielec.sh
=p2_dielec=
[teac14@cmd2 Al_s]$
```

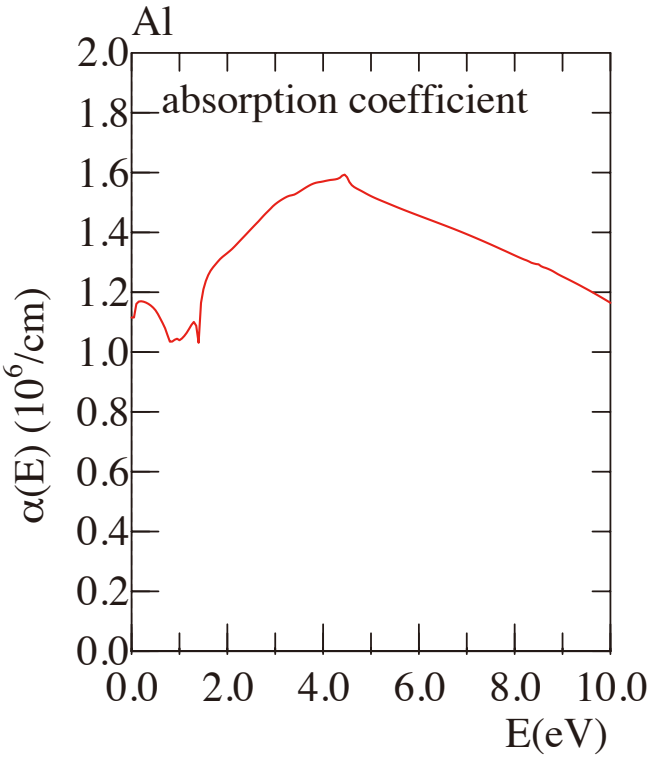


p2_optnk.data (~/abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys001

```
0     0                jpr, kpaper
2                      iconv(2:Hr->eV)
0.0    6.0  1.0        emin, emax, de          (eV)
0.0   20.0   2.0        dmin, dmax, dd(integer)
12.0    5.0            xe, yd  (mm/u, mm/u)
Al
1             ncurve
xx,yy,zz
0               ndata, jdata(ndata)
-------------------------------------------------
3             ncurve
average
0               ndata, jdata(ndata)
zz
1  11           ndata, jdata(ndata)
xx+yy
2  1  7         ndata, jdata(ndata)
-------------------------------------------------
0     0                jpr, kpaper
2                      iconv(2:Hr->eV)
0.0   14.0  1.0        emin, emax, de          (eV)
0.0   1.5   0.5        dmin, dmax, dd(integer)
8.0     50.0           xe, yd  (mm/u, mm/u)
ZnO
1             ncurve
xx,yy,zz
0               ndata, jdata(ndata)
~
~
~
 NORMAL  p2_optnk.data                  unix iso-2022-jp no     5/27:  9
```

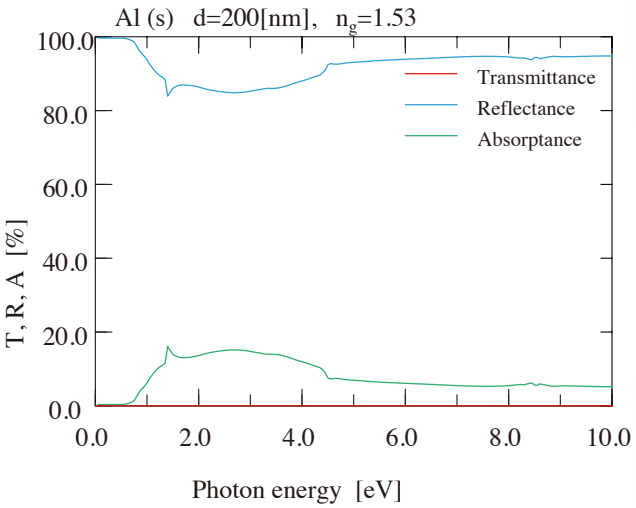
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys001

```
[teac14@cmd2 Al_s]$ ./p2_optnk.sh
=p2_optnk=
[teac14@cmd2 Al_s]$
```




```
p2_absorb.data (~/abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys001
0    0                jpr, kpaper
2                     iconv(2:Hr->eV)
0.0   10.0  1.0       emin, emax, de        (eV)
0.0   2.0   0.2       dmin, dmax, dd(integer)
8.0    50.0           xe, yd  (mm/u, mm/u)
Al
1             ncurve
xx,yy,zz
0               ndata, jdata(ndata)
-----------------------------------------------
3             ncurve
average
0               ndata, jdata(ndata)
zz
1  11           ndata, jdata(ndata)
xx+yy
2  1  7         ndata, jdata(ndata)
-----------------------------------------------
~
~
NORMAL  p2_absorb.data          unix iso-2022-jp no    1/18:  1
```

```
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys001
[teac14@cmd2 Al_s]$ p2_absorb.sh
=p2_absorb=
[teac14@cmd2 Al_s]$
```




```
optra.data (~/abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys001
6                       ij_epsilon(1:xx,4:yy,6:zz)
200.0                   ddd [nm]
1.0d0    1.53d0         n-incident, n-substrate
-----------------------------------------------------------
  ij_epsilon: tensor component of the dielectric constant
              (direction of the incident beam)
  ddd  : thickness of the material [nm]
  n-incident  : refractive index in front of the material
  n-substrate : refractive index of substrate


  1.0d0    1.53d0         n-incident, n-substrate
  1.0d0    1.46d0         n-incident, n-substrate
~
~
NORMAL  optra.data              unix iso-2022-jp no    1/13:  1
```

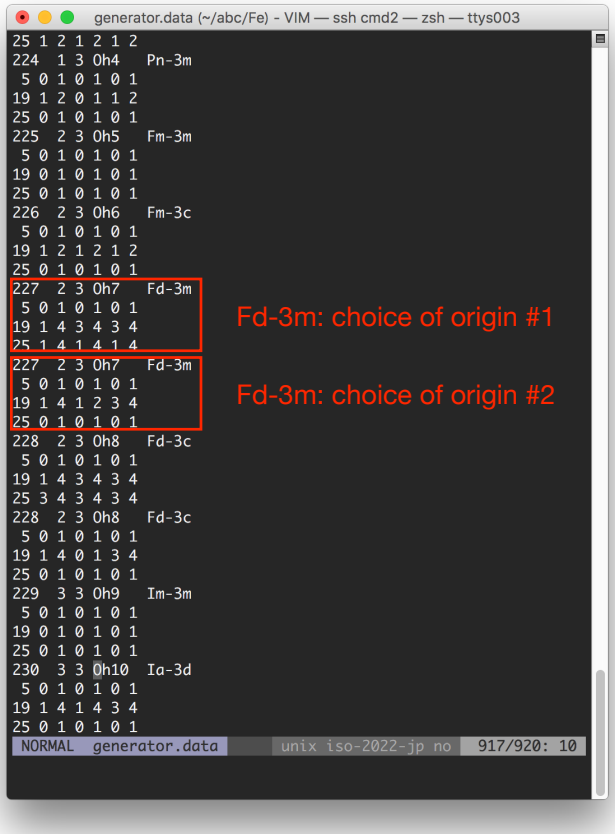
```
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys001
[teac14@cmd2 Al_s]$ ./optra.sh
=optra =
[teac14@cmd2 Al_s]$
```

```
p2_optra.data (~/abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys001
1  0                    jpr, kpaper(0,1)
1                       iscale(0,1)
   Al (s)   d=200[nm],   n$dg=1.53
              Photon energy  [eV]
0  0.0 10.0   1.0  'F'       iautox,xmin,xmax,dx,FEIx(F,E,I)
         T, R, A  [%]
0   0.0  100.0    20.0   'F'       ymin,ymax,dy,FEIy(F,E,I)
1    0.6  0.1                isize,ux,uy (cm/unit)
1 3                          ifmt(0:sut format,1:gnu format),# of lines
'f_TRAeV.dta',1 2 1   'Transmittance'        iix,iiy,type of line
'f_TRAeV.dta',1 3 2   'Reflectance'          iix,iiy,type of line
'f_TRAeV.dta',1 4 3   'Absorptance'          iix,iiy,type of line

NORMAL  p2_optra.data           unix iso-2022-jp no    6/27: 12
```

```
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys001
[teac14@cmd2 Al_s]$ p2_optra.sh
=p2_l=
[teac14@cmd2 Al_s]$
```

Additional Information

Space group information



Generator of the space group

File: **generator.data**

---

index of space group
lattice type(=il)
# of generator
Schöenflies Symbol
Hermann-Mauguin Symbol

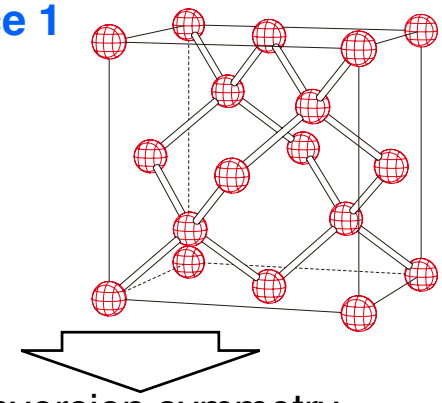
```
227  2 3 Oh7  Fd-3m
  5  0 1 0 1 0 1
 19  1 4 3 4 3 4
 25  1 4 1 4 1 4
```

rotation translation

How do you define the origin of Nonsymmorphic Crystal?

Example: diamond structure $\mathrm{Fd\bar{3}m(O_h^7)}$

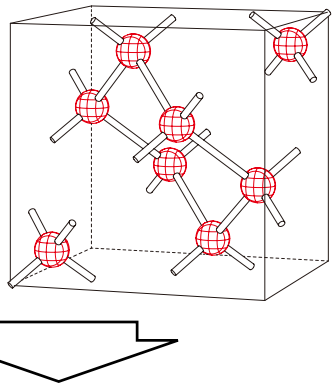
choice 1



× inversion symmetry

○ atom on origin

choice 2



○ inversion symmetry

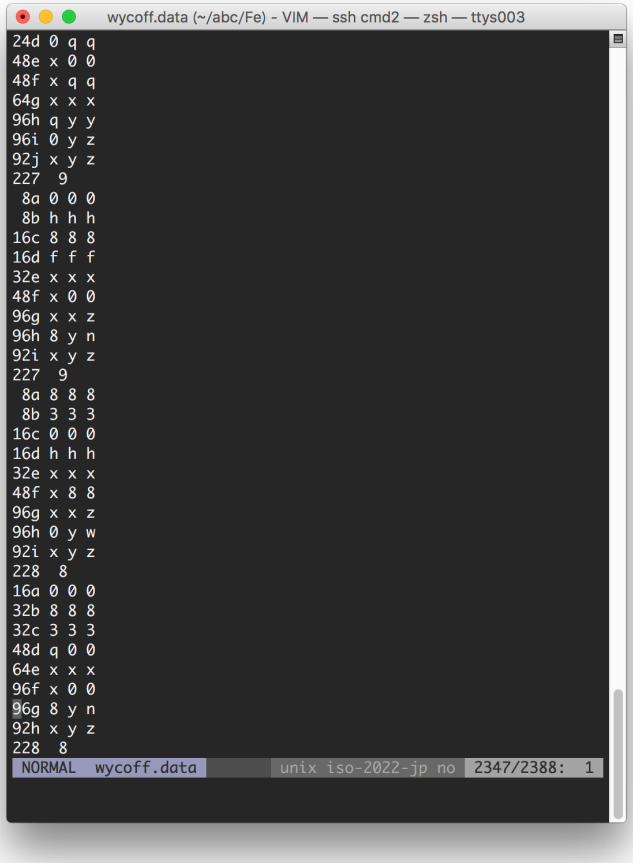
× atom on origin

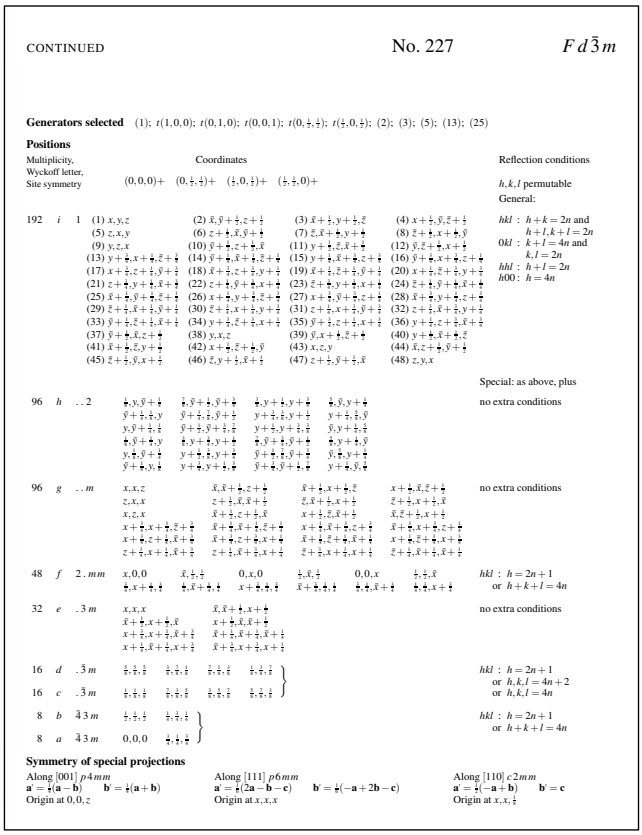
	atomic position	inversion center
choice 1	(0,0,0) and (1/4,1/4,1/4)	No
choice 2	(±1/8,±1/8,±1/8)	Yes

which is better?

Generator of the space group

File: **wycoff.data**





CONTINUED No. 227 $Fd\bar{3}m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates (0,0,0)+ $(0,\frac{1}{2},\frac{1}{2})$+ $(\frac{1}{2},0,\frac{1}{2})$+ $(\frac{1}{2},\frac{1}{2},0)$+	Reflection conditions
		h,k,l permutable
		General:
192 i 1	(1) x,y,z (2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$ (5) z,x,y (6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$ (7) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$ (8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$ (9) y,z,x (10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$ (11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$ (12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$ (13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$ (18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$ (19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$ (20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$ (21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$ (22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$ (23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$ (24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$ (25) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (27) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$ (29) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$ (30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$ (31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$ (32) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$ (33) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$ (34) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$ (35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$ (36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$ (37) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{1}{2}$ (38) y,x,z (39) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$ (41) $\bar{x}+\frac{1}{2},\bar{z},y+\frac{1}{2}$ (42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}$ (43) x,z,y (44) $\bar{x},z+\frac{1}{2},\bar{y}+\frac{1}{2}$ (45) $\bar{z}+\frac{1}{2},\bar{y},x+\frac{1}{2}$ (46) $\bar{z},y+\frac{1}{2},\bar{x}+\frac{1}{2}$ (47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}$ (48) z,y,x	
		Special: as above, plus
96 h ..2	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$ $\frac{3}{4},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2}$ $\frac{3}{4},y+\frac{1}{2},y+\frac{1}{2}$ $\frac{1}{4},\bar{y},y+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},y$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}+\frac{1}{2}$ $y+\frac{1}{2},\frac{3}{4},y+\frac{1}{2}$ $y+\frac{1}{2},\frac{1}{4},\bar{y}$ $y,\bar{y}+\frac{1}{2},\frac{1}{4}$ $\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{3}{4}$ $y+\frac{1}{2},y+\frac{1}{2},\frac{3}{4}$ $\bar{y},y+\frac{1}{2},\frac{1}{4}$ $\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\frac{3}{4},y+\frac{1}{2},y+\frac{1}{2}$ $\frac{3}{4},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2}$ $\frac{1}{4},y,y+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$ $y+\frac{1}{2},\frac{3}{4},y$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}+\frac{1}{2}$ $y+\frac{1}{2},\frac{1}{4},y+\frac{1}{2}$ $\bar{y},\frac{1}{4},\bar{y}+\frac{1}{2}$ $y,\bar{y}+\frac{1}{2},\frac{1}{4}$ $\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{3}{4}$ $y+\frac{1}{2},y+\frac{1}{2},\frac{3}{4}$ $\bar{y},y+\frac{1}{2},\frac{1}{4}$	no extra conditions
96 g ..m	x,x,z $\bar{x},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}$ $x+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$ z,x,x $z+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$ $\bar{z},\bar{x}+\frac{1}{2},x+\frac{1}{2}$ $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{x}$ x,z,x $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{x}$ $x+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$ $\bar{x},\bar{z}+\frac{1}{2},x+\frac{1}{2}$ $x+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ $x+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$ $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$ $x+\frac{1}{2},\bar{z},x+\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$ $z+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$ $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$ $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$ $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	no extra conditions
48 f 2..mm	$x,0,0$ $\bar{x},\frac{1}{2},\frac{1}{2}$ $0,x,0$ $\frac{1}{2},\bar{x},\frac{1}{2}$ $0,0,x$ $\frac{1}{2},\frac{1}{2},\bar{x}$ $\frac{1}{4},x,\frac{1}{4}$ $\frac{3}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$ $\frac{1}{4},x+\frac{1}{2},\frac{3}{4}$ $\frac{3}{4},\bar{x},\frac{3}{4}$ $\frac{1}{4},\frac{1}{4},x$ $\frac{3}{4},\frac{3}{4},\bar{x}+\frac{1}{2}$ $\frac{1}{4},\frac{3}{4},x+\frac{1}{2}$ $\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$	hkl : $h=2n+1$ or $h+k+l=4n$
32 e .3m	x,x,x $\bar{x},\bar{x}+\frac{1}{2},x+\frac{1}{2}$ $x+\frac{1}{2},x+\frac{1}{2},\bar{x}$ $\bar{x}+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	no extra conditions
16 d .$\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$	hkl : $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16 c .$\bar{3}m$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},\frac{5}{8}$ $\frac{1}{8},\frac{5}{8},\frac{1}{8}$ $\frac{5}{8},\frac{1}{8},\frac{1}{8}$	
8 b $\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$	hkl : $h=2n+1$ or $h+k+l=4n$
8 a $\bar{4}3m$	$0,0,0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	

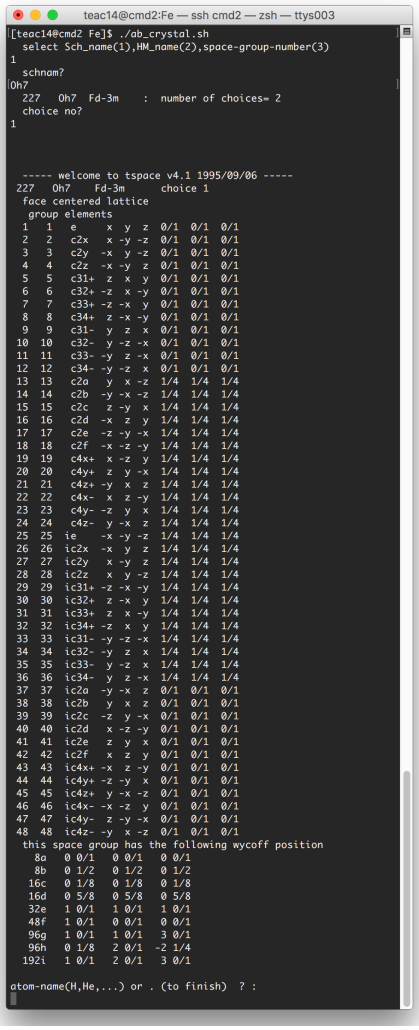
Symmetry of special projections

Along [001] $p4mm$ $\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$ Origin at $0,0,z$

Along [111] $p6mm$ $\mathbf{a}'=\frac{1}{2}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{2}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$ Origin at x,x,x

Along [110] $c2mm$ $\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$ Origin at $x,x,\frac{1}{4}$

International Table of Crystallography A



To make **ab_prp.data**, there is a tool, **ab_crystal.sh**.

Crystal Structure

NIMS database:

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

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