



2nd-6th September 2019

ABCAP: advanced course

ABCAP(All electron BAnd Calculation Package): FLAPW code

Noriaki Hamada, Tokyo University of Science, Osaka University
Hiroki Funashima, Kobe University

Purpose

- ① Study the symmetry of crystal and electronic structure (symmetry operations).
- ② Study the symmetry of wavefunction (irreducible representations).
- ③ Study the optical transition between valence and conduction bands (dipole allowed).
- ④ Calculate the optical absorption spectrum.
- ⑤ Treat magnetic materials.
- ⑥ Use the $+U$ method.

1-1. 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
```



```
ターミナル — ssh rl — zsh — ttys003
ssh rl
[teac14@r101]~-% cat /home/CMD/teac02/abcap1707/Envvs_sh >> ~/.bashrc
[teac14@r101]~-% source ~/.bashrc
```

```
#-----
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/
```



```
teac14@cmd2:~ — ssh cmd2 — zsh — ttys003
teac14@cmd2:~ — ssh cmd2
[teac14@cmd2 ~]$ cd ~
[teac14@cmd2 ~]$ mkdir abc
[teac14@cmd2 ~]$ cp $ABCAP/samples/Setnew.sh abc/
[teac14@cmd2 ~]$
```

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/**.

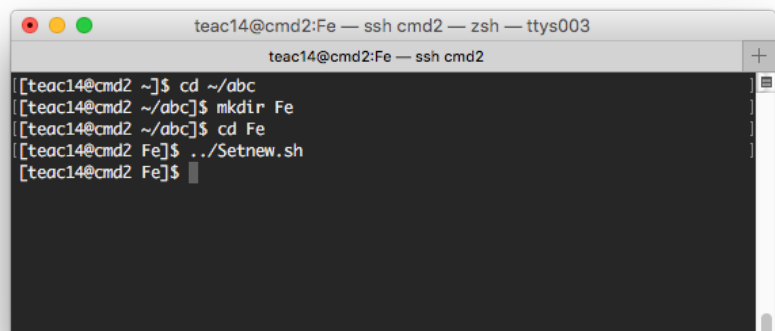
Hands on DFT simulation

- Ferromagnetic Fe
- Nonmagnetic Si

2-1. Ferromagnetic Fe

Prepare a directory for the calculation:

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



```
teac14@cmd2:Fe — ssh cmd2 — zsh — ttys003  
teac14@cmd2:Fe — ssh cmd2  
[teac14@cmd2 ~]$ cd ~/abc  
[teac14@cmd2 ~/abc]$ mkdir Fe  
[teac14@cmd2 ~/abc]$ cd Fe  
[teac14@cmd2 Fe]$ ../Setnew.sh  
[teac14@cmd2 Fe]$
```

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`

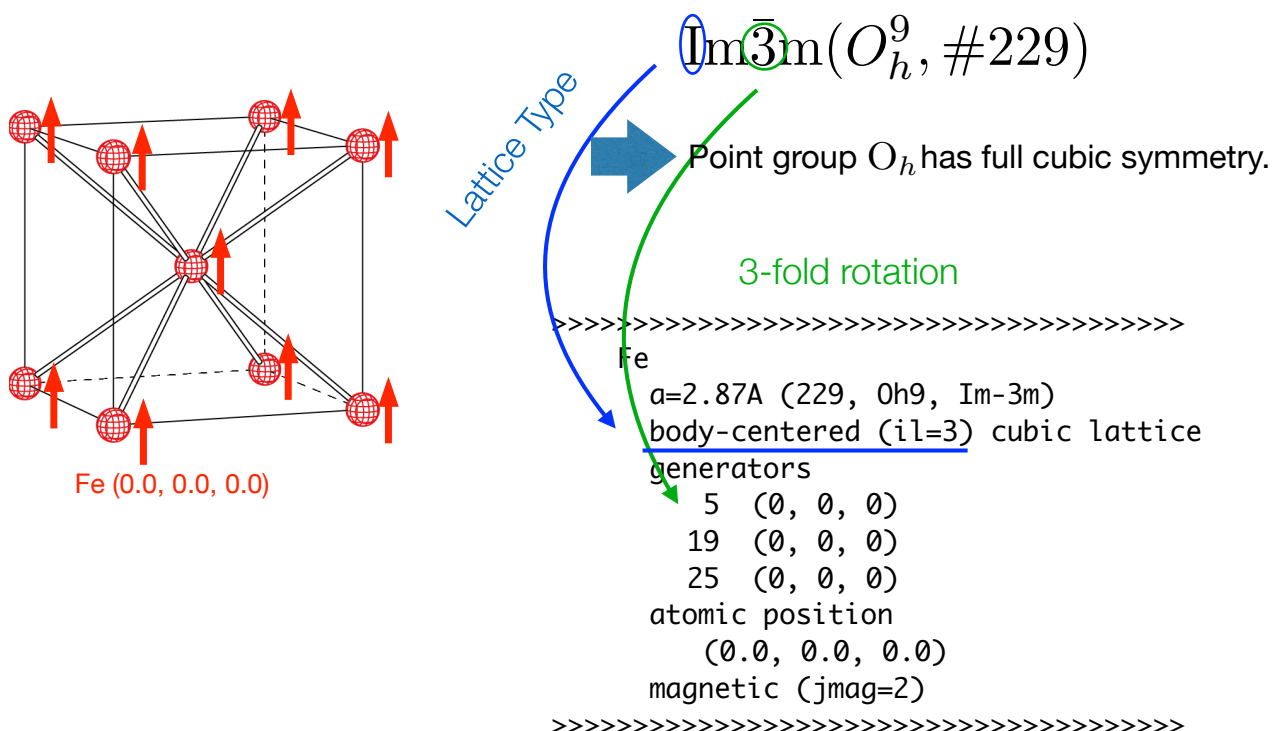
```

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) <noS0i> (bnpl.data)  bnpl.sh
<noS0i> (angle.data)  brzone.sh --> brzone.ps
<S0i> 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



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	Subgroup of O_h/D_{6h}
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	

symmetry Operation

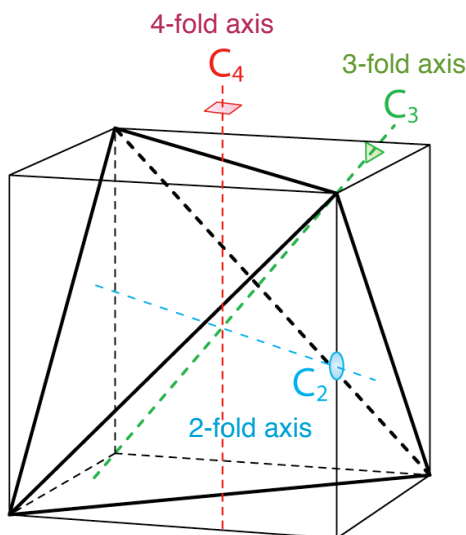
$$(\alpha|\vec{t} + \vec{u}_\alpha) = \alpha\vec{u} + \vec{t} + \vec{u}_\alpha$$

$$(\alpha|\vec{a})(\beta|\vec{b}) = (\alpha\beta|\alpha\vec{b} + \vec{a})$$

$$(\alpha|\vec{b})^{-1} = (\alpha^{-1}|\alpha^{-1}\vec{b})$$

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

Point Group: O_h



Cubic Symmetry O_h

$E \dots \dots 1$ identity operation

$C_4 \dots \dots 6$ $\pm\pi/2$

$C_4^2 \dots \dots 3$ $\pm\pi$

$C_2 \dots \dots 6$ $\pm\pi$

$C_3 \dots \dots 8$ $\pm 2\pi/3$

24 rotational operation

+ inversion, rotation inversion,
 reflection and rotational reflection

48 symmetry Operation

subgroup of O_h

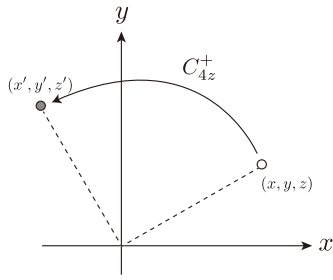
example

Tetrahedral Symmetry $\rightarrow T_d$

$$T_d \otimes C_4 = O_h$$

Rotational Operation

example: C_{4z}^+



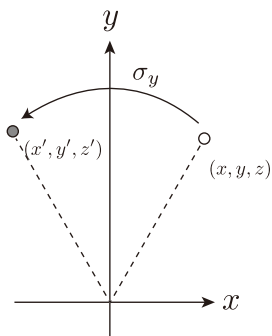
$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -y \\ x \\ z \end{bmatrix}$$

matrix representation of C_{4z}^+

C_{4z}^+	$(-y, x, z)$
------------	--------------

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}

IC_{2x}	$(-x, y, z)$
-----------	--------------

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

space inversion(I)

C_{2x}

x-axis is the normal direction of yz-plane

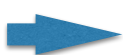
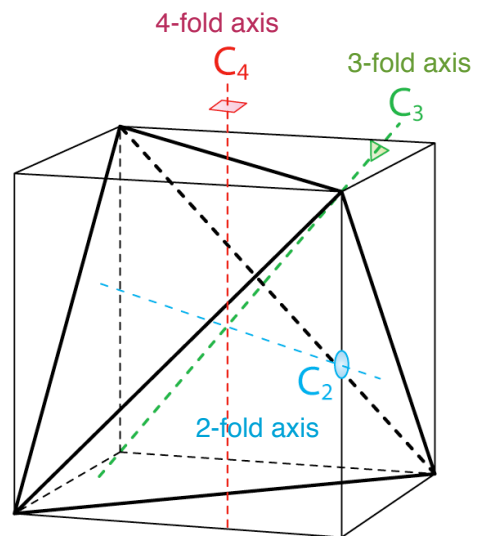
Generally speaking, reflectional operation is written as production between space inversion and 2-fold rotation, C_2

rotational operation code for O_h and subgroup in TSPACE

identity	(1) E	(x, y, z)
C_4^\pm	(2) C_{2x}	(x, -y, -z)
	(3) C_{2y}	(-x, y, -z)
	(4) C_{2z}	(-x, -y, z)
	(5) C_{31}^+	(z, x, y)
C_3^\pm	(6) C_{32}^+	(-z, x, -y)
	(7) C_{33}^+	(-z, -x, y)
	(8) C_{34}^+	(z, -x, -y)
	(9) C_{31}^-	(y, z, x)
	(10) C_{32}^-	(y, -z, -x)
	(11) C_{33}^-	(-y, z, -x)
C_2	(12) C_{34}^-	(-y, -z, x)
	(13) C_{2a}	(y, x, -z)
	(14) C_{2b}	(-y, -x, -z)
	(15) C_{2c}	(z, -y, x)
	(16) C_{2d}	(-x, z, y)
	(17) C_{2e}	(-z, -y, -x)
C_4^\pm	(18) C_{2f}	(-x, -z, -y)
	(19) C_{4x}^+	(x, -z, y)
	(20) C_{4y}^+	(z, y, -x)
	(21) C_{4z}^+	(-y, x, z)
	(22) C_{4x}^-	(x, z, -y)
	(23) C_{4y}^-	(-z, y, x)
	(24) C_{4z}^-	(y, -x, z)

(25) IE	(-x, -y, -z)
(26) IC_{2x}	(-x, y, z)
(27) IC_{2y}	(x, -y, z)
(28) IC_{2z}	(x, y, -z)
(29) IC_{31}^+	(-z, -x, -y)
(30) IC_{32}^+	(z, -x, y)
(31) IC_{33}^+	(z, x, -y)
(32) IC_{34}^+	(-z, x, y)
(33) IC_{31}^-	(-y, -z, -x)
(34) IC_{32}^-	(-y, z, x)
(35) IC_{33}^-	(y, -z, x)
(36) IC_{34}^-	(y, z, -x)
(37) IC_{2a}	(-y, -x, z)
(38) IC_{2b}	(y, x, z)
(39) IC_{2c}	(-z, y, -x)
(40) IC_{2d}	(x, -z, -y)
(41) IC_{2e}	(z, y, x)
(42) IC_{2f}	(x, z, y)
(43) IC_{4x}^+	(-x, z, -y)
(44) IC_{4y}^+	(-z, -y, x)
(45) IC_{4z}^+	(y, -x, -z)
(46) IC_{4x}^-	(-x, -z, y)
(47) IC_{4y}^-	(z, -y, -x)
(48) IC_{4z}^-	(-y, x, -z)

space inversion



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

production between group elements

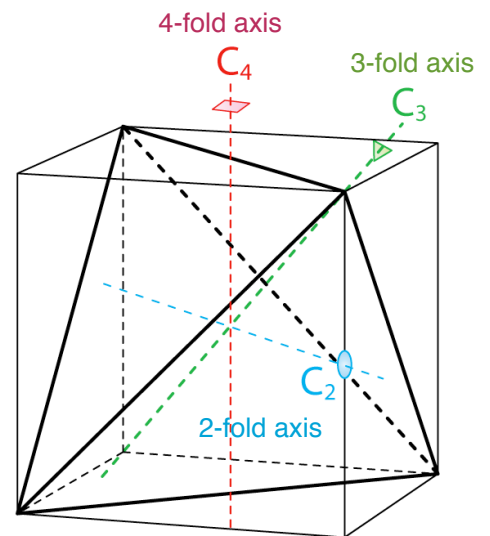
e.g. $C_{2b} \cdot C_{2x} = ?$

$$\begin{array}{l} (2) \quad C_{2x} \quad (x, -y, -z) \\ (14) \quad C_{2b} \quad (-y, -x, -z) \end{array}$$

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

rotational operation code for O_h and subgroup in TSPACE

identity	(1) E	(x, y, z)	(25) IE	(-x, -y, -z)	inversion
C_4^2	(2) C _{2x}	(x, -y, -z)	(26) IC _{2x}	(-x, y, z)	
	(3) C _{2y}	(-x, y, -z)	(27) IC _{2y}	(x, -y, z)	
	(4) C _{2z}	(-x, -y, z)	(28) IC _{2z}	(x, y, -z)	
	(5) C ₃₁₊	(z, x, y)	(29) IC ₃₁₊	(-z, -x, -y)	
C_3^\pm	(6) C ₃₂₊	(-z, x, -y)	(30) IC ₃₂₊	(z, -x, y)	
	(7) C ₃₃₊	(-z, -x, y)	(31) IC ₃₃₊	(z, x, -y)	
	(8) C ₃₄₊	(z, -x, -y)	(32) IC ₃₄₊	(-z, x, y)	
	(9) C ₃₁₋	(y, z, x)	(33) IC ₃₁₋	(-y, -z, -x)	
	(10) C ₃₂₋	(y, -z, -x)	(34) IC ₃₂₋	(-y, z, x)	
	(11) C ₃₃₋	(-y, z, -x)	(35) IC ₃₃₋	(y, -z, x)	
	(12) C ₃₄₋	(-y, -z, x)	(36) IC ₃₄₋	(y, z, -x)	
	C_2	(13) C _{2a}	(y, x, -z)	(37) IC _{2a}	(-y, -x, z)
(14) C _{2b}		(-y, -x, -z)	(38) IC _{2b}	(y, x, z)	
(15) C _{2c}		(z, -y, x)	(39) IC _{2c}	(-z, y, -x)	
(16) C _{2d}		(-x, z, y)	(40) IC _{2d}	(x, -z, -y)	
(17) C _{2e}		(-z, -y, -x)	(41) IC _{2e}	(z, y, x)	
(18) C _{2f}		(-x, -z, -y)	(42) IC _{2f}	(x, z, y)	
C_4^\pm	(19) C _{4x+}	(x, -z, y)	(43) IC _{4x+}	(-x, z, -y)	
	(20) C _{4y+}	(z, y, -x)	(44) IC _{4y+}	(-z, -y, x)	
	(21) C _{4z+}	(-y, x, z)	(45) IC _{4z+}	(y, -x, -z)	
	(22) C _{4x-}	(x, z, -y)	(46) IC _{4x-}	(-x, -z, y)	
	(23) C _{4y-}	(-z, y, x)	(47) IC _{4y-}	(z, -y, -x)	
	(24) C _{4z-}	(y, -x, z)	(48) IC _{4z-}	(-y, x, -z)	



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	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

```
abcap-ab_prp.data
0
!jpr
Fe body centered cubic ferromag.
lattice parameter -2---*---3---*---4---*---5---*---6---*---7
2.87 2.87 2.87 90.0 90.0 90.0 !a,b,c[A], alpha,beta,gamma[degree]
space group -2---*---3---*---4---*---5---*---6---*---7
3 3 3 1 !ldim, 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 Fe !jpos,position,name
magnetic state -2---*---3---*---4---*---5---*---6---*---7
2 !jmag0 !noS0:(0(N),1(AF),2(M)), S0:(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
6 6 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 1/23: 17
"ab_prp.data" [converted] 23L, 1490C
```

1. Crystal Structure

```
[teac14@cmd2 Fe]$ Hqc
-----
(0) (ab_prp.data, atom.data) ab_prp.qc ←
```

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.

```
teac14@cmd2:Fe — ssh cmd2 — zsh — ttys003
teac14@cmd2:Fe — ssh cmd2
[teac14@cmd2 Fe]$ ab_prp.qsub
rm: cannot remove `ab_prp.e*': No such file or directory
rm: cannot remove `ab_prp.o*': No such file or directory
Your job 138846 ("ab_prp.sh") has been submitted
[teac14@cmd2 Fe]$
```

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...

```
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
```

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)

```
teac14@cmd2:Fe — ssh cmd2 — zsh — ttys003
teac14@cmd2:Fe — ssh cmd2
[teac14@cmd2 Fe]$ ab_in.qsub
rm: cannot remove `ab_in.e*': No such file or directory
rm: cannot remove `ab_in.o*': No such file or directory
Your job 138847 ("ab_in.sh") has been submitted
[teac14@cmd2 Fe]$
```

3. Self-Consistent Field(SCF) Calculation

```
teac14@cmd2:Fe — ssh cmd2 — zsh — ttys003
-----
(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
```

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

contents of "*fl06.sh*"

```
fl06.csh (~/.abc/Fe) - VIM — ssh cmd2 — zsh — ttys003
#!/bin/csh -f
#PBS -q PCC
#PBS -l cpunum_job=1,elapstim_req=6:00:00,memsz_job=900MB
#PBS -o fl06.out
#PBS -e fl06.err
if($?PBS_0_WORKDIR) then
  cd $PBS_0_WORKDIR
endif

#=====
set ITER_MAIN = 8
set ITER_PLUS = 1
#=====
echo $PWD

date                >>& iter.log
echo $HOSTNAME      >>& Current
date                >>& Current
echo =====      >>& Current

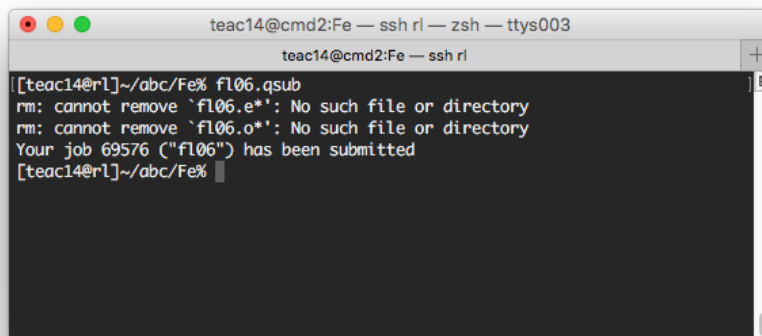
unlimit datasize
rm -f f_energy.dta
$ABCAP/bin/jmag0.exe
set JMAG0=`cat jmag0.dta`
set JMAG00=`expr $JMAG0 / 10`
echo `jmag0=$JMAG0

NORMAL fl06.csh          unix iso-2022-jp tcsh      8/138: 5
```

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

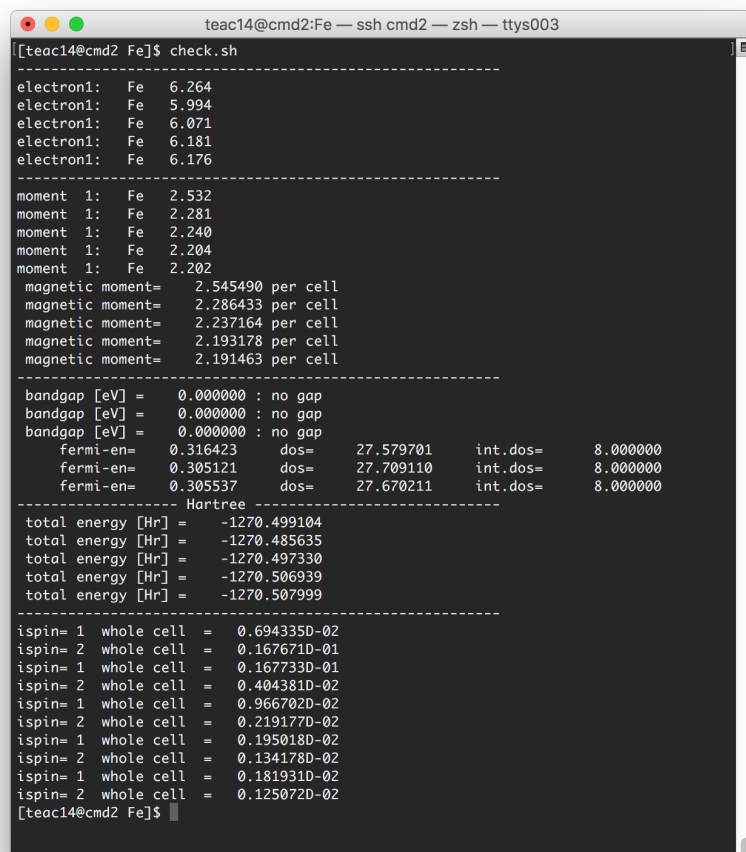
- **fl_pot.exe**: makes the potential from the charge density.
- **fl_potuj.exe**: makes the $+U$ potential from the local density matrix.
- **fl_bnd.exe**: calculates eigen functions through a standard diagonalization.
- **fl_chg.exe**: determines the Fermi energy and calculate the charge density from 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 $\text{lda}+u > 0$.



```
teac14@cmd2:Fe — ssh rl — zsh — ttys003
teac14@cmd2:Fe — ssh rl
[teac14@rl]~/abc/Fe% fl06.qsub
rm: cannot remove `fl06.e*': No such file or directory
rm: cannot remove `fl06.o*': No such file or directory
Your job 69576 ("fl06") has been submitted
[teac14@rl]~/abc/Fe%
```

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**

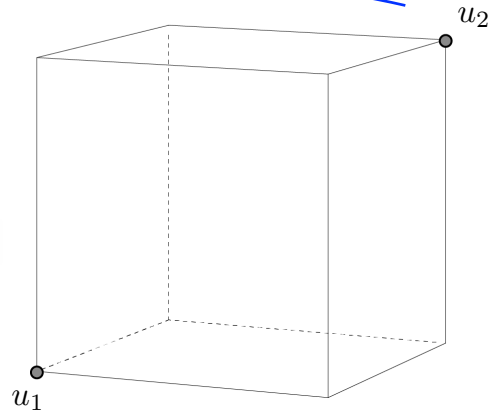


```
teac14@cmd2:Fe — ssh cmd2 — zsh — ttys003
[teac14@cmd2 Fe]$ check.sh
-----
electron1: Fe 6.264
electron1: Fe 5.994
electron1: Fe 6.071
electron1: Fe 6.181
electron1: Fe 6.176
-----
moment 1: Fe 2.532
moment 1: Fe 2.281
moment 1: Fe 2.240
moment 1: Fe 2.204
moment 1: Fe 2.202
magnetic moment= 2.545490 per cell
magnetic moment= 2.286433 per cell
magnetic moment= 2.237164 per cell
magnetic moment= 2.193178 per cell
magnetic moment= 2.191463 per cell
-----
bandgap [eV] = 0.000000 : no gap
bandgap [eV] = 0.000000 : no gap
bandgap [eV] = 0.000000 : no gap
fermi-en= 0.316423 dos= 27.579701 int.dos= 8.000000
fermi-en= 0.305121 dos= 27.709110 int.dos= 8.000000
fermi-en= 0.305537 dos= 27.670211 int.dos= 8.000000
-----
Hartree
total energy [Hr] = -1270.499104
total energy [Hr] = -1270.485635
total energy [Hr] = -1270.497330
total energy [Hr] = -1270.506939
total energy [Hr] = -1270.507999
-----
ispin= 1 whole cell = 0.694335D-02
ispin= 2 whole cell = 0.167671D-01
ispin= 1 whole cell = 0.167733D-01
ispin= 2 whole cell = 0.404381D-02
ispin= 1 whole cell = 0.966702D-02
ispin= 2 whole cell = 0.219177D-02
ispin= 1 whole cell = 0.195018D-02
ispin= 2 whole cell = 0.134178D-02
ispin= 1 whole cell = 0.181931D-02
ispin= 2 whole cell = 0.125072D-02
[teac14@cmd2 Fe]$
```

4-1. Drawing the Crystal Structure

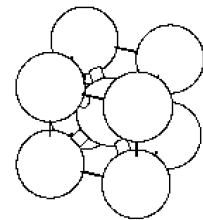
- ① Edit **bn_atps.data**. Give the region of drawing in the file.
- ② Run **bn_atps.sh** and **p3_atps.sh**.
- ③ A postscript file, **plot.ps**, is obtained.

```
bn_atps.data (~/.abc/Fe) - VIM — ssh cmd2 — zsh — ttys003
1      jdata
0.0 0.0 0.0 1.0 1.0 1.0 u1(3),u2(3)
~
~
NORMAL bn_atps.data          unix iso-2022-jp no 1/2: 1
```



```
teac14@cmd2:Fe — ssh cmd2 — zsh — ttys003
[teac14@cmd2 Fe]$ ./bn_atps.sh
=bn_atps=
[teac14@cmd2 Fe]$ p3_atps.sh
=p3_atps=
[teac14@cmd2 Fe]$
```

```
teac14@cmd2:Fe — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 Fe]$ gs plot.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.
>>showpage, press <return> to continue<<
```



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

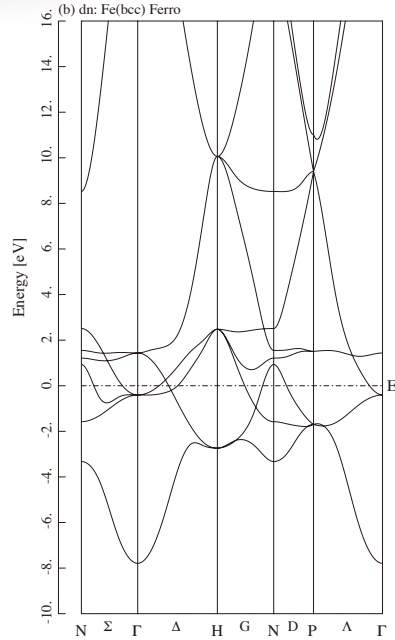
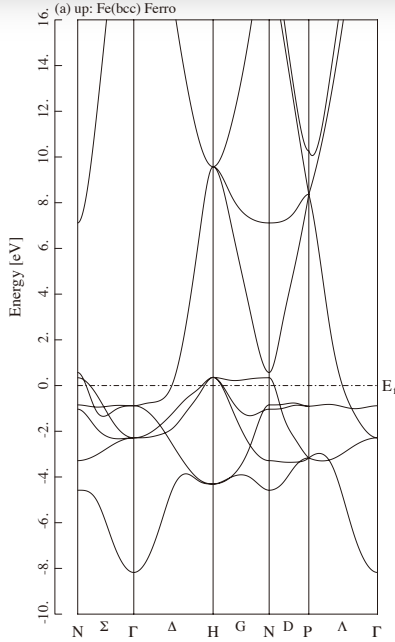
- ① Edit **bnpl.data** and **a_bnpl.data**. Give paths in the k-space to be drawn.
- ② Run **bnpl.sh**.
- ③ **plot.ps** is obtained for the nonmagnetic case ($j_{\text{mag}}=0$) or the antiferromagnetic case ($j_{\text{mag}}=1$); **plot1.ps** and **plot2.ps** are obtained for the magnetic case ($j_{\text{mag}}=2$).

```
bnpl.data + (~/.abc/Fe) - VIM — ssh -X cmd2 — zsh — ttys003
abcap-bnpl.data
6 0          nlcomponent(6), nspin(0,3)
3 0          jpr, jmark(0,1: irrep.off,on)
30.0 10.0    xscale(mm/unit), yscale(mm/unit)
-10.0 16.0 2.0 emin, emax, ed
-1          # of axes
bcc
Fe(bcc) Ferro
-----
-1          # of axes
sc
bcc
fcc
h
4          # of axes
1 1 0 2     1 1 1 2     M R
1 1 1 2     0 0 0 1     R gamma
0 0 0 1     1 0 0 2     gamma X
NORMAL bnpl.data +          unix iso-2022-jp no 5/22: 3
```

```
a_bnpl.data (~/.abc/Fe) - VIM — ssh -X cmd2 — zsh — ttys003
@bcap-a_bnpl.data
sc          crystal structure (simple cubic)
5          # of axes
1 1 0 2     1 1 1 2     M R
1 1 1 2     0 0 0 1     R gamma
0 0 0 1     1 0 0 2     gamma X
1 0 0 2     1 1 0 2     X M
1 1 0 2     0 0 0 1     M gamma
fcc          crystal structure (face-centered cubic)
6          # of axes
1 1 0 1     3 3 0 4     X K
3 3 0 4     0 0 0 1     K gamma
0 0 0 1     1 0 0 1     gamma X
1 0 0 1     2 1 0 2     X W
2 1 0 2     1 1 1 2     W L
1 1 1 2     0 0 0 1     L gamma
bcc          crystal structure (body-centered cubic)
5          # of axes
1 1 0 2     0 0 0 1     N gamma
0 0 0 1     1 0 0 1     gamma H
1 0 0 1     1 1 0 2     H N
1 1 0 2     1 1 1 2     N P
1 1 1 2     0 0 0 1     P gamma
r          crystal structure (rhombohedral)
4          # of axes
0 0 3 2     0 0 0 1     Z gamma
0 0 0 1     1 1 0 2     gamma F
1 1 0 2     1 1 3 2     F L
NORMAL a_bnpl.data          unix iso-2022-jp no 1/161: 1
```

```
teac14@cmd2:Fe — ssh -X cmd2 — zsh — ttys003
[[teac14@cmd2 Fe]$ bnp1.sh
=reform_h=
=bnpl =
[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 d
etails.
Can't find (or can't open) font file /usr/share/ghostscript/8.7
0/Resource/Font/NimbusRomNo9L-Regu.
Can't find (or can't open) font file NimbusRomNo9L-Regu.
Can't find (or can't open) font file /usr/share/ghostscript/8.7
0/Resource/Font/NimbusRomNo9L-Regu.
```

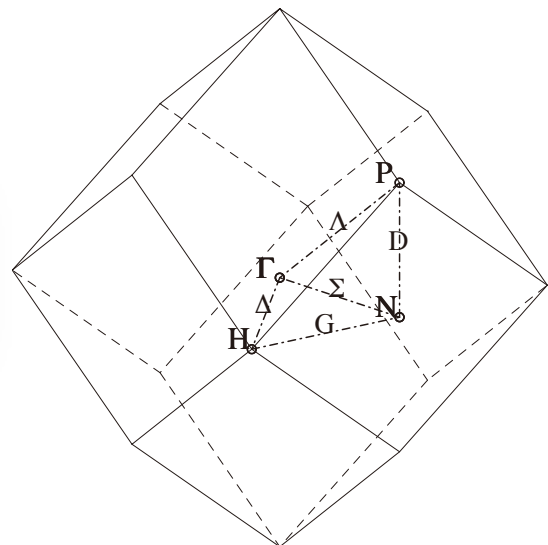


4-2. Drawing the k-space path and BZ

- ① Run **brzone.sh**.
- ② **brzone.ps** is obtained, which shows the k-space path in the e-k curve.

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

```
teac14@cmd2:Fe — ssh -X cmd2 — zsh — ttys003
[[teac14@cmd2 Fe]$ gs brzone.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 d
etails.
```



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 ($jmag=2$).

```
bn_pdos.data + (~/abc/Fe) - VIM — ssh -X cmd2 — zsh — ttys003
0      jpr
1000   # mesh
-10.0 20.0 energy range (eV relative to Ef)
1      500 neig1,neig2
```

calculate DOS

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

```
p2_dos.data (~/cmd35/abc/Fe) - VIM — ssh -Y rl — zsh — ttys004
0      0      jpr, kpaper
10     atomic sphere choice (00:mts, 10:as1)
1      iscale(1): not used now
2      2      ifermi(1,2), iconv(0:Hr, 2:Hr-eV)
-8.0   6.0   2.0   emin,emax,de (eV)
8.0    2.0    dmax,dd
8.0    5.0    (scale) xe, yd (mm/u, mm/u)
0      104    ncurve,jtype(1,4,16)
total  1 0 0 0.0 nl, (kind(j),l(j), j=1,nl), dmax1
Fe-3d  1 1 2 6.0 nl, (kind(j),l(j), j=1,nl), dmax1
Fe-4s  1 1 0 6.0 nl, (kind(j),l(j), j=1,nl), dmax1
-----
s:l=0, p:l=1, d:l=2, d:l=3
-----
~
NORMAL p2_dos.data unix iso-2022-jp no 11/18: 18
"p2_dos.data" [converted] 18L, 784C
```

number of curves

number of components

index for kind of atom
Azimuthal quantum number

$$\begin{matrix} 1 & 2 \\ \left. \begin{matrix} l=0 & (s) \\ l=1 & (p) \\ l=2 & (d) \\ l=3 & (f) \end{matrix} \right\} \end{matrix}$$

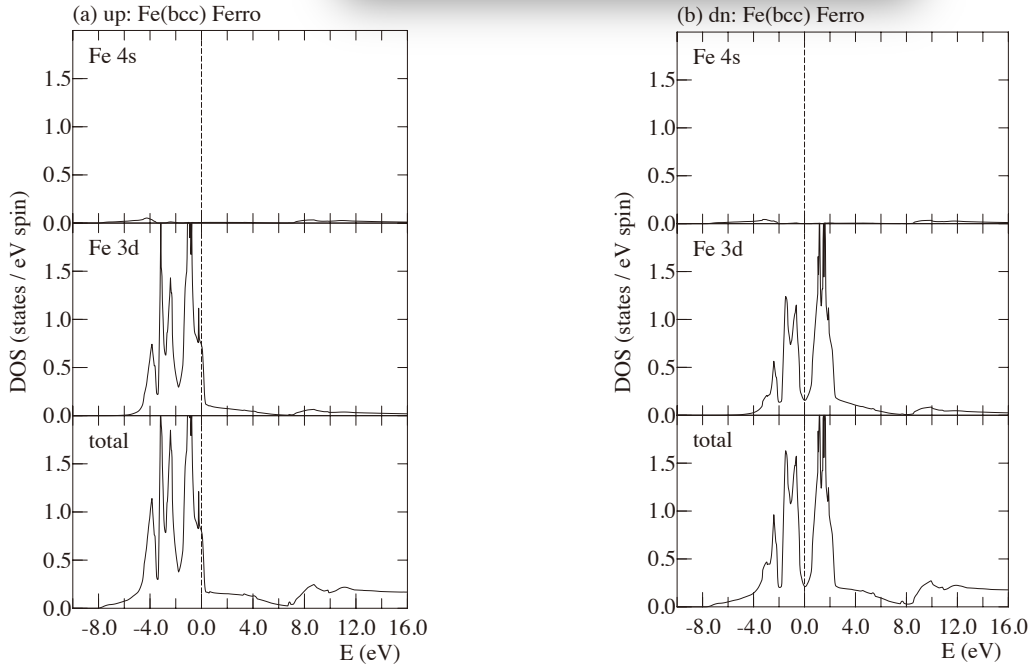
ref.)

```
p2_dos.data (~/abc/Fe.org) - VIM — ssh -X cmd2 — zsh — ttys003
0      0      jpr, kpaper
0      nspin(0)
1      iscale(0,1)
2      2      ifermi(1,2), iconv(0:Hr, 2:Hr-eV)
-8.0   6.0   2.0   emin,emax,de (eV)
7.0    2.0    dmax,dd
8.0    5.0    (scale) xe, yd (mm/u, mm/u)
LaMnO5d3
4      4      ncurve,jtype(1,4,16)
total  1 0 0 0.0 nl, (kind(j),l(j), j=1,nl)
La 4f+5d 2 1 3 1 2 nl, (kind(j),l(j), j=1,nl)
Mn 3d 1 2 2 nl, (kind(j),l(j), j=1,nl)
0 2p 1 3 1 nl, (kind(j),l(j), j=1,nl)
-----
s:l=0, p:l=1, d:l=2, d:l=3
-----
LaMnO5d3
4      1      ncurve,jtype(1,4,16)
total  1 0 0 0.0 nl, (kind(j),l(j), j=1,nl)
NORMAL p2_dos.data unix iso-2022-jp no 1/66: 1
"../Fe.org/p2_dos.data" [converted] 66L, 2200C
```

drawing DOS curves

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

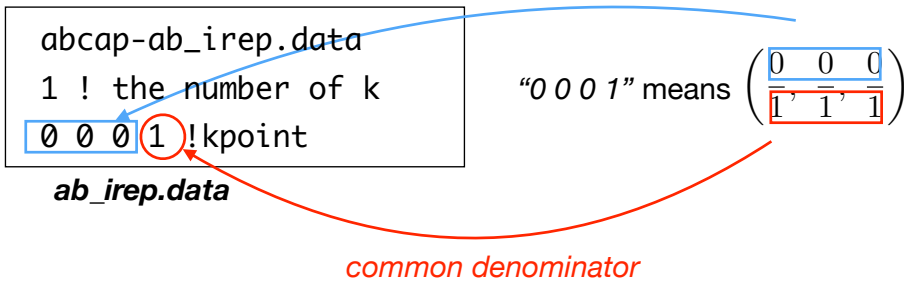
[teac14@cmd2:Fe — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 Fe]$ gs plot1.ps
GPL Ghostscript 8.70 (2009-07-31)
Copyright (C) 2009 Artifex Software, Inc. All rights reserved.
This software comes with NO WARRANTY: see the file PUBLIC for details.
Can't find (or can't open) font file /usr/share/ghostscript/8.70/Resource/Font/NimbusRomNo9L-Regu.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



4. The *k* group

1. irreducible representation for *k* group

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



(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
     -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
--- irreducible decomposition of Jones faithful rep.---
irrep= 6 : ndim= 3
-----
```

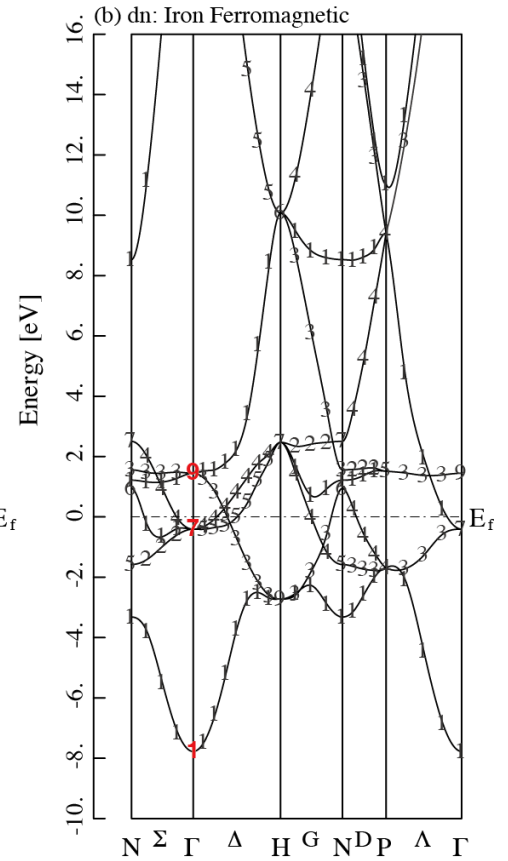
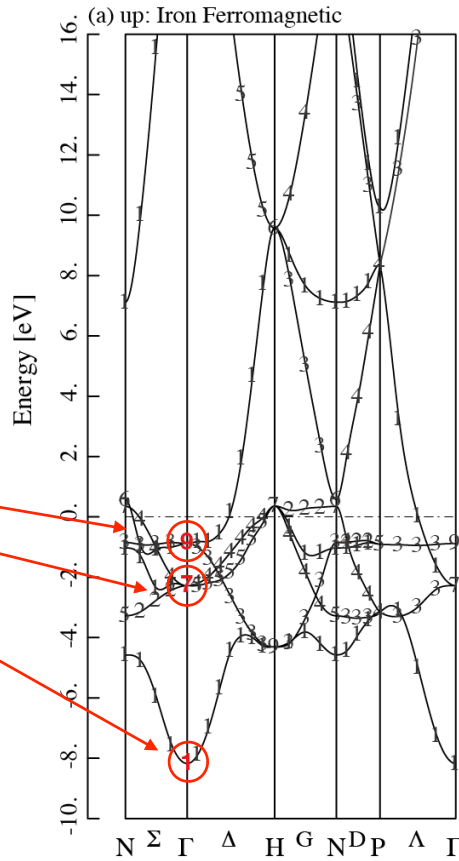
character of irreducible representation (case:Fe)

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)

IMR NO **1** DIMENSION= 1

MATRIX REPRESENTATION

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 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 1 + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
```

IMR NO **7** DIMENSION= 3

MATRIX REPRESENTATION

7

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

IMR NO **9** DIMENSION= 2

MATRIX REPRESENTATION

9

```
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 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 1 + + + + V V V V W W W W 0 0 0 0 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 0 0 + + V W V W W V + W V + 0 0 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 0 0 + + W V W V V W + V W + 0 0 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 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 “ $\exp\left(\frac{2\pi i}{3}\right)$ ”
 “W” indicates “ $\exp\left(\frac{4\pi i}{3}\right)$ ” 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) (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) (0.00 0.00) (0.00 0.00)

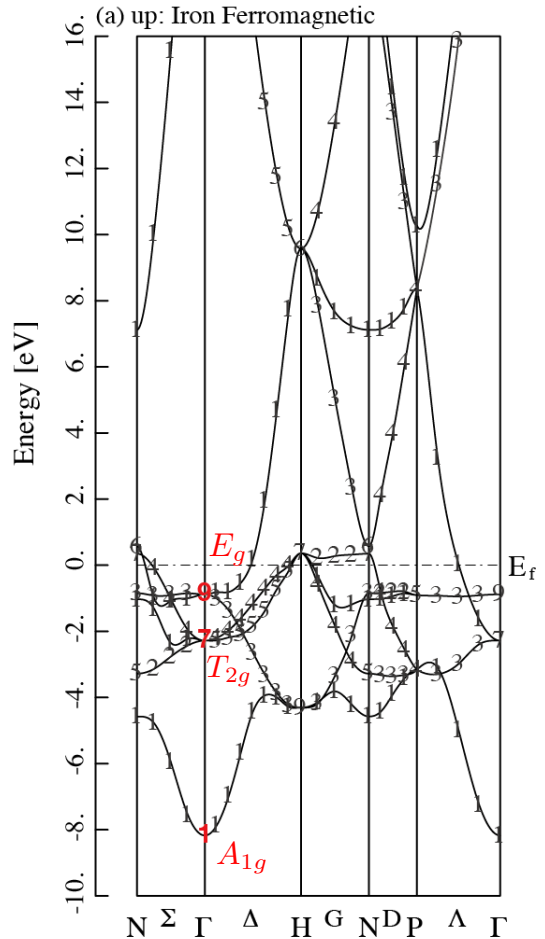
1. 立方晶系の点群

O_h	E	$6C_4$	$3C_2^2, 6C_2'$	$8C_3$	I	$6IC_4$	$3\sigma_h, 6\sigma_d$	$8IC_3$	Γ, R, H	
$A_{1g} \Gamma_1^+$	1	1	1	1	1	1	1	1	Γ_1	
$A_{2g} \Gamma_2^+$	1	-1	1	-1	1	-1	1	-1	Γ_2	
$E_g \Gamma_3^+$	2	0	2	0	-1	2	0	-1	Γ_{12}	
$T_{1g} \Gamma_4^+$	3	1	-1	-1	0	3	1	-1	Γ_{15}^+	
$T_{2g} \Gamma_5^+$	3	-1	-1	1	0	3	-1	1	Γ_{25}^+	
$A_{1u} \Gamma_1^-$	1	1	1	1	-1	-1	-1	-1	Γ_1^-	
$A_{2u} \Gamma_2^-$	1	-1	1	-1	-1	1	-1	1	Γ_2^-	
$E_u \Gamma_3^-$	2	0	2	0	-1	-2	0	-2	Γ_{12}^-	
$T_{1u} \Gamma_4^-$	3	1	-1	-1	0	-3	1	1	Γ_{15}^-	
$T_{2u} \Gamma_5^-$	3	-1	-1	1	0	-3	1	-1	Γ_{25}^-	
$E_{1/2g} \Gamma_6^+$	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	1	-1	Γ_6^+	
$E_{3/2g} \Gamma_7^+$	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	1	-1	Γ_7^+	
$G_{3/2g} \Gamma_8^+$	4	-4	0	0	0	-1	1	4	-4	Γ_8^+
$E_{1/2u} \Gamma_6^-$	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	1	-1	Γ_6^-	
$E_{3/2u} \Gamma_7^-$	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	1	-1	Γ_7^-	
$G_{3/2u} \Gamma_8^-$	4	-4	0	0	0	-1	1	4	-4	Γ_8^-

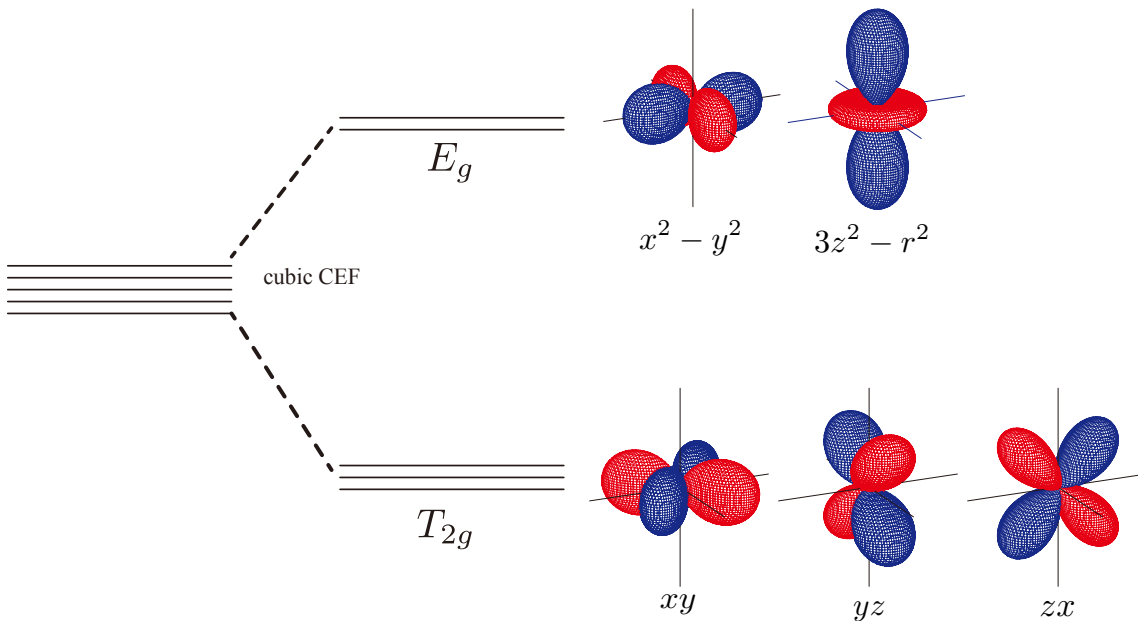
- A_{1g} : $r^2, x^4 + y^4 + z^4 - \frac{3}{5}r^4$ **1**
 A_{2g} : $x^4(y^2 - z^2) + y^4(z^2 - x^2) + z^4(x^2 - y^2)$
 E_g : $\{u, v\}, u \equiv 2z^2 - x^2 - y^2, v \equiv \sqrt{3}(x^2 - y^2)$
 T_{1g} : $\{yz, yz - x^2, zx(x^2 - x^2), xy(x^2 - y^2)\}$
 T_{2g} : $\{xy, zx, xy\}$ **7**
 Γ_6^+ : $\{\alpha, \beta\}$
 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^- : $\{xyza, xyz\beta\}$
 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).

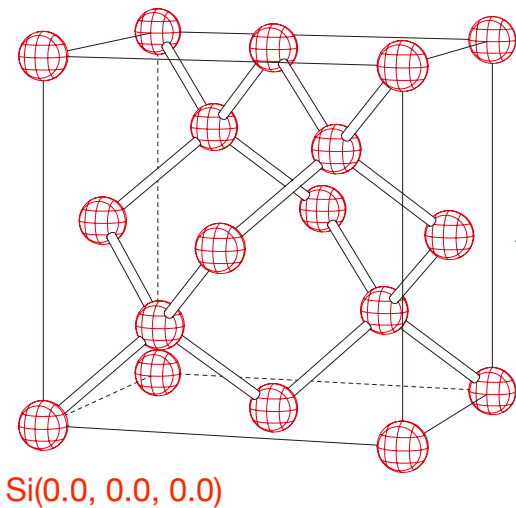
$$\begin{cases} E_g : d\gamma(x^2 - y^2, 3z^2 - r^2) \\ T_{2g} : d\varepsilon(xy, yz, zx) \\ A_{1g} : s \end{cases}$$



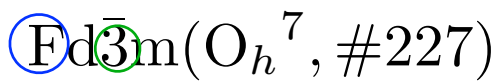
Cubic Crystal Electric Field(CEF) for 3d



2-2. Si



Diamond Structure



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 >>>>>>>>>
    
```

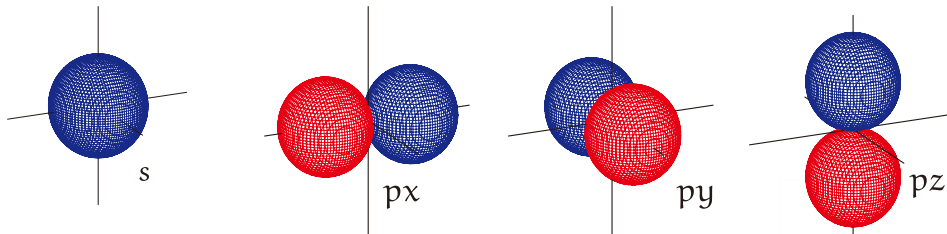
Symmetry operation for Si

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

rotation
translation

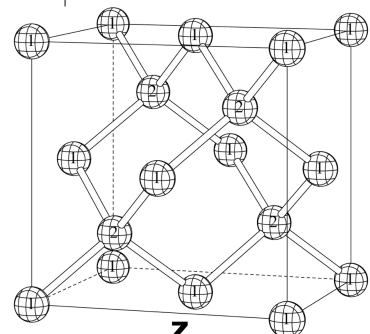
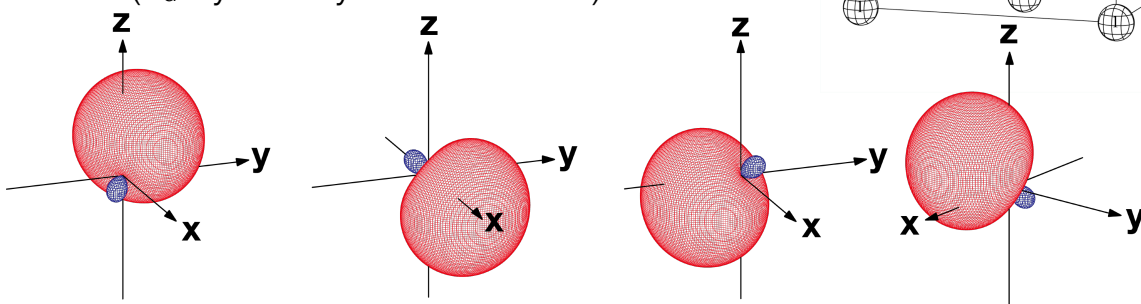
result of "ab_in.log"

sp³ basis function

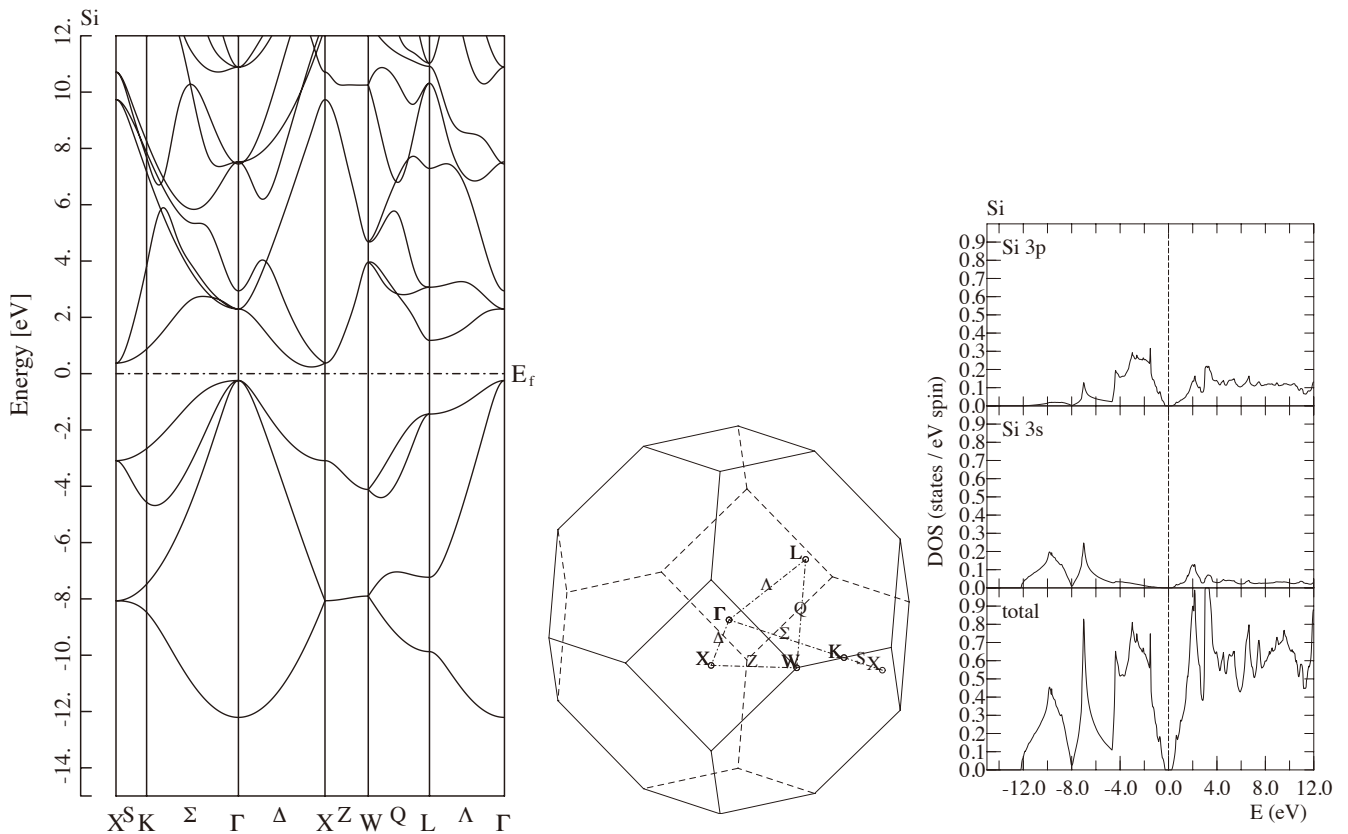


$$\begin{cases}
 |h_1\rangle = \frac{1}{2} \{|s\rangle + |p_x\rangle + |p_y\rangle + |p_z\rangle\} & [111] \\
 |h_2\rangle = \frac{1}{2} \{|s\rangle + |p_x\rangle - |p_y\rangle - |p_z\rangle\} & [1\bar{1}\bar{1}] \\
 |h_3\rangle = \frac{1}{2} \{|s\rangle - |p_x\rangle + |p_y\rangle - |p_z\rangle\} &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

(T_d-Symmetry basis function)



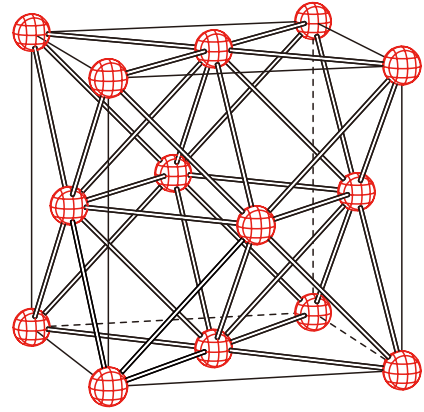
Electronic structure of Silicon



Magnetic states and LDA +U

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

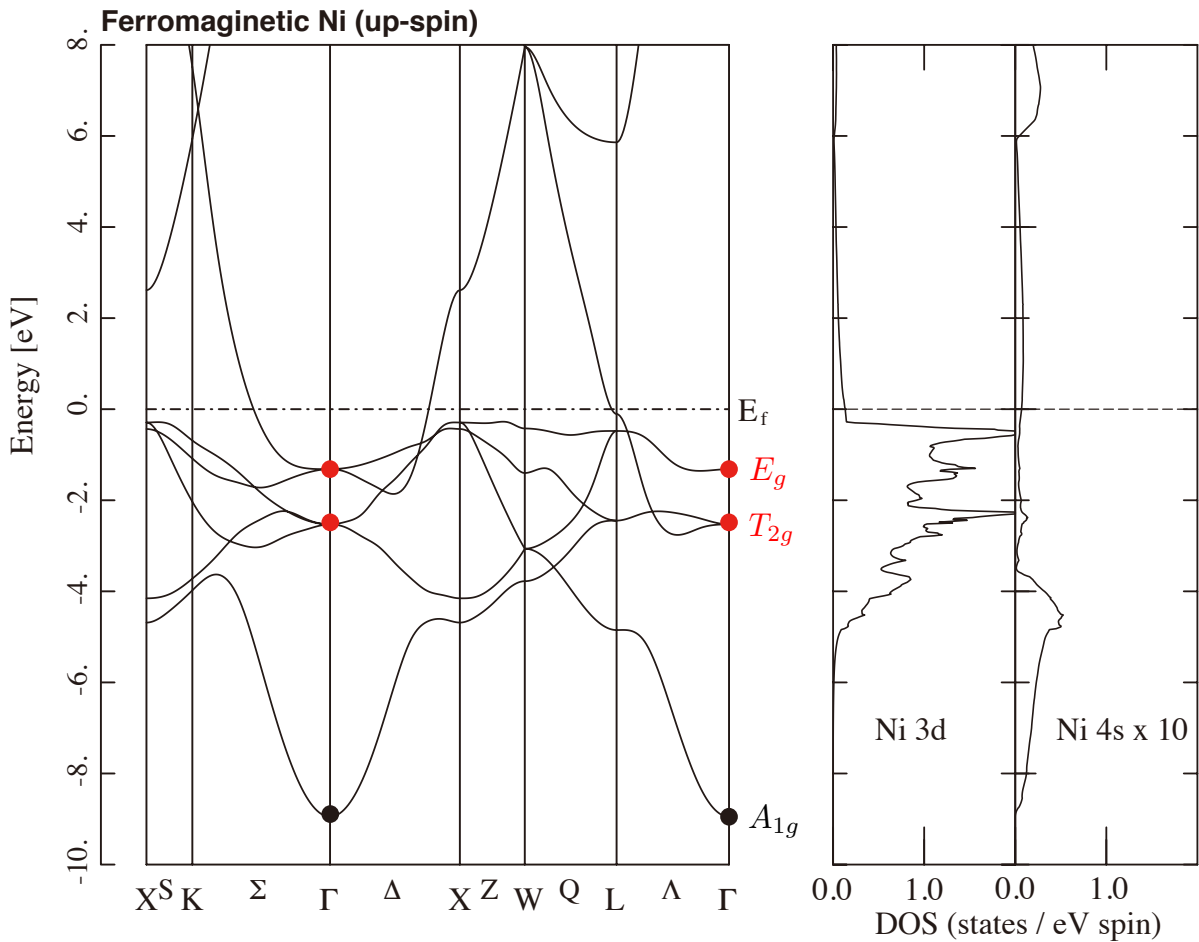
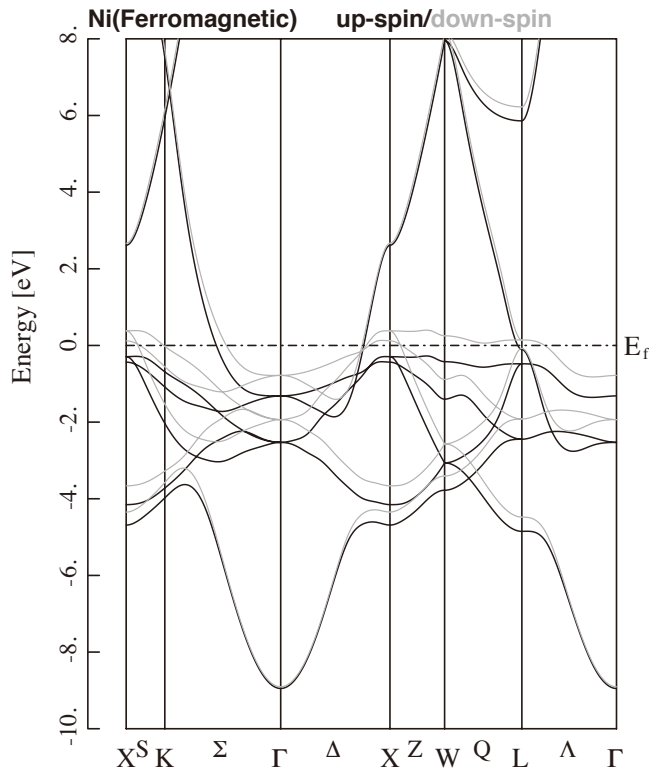
Ref: Ni



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

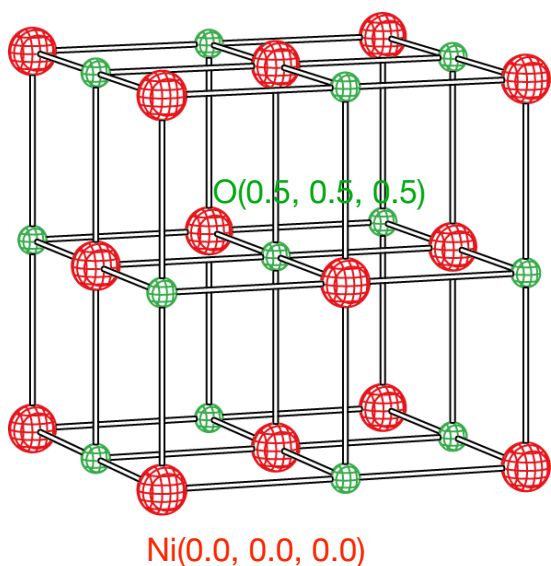
```

>>>>>>> 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

```

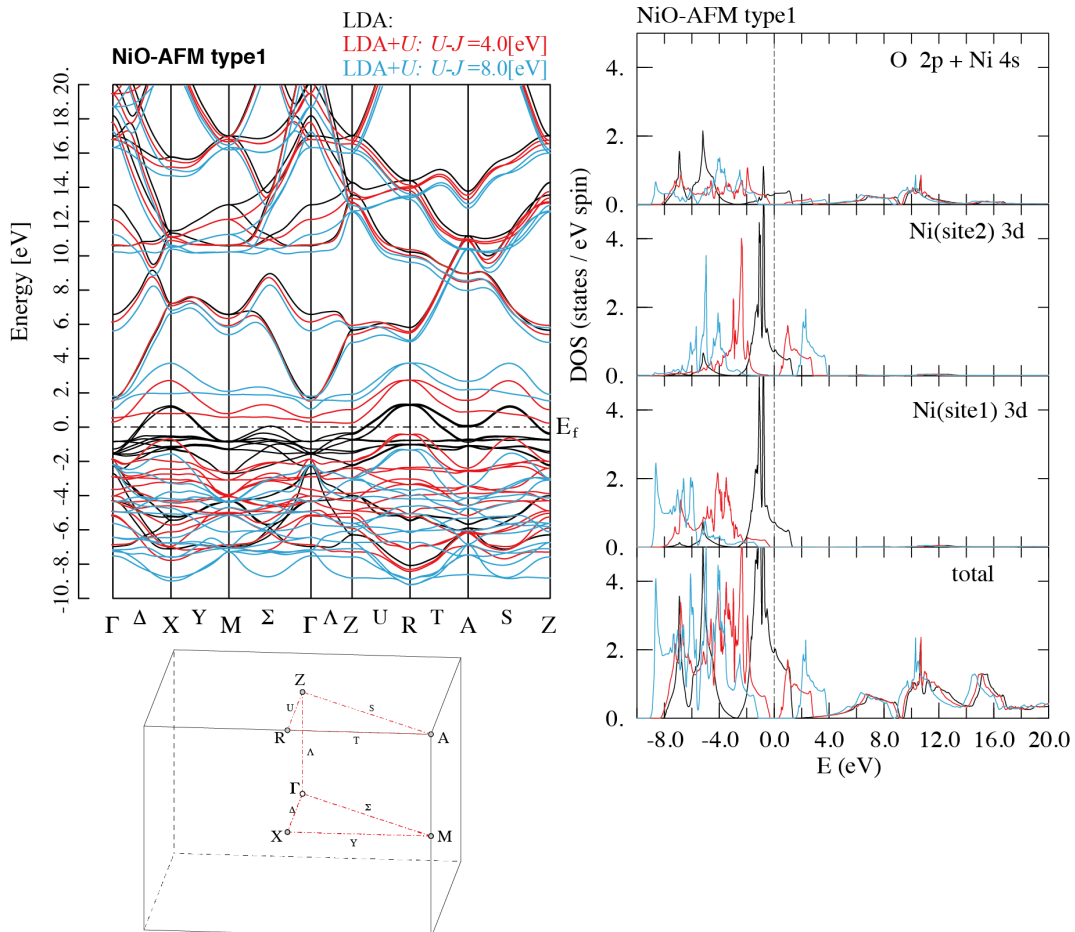
abcap-ab_prp.data
0
!jpr
NiO Ferromagnetic
Lattice parameter -2---*---3---*---4---*---5---*---6---*---7
4.17 4.17 4.17 90.0 90.0 90.0 !a,b,c[A], alpha,beta,gamma[degree]
space group -2---*---3---*---4---*---5---*---6---*---7
3 2 3 0 !idim, il(-1(r),0(h),1(s),2(f),3(b),4(c),5(a),6(b)),ngen,inv(0))
5 0 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))
!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
    
```


"ab_prp.data" for NiO-AFM type1

```

abcap-ab_prp.data
0
NiO-antiferro type1
lattice parameter 2.948635 2.948635 4.17 90.0 90.0 90.0 !a,b,c[A], alpha,beta,gamma[degree]
space group 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 4
1 0.0 0.0 0.0 Ni !# of kinds
1 0.5 0.5 0.5 Ni ! Ni up-spin
1 0.5 0.5 0.0 0 ! Ni down-spin
1 0.0 0.0 0.5 0 !
magnetic state 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 24.0 6 !cut-off energy[Hr],Lmax
k-points (# of division) 12 12 8
iteration 4 6 0.05 0.05 !method, n-method, pmix, amix
!
NORMAL ab_prp.data

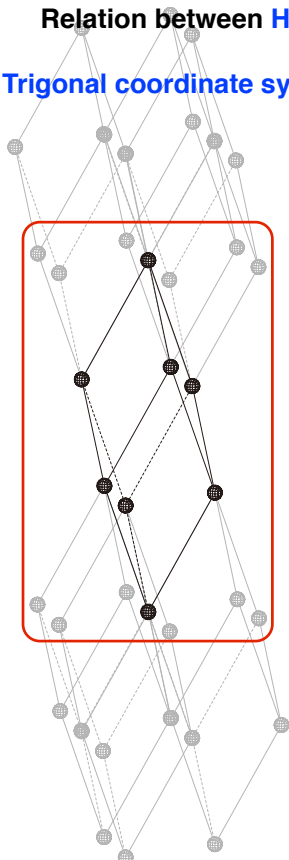
```



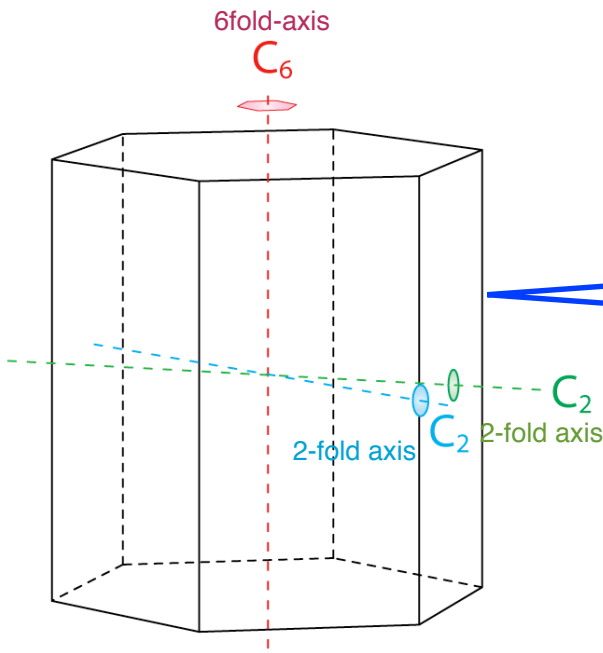
“ab_prp.data” for NiO-AFM type2

```
abcap-ab_prp.data
0
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 !ldim, 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 0 !
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 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}

$E \dots\dots 1$ identity operation

$C_6 \dots\dots 2 \quad \pm\pi/3$

$C_6^2 \dots\dots 2 \quad \pm 2\pi/3$

$C_6^3 \dots\dots 1 \quad \pm\pi$

$C_2' \dots\dots 3 \quad \pm\pi$

$C_2'' \dots\dots 3 \quad \pm\pi$

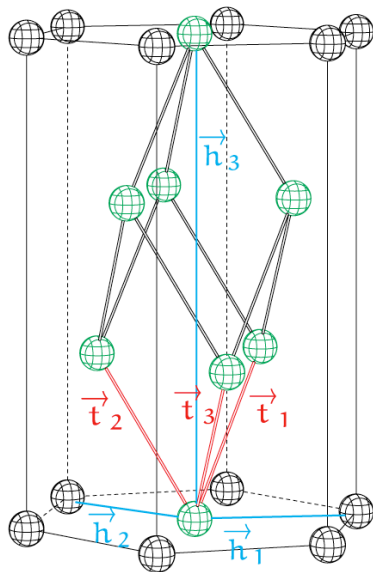
12 rotational operation
+ inversion, rotation inversion,
reflection and rotational reflection

24 symmetry operation

subgroup of D_{6h}

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

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



transformation basis

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

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

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

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

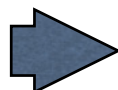
$$\vec{h}_2 = \vec{t}_2 - \vec{t}_3$$

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

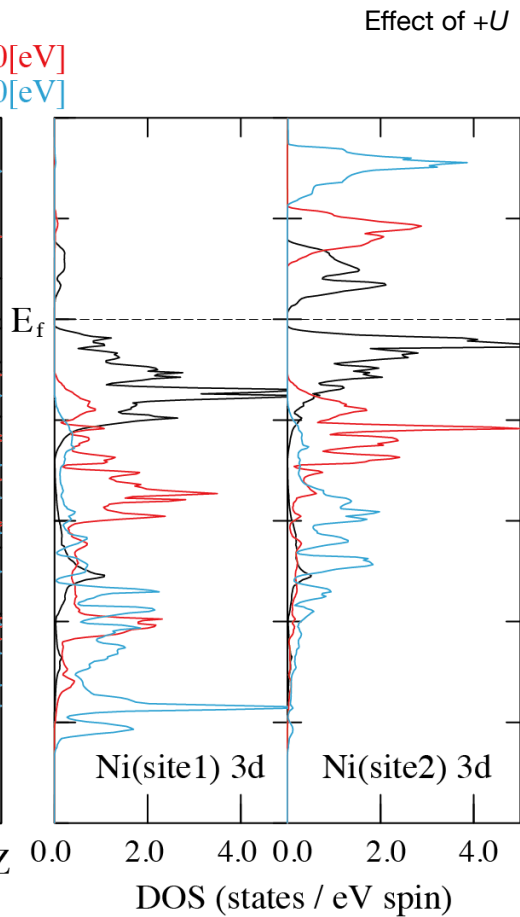
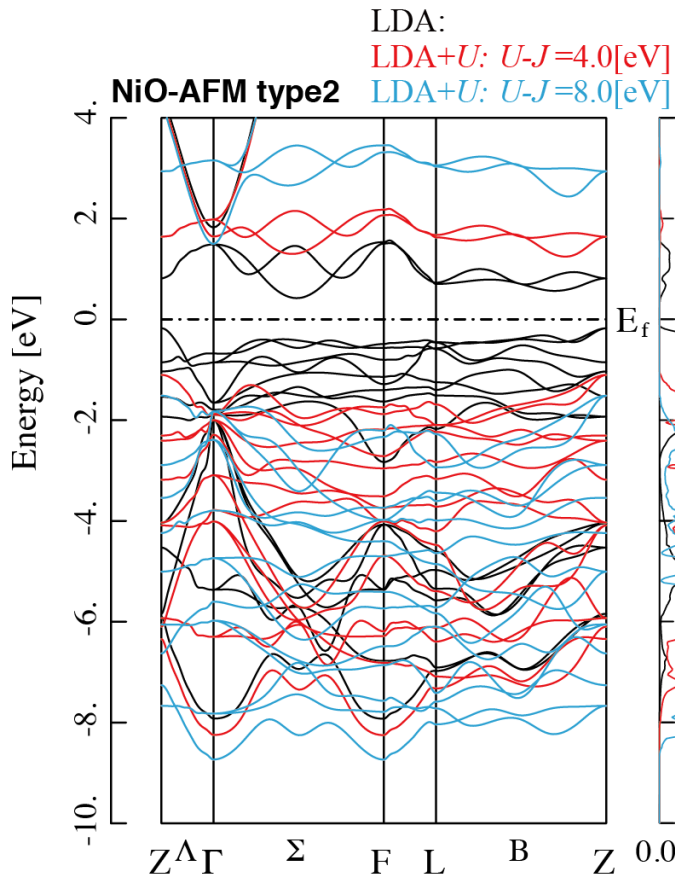
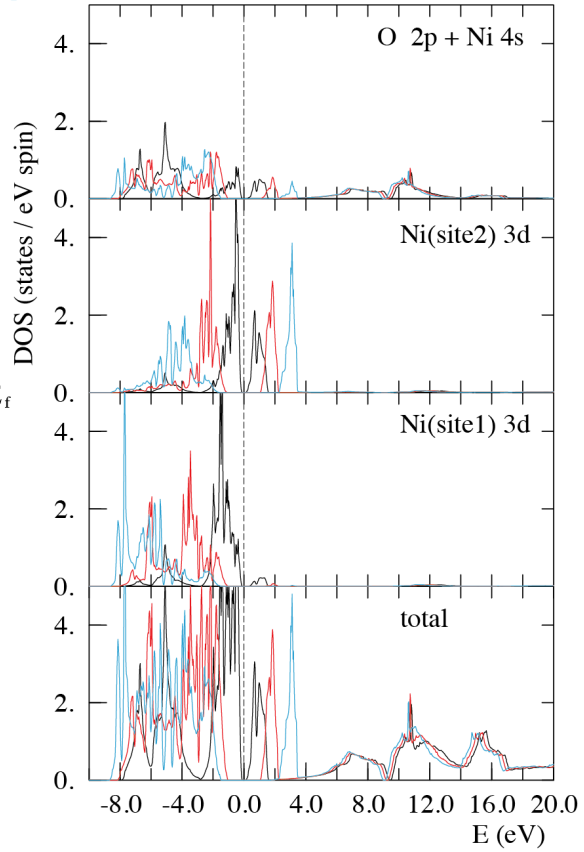
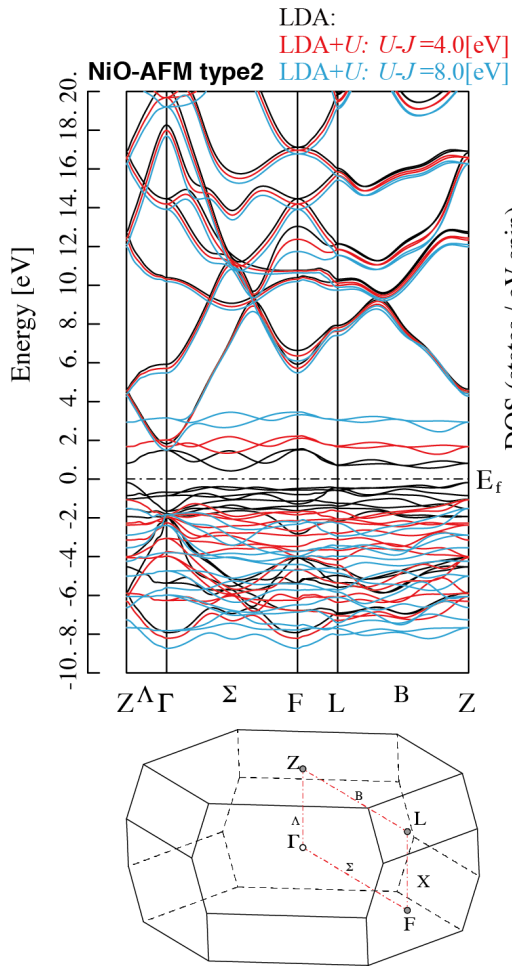
primitive trigonal lattice

+

add lattice point



Hexagonal Lattice



Optical property for semiconductor and metal

- AIP (semiconductor)
- Al(metal)

Optical property

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

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

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

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

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

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

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

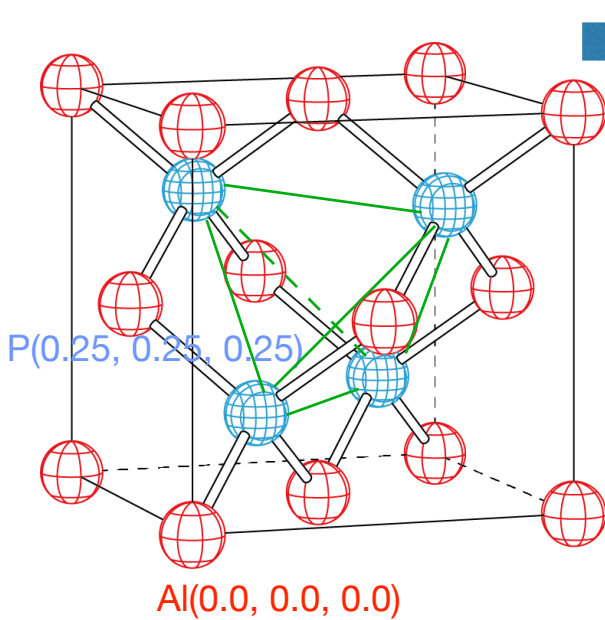
$$v_{\mathbf{k},n} = \left\langle \psi_{\mathbf{k},n} \left| \frac{\mathbf{p}}{m} \right| \psi_{\mathbf{k},n} \right\rangle$$

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

4-1. AIP

Zincblende Structure

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

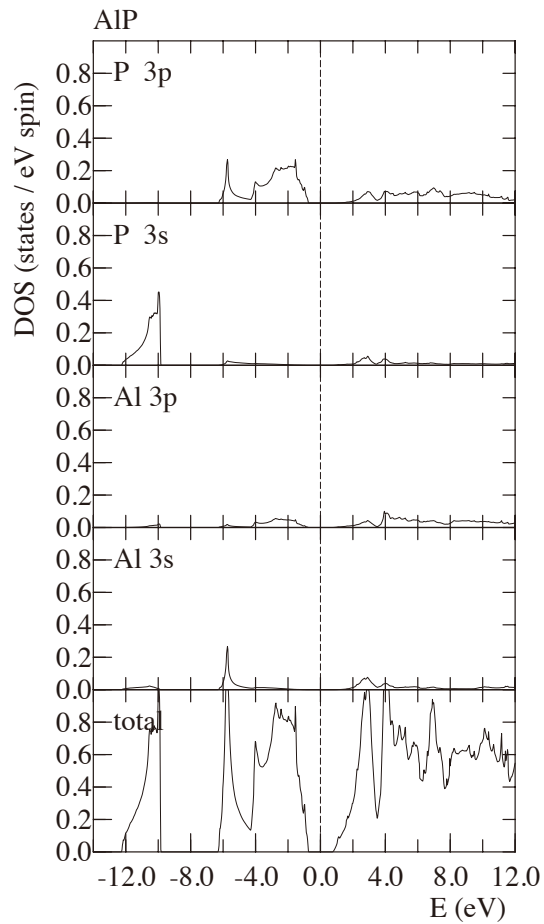
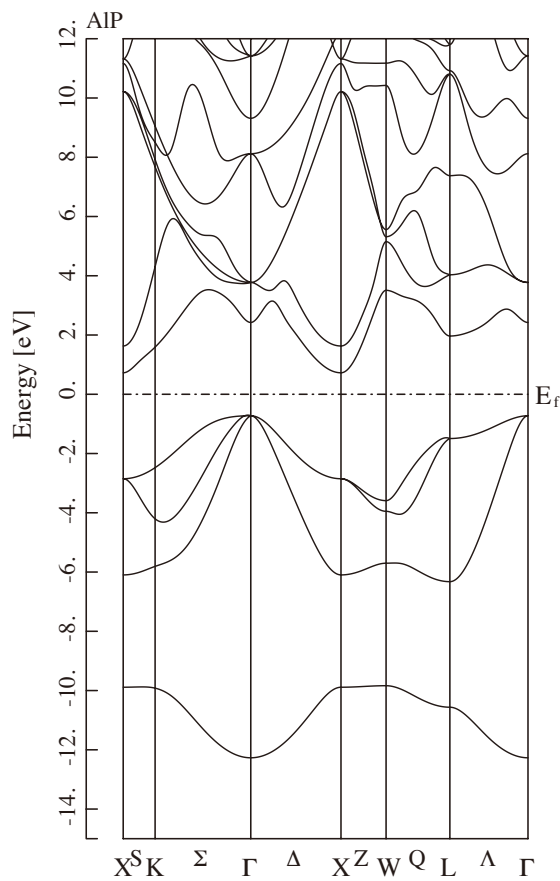


Point group T_d has full tetrahedral symmetry.

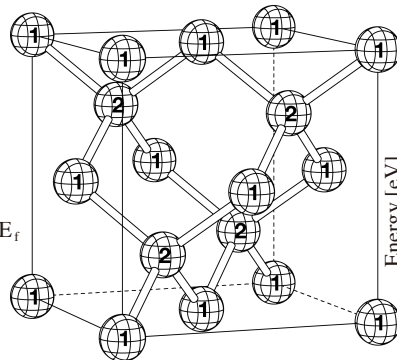
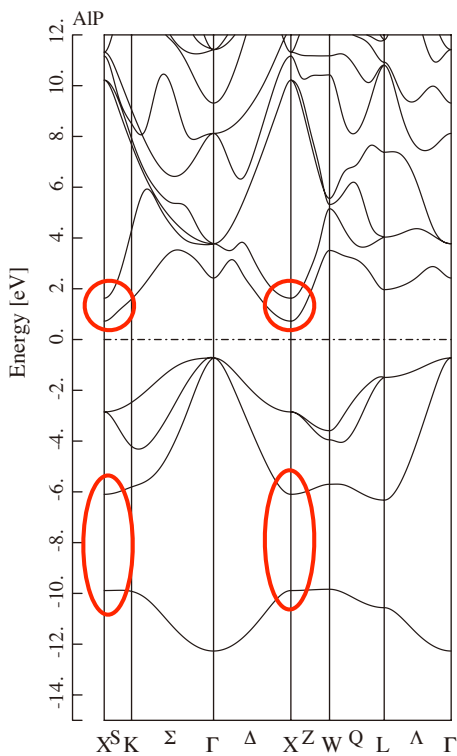
```
>>>>>>> ab_prp.data >>>>>>>>
ALP (216, Td2, F-43m) zinc blende
a=5.45 A
face-centered (il=2)
generators      5 (0, 0, 0)
                 43 (0, 0, 0)
atomic positions
(0.0, 0.0, 0.0) Al
(0.25, 0.25, 0.25) P
nonmagnetic (jmag=0)
>>>>>>> ab_prp.data >>>>>>>>
```

“ab_prp.data” for AIP

```
abcap-ab_prp.data
0
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 !ldim, 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
```

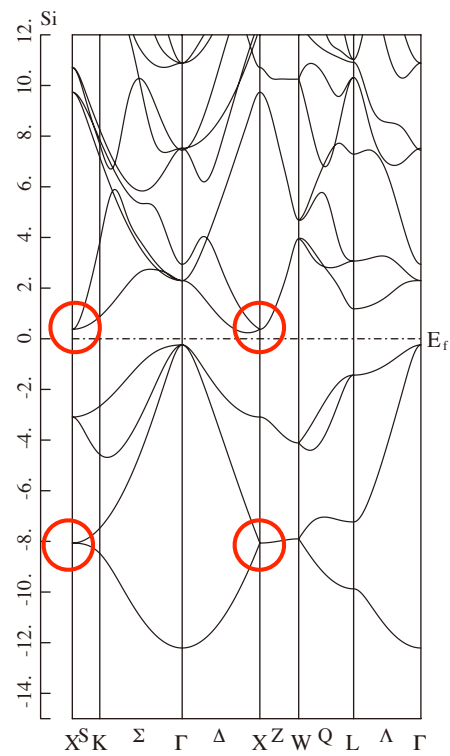



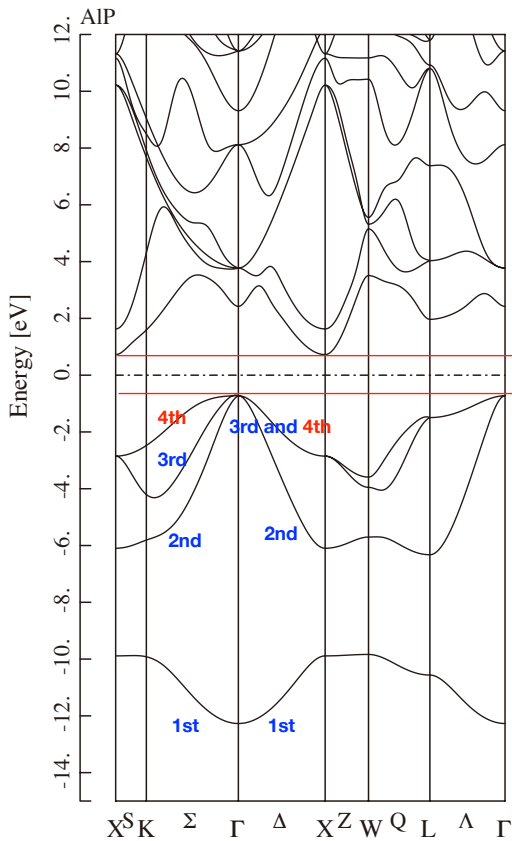
Comparison between E-k curves
(Zincblende and Diamond Structure)



$$\begin{cases} \frac{\epsilon_s^1 + \epsilon_p^2}{2} \pm \sqrt{\left(\frac{\epsilon_s^1 - \epsilon_p^2}{2}\right)^2 + (4E_{sp})^2} \\ \frac{\epsilon_p^2 + \epsilon_s^1}{2} \pm \sqrt{\left(\frac{\epsilon_p^1 - \epsilon_s^2}{2}\right)^2 + (4E_{sp})^2} \end{cases}$$

$$\left(E_{sp} \equiv \frac{1}{3^{1/3}} V_{sp\sigma}\right)$$





result of “**check.sh**”

```

teac14@cmd2:AIP — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 AIP]$ check.sh
-----
electron1: Al 0.639 P 2.217
electron1: Al 0.639 P 2.217
electron1: Al 0.639 P 2.217
electron1: Al 0.639 P 2.217
-----
bandgap [eV] = 1.449960
bandgap [eV] = 1.449960
bandgap [eV] = 1.449960
fermi-en= 0.176817 dos= 0.000000 int.dos= 8.000000
fermi-en= 0.176817 dos= 0.000000 int.dos= 8.000000
fermi-en= 0.176817 dos= 0.000000 int.dos= 8.000000
  
```

E_f \updownarrow 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**”

```

f_ef.dta (~/.abc/AIP) - VIM — ssh -X cmd2 — zsh — ttys002
abcap-ef[Hr]: Fermi-level, dos, vale, band-E (/spin)
0.1768167130061111E+00 1 40
4 4 40 # of fully-occ. bands, # of occ. bands
0.0000000000000000E+00 0.4000000000000000E+01 -0.5711363479187916E-01 spin=1
  
```

preparation to calculation for optical properties

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

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

```

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

```

teac14@cmd2:~/abc — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 ~]$ cd ~
[teac14@cmd2 ~]$ cp $ABCAP/samples/Setopt.sh abc
[teac14@cmd2 ~]$ cd abc
[teac14@cmd2 ~/abc]$ ./Setopt.sh AIP
[teac14@cmd2 ~/abc]$
  
```

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 “**AIP_s**”.
- ② results for SCF calculation for “AIP” is copied from “AIP” to “AIP_s”
- ③ files needed for the optical calculation are copied from the directories, **\$ABCAP/samples/ZnO_5_s0/** .

```

teac14@cmd2:~/abc — ssh -X
[teac14@cmd2 ~/abc]$ ls -l
total 128
drwxr-xr-x 15 teac14 4096 Aug 16 16:27 ./
drwxr-xr-x 33 teac14 4096 Aug 16 16:27 ../
drwxr-xr-x 6 teac14 8192 Aug 15 18:08 AIP/
drwxr-xr-x 6 teac14 8192 Aug 4 12:02 AIP_s/
drwxr-xr-x 2 teac14 4096 Aug 16 16:18 AIP_s/
  
```

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

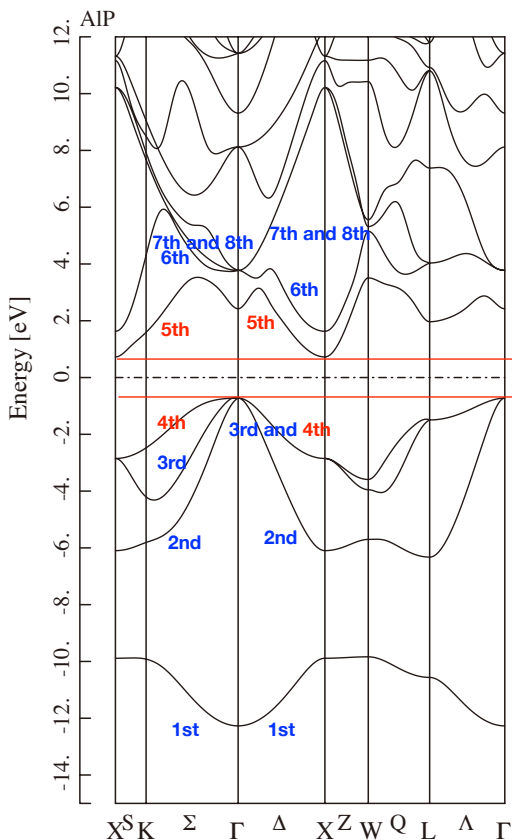
Firstly, we enter the working directory, "AIP_s"

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

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

```
teac14@cmd2:AIP_s — ssh -X cmd2 — zsh — ttys002
[teac14@cmd2 AIP_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|pw>
    bn_evp2.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 AIP_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.

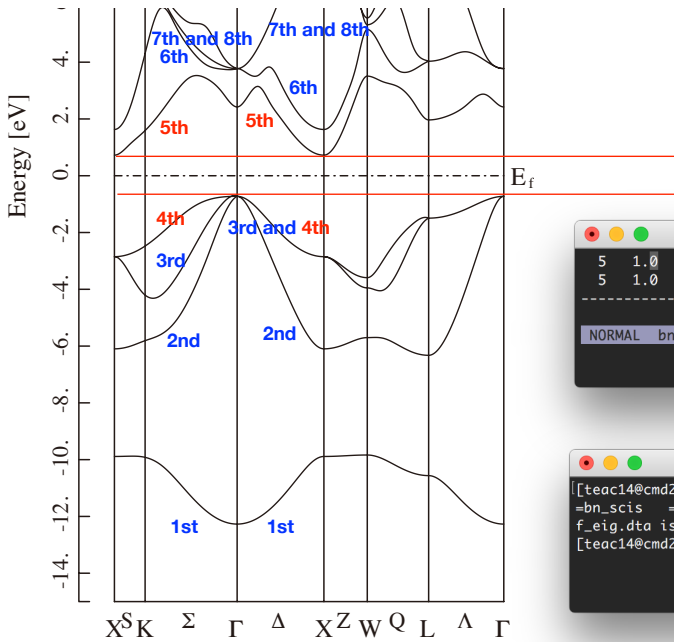
① Edit **bn_scis.data** Set band indexes which

Scissors operator operate.

② Run **bn_scis.sh**.

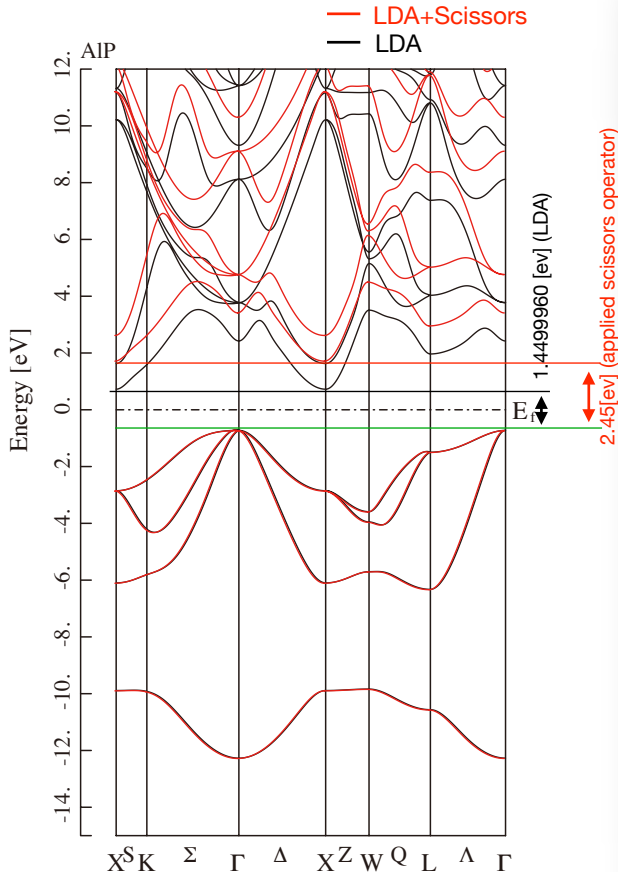
③ **bngap.sh** show the information about optical band gap

```
teac14@cmd2:AIP_s — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 AIP_s]$ H
-----
(0) (bn_scis.data) bn_scis.sh (do this just once)
                   bngap.sh !optical gap
```



```
bn_scis.data (~/.abc/AIP_s) - VIM — ssh -X cmd2 — zsh — ttys003
5 1.0 i-conduction-band, scissors[eV] (for up spin)
5 1.0 i-conduction-band, scissors[eV] (for down spin)
-----
NORMAL bn_scis.data unix iso-2022-jp no 1/4: 9
```

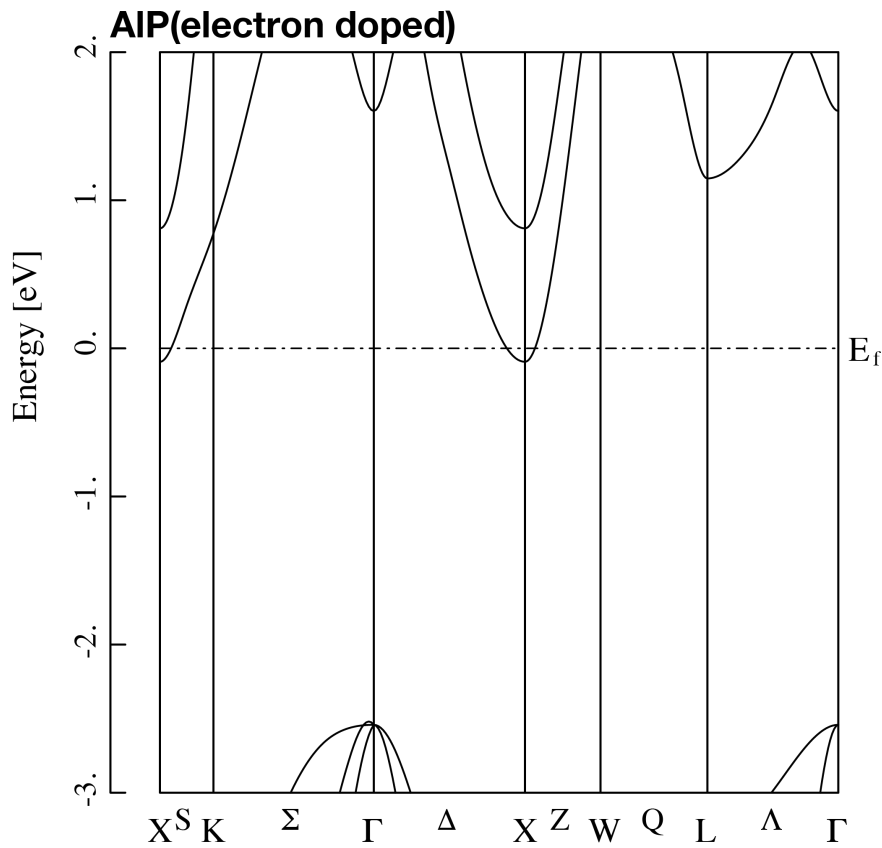
```
teac14@cmd2:AIP_s — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 AIP_s]$ bn_scis.sh
=bn_scis =
f_eig.dta is modified.
[teac14@cmd2 AIP_s]$
```



```
teac14@cmd2:AIP_s — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 AIP_s]$ bngap.sh
--- m_bn_e eig_set ---
--- m_bn_e eig_set ---
np2,neig5,nspin1= 125 40 1
--- f_eig.dta has been read. ---
--- m_bn_e eig_unset ---
--- m_bn_e eig_unset ---
=bngap=
[teac14@cmd2 AIP_s]$
```

```
bngap.txt (~/.abc/AIP_s) - VIM — ssh -X cmd2 — zsh — ttys003
Eigenenergy at Gamma point
up-spin[eV] down-spin[eV]
1 -12.270 1
2 -0.725 4
3 -0.725 4
4 -0.725 4
5 3.422 1
6 4.775 4
7 4.775 4
8 4.775 4
9 9.119 5
10 9.119 5
11 10.314 1
12 12.420 4
13 12.420 4
14 12.420 4
15 16.261 1
16 24.076 4
17 24.076 4
18 24.076 4
19 25.372 5
20 25.372 5
21 26.491 4
22 26.491 4
23 26.491 4
24 30.657 3
25 30.657 3
26 30.657 3
27 36.085 4
28 36.085 4
29 36.085 4
30 39.089 1
31 39.290 5
32 39.290 5
33 42.219 5
34 42.219 5
35 43.008 4
36 43.008 4
37 43.008 4
38 45.212 4
39 45.212 4
40 45.212 4
```

```
bngap.log (~/.abc/AIP_s) - VIM — ssh -X cmd2 — zsh — ttys003
@fermi= 0.176817Hr = 4.811eV
-----
spin = 1 val.band.structure= 4 4
direct gap = 0.152406Hr 4.147eV at ip2= 1 k= 0.000 0.000 0.000
-----
val. top = 0.150174Hr 4.086eV at ip2= 1 k= 0.000 0.000 0.000
Fermi level= 0.176817Hr 4.811eV
cond.bottom= 0.240209Hr 6.536eV at ip2= 9 k= 1.000 0.000 0.000
band gap = 0.090034Hr 2.450eV for spin= 1
-----
NORMAL bngap.log unix iso-2022-jp no 1/9: 1
```



Calculation for

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

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

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

$$\chi_{ij}^{cv}(z) = -\frac{1}{N} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}v} (1 - f_{\mathbf{k}c}) \langle v | p_i | c \rangle \langle c | p_j | v \rangle}{z - (\epsilon_{\mathbf{k}c} - \epsilon_{\mathbf{k}v})}$$

```
df01.data (~/abc/AIP_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      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      emax r8 (0) : max. value of Re(z) (when ipath=1)
c      esift r8 (0) : max. value of Im(z) (when ipath=2)
c      esift r8 (0) : imaginary part of z (when ipath=2)
c      real part of z (when ipath=1)
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
"df01.data" [converted] 39L, 1738C
```

```
teac14@cmd2:AIP_s -- ssh -X cmd2 -- zsh -- ttys009
[teac14@cmd2 AIP_s]$ df01.qc
Your job 84216 ("df01.csh") has been submitted
[teac14@cmd2 AIP_s]$
```

Calculation for the velocity

```
wpw.data (~/.abc/AIP_s) - VIM — ssh -X cmd2 — zsh — ttys008
-3 4  bnbgn+, bndend+ (spin up)
-3 4  bnbgn+, bndend+ (spin down)
~
NORMAL wpw.data          unix iso-2022-jp no  2/2: 5
"wpw.data" [converted] 2L, 76C
```

```
teac14@cmd2:AIP_s — ssh -X cmd2 — zsh — ttys008
[teac14@cmd2 AIP_s]$ wpw.sh
=wpw =
[teac14@cmd2 AIP_s]$
```

```
wpw.log + (~/.abc/AIP_s) - VIM — ssh -X cmd2 — zsh — ttys000
npw9= 189  neig9= 40
npw9= 180  neig9= 40

ispin = 1
2 band      <px>          <py>          <pz>
1  0.0000000000000000  -0.0000000000000000  0.0000000000000000
2  -0.3106594831987   -0.0000000000000000  0.0000000000000000
3  -0.416184783701    0.0000000000000000  0.0000000000000000
4  -0.436564647111    0.0000000000000000  -0.0000000000000000
5  -0.428526895962    -0.0000000000000000  0.0000000000000000
6  -0.399840889706    0.0000000000000000  0.0000000000000000
7  -0.337197468719    0.0000000000000000  0.0000000000000000
8  -0.209523773776    0.0000000000000000  -0.0000000000000000
9  -0.0000000000000000  0.0000000000000000  -0.0000000000000000
10 -0.319525616057    -0.319525616057     -0.0000000000000000
11 -0.369644936101    -0.302128644337     -0.0000000000000000
12 -0.381029828053    -0.244773927385     0.0000000000000000
13 -0.377409671605    -0.168290632212     0.0000000000000000
14 -0.358474769104    -0.089767639685     0.0000000000000000
15 -0.307159302117    -0.022727481425     -0.0000000000000000
16 -0.192146329511    -0.024495544411     0.0000000000000000
17 -0.0000000000000000  0.042569280745     -0.0000000000000000
18 -0.331146689585    -0.331146689585     -0.0000000000000000

NORMAL wpw.log +          unix iso-2022-jp no  839/1724: 5
117 0.126067430781    -0.133909906667     -0.133909906667
118 0.227800476800    -0.186462818440     -0.186462818440
119 0.063818681539    0.063818681539     -0.121408303448
120 0.258601091511    0.0000000000000000  -0.258601091535
121 0.186462818438    0.186462818438     -0.22780047679
122 -0.133909906667    -0.126067430781     -0.133909906667
123 0.063818681539    -0.063818681539     -0.121408303448
124 -0.040577521040    -0.040577521040     -0.040577521040
125 -0.0000000000000000  -0.0000000000000000  -0.0000000000000000

8 band      <px>          <py>          <pz>
1  0.0000000000000000  0.0000000000000000  -0.0000000000000000
2  0.202692821443     0.0000000000000000  0.0000000000000000
3  0.343306505478     0.0000000000000000  -0.0000000000000000
4  0.425387619533     0.0000000000000000  0.0000000000000000
5  0.474367219485     0.0000000000000000  0.0000000000000000
6  0.504470227333     -0.0000000000000000  -0.0000000000000000
7  0.525264031176     0.0000000000000000  0.0000000000000000
8  0.514307213681     -0.0000000000000000  -0.0000000000000000
9  0.0000000000000000  0.0000000000000000  -0.0000000000000000
10 0.242404580245     0.242404580245     0.0000000000000000
11 0.237687358120     0.20623993908      0.0000000000000000
12 0.438579602866     -0.097011318680     -0.0000000000000000

NORMAL wpw.log +          unix iso-2022-jp no  1503/1724: 1
```

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

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

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

```
teac14@cmd2:AIP_s — ssh -X cmd2 — zsh — ttys001
[teac14@cmd2 AIP_s]$ bn_efp2.sh
=bn_efp2 =
[teac14@cmd2 AIP_s]$
```

```
bn_efp2.log (~/.hamada/CMD/29/occal/AIP_s16) - VIM — vim bn_efp2.log — zsh — ttys004
isp,ibn,teig= 1 6 7
isp,ibn,teig= 1 7 8

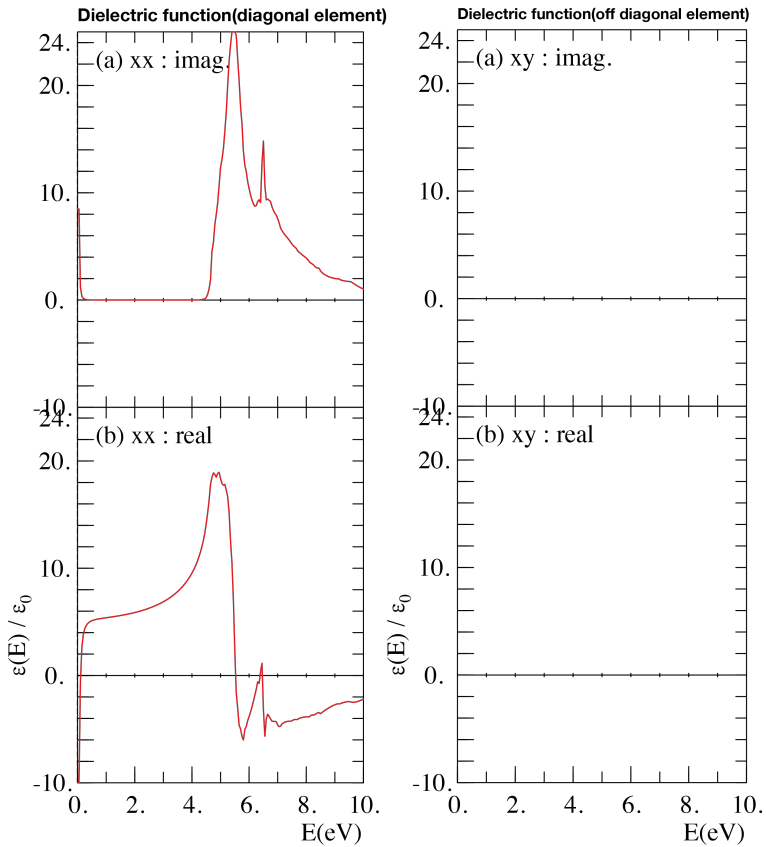
--- p**2 (atomic unit) --- (each band)
--- p**2 (anisotropy) --- (each band)
--- DOS[Hz], v [m/s] (SI unit) --- (each band)
--- p**2 (atomic unit) --- (each spin)
1 0.001820 0.000496 0.000000 -0.000000 0.000496 0.000000 0.000496
--- DOS[Hz], v [m/s] (SI unit) --- (each spin)
1 0.001820 48703. 48703.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

--- DOS, xx, yx,yy, zx,zy,zz --- =(whole bands)=
DOS[Hz]= 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_eig_unset ---
--- m_bn_kp_unset ---
--- end m_input_unset ---
NORMAL bn_efp2.log          unix iso-2022-jp no  14873/14873: 1
```


diagonal and off diagonal element of dielectric function tensor



```
p2_dielec.data + (~/hamada/CMD/29/local/AIP_s16) - VIM - vim p2_dielec.data - zsh...
0 0 jpr, kpaper
2 iconv(2:Hr->eV)
0.0 10.0 1.0 emin, emax, de (eV)
-10.0 25.0 2.0 dmin, dmax, dd(integer)
8.0 3.0 xe, yd (mm/u, mm/u)
AIP Dielectric function(diagonal element)
2 ncurve
(Real part) xy
1 nm(i),(im(j,i),j=1,nm(i))
(Imaginary part) xy
1 2 nm(i),(im(j,i),j=1,nm(i))
~
~
NORMAL p2_dielec.data + unix iso-2022-jp no 11/11: 8
p2_dielec.data" [converted] 11L, 453C written
```

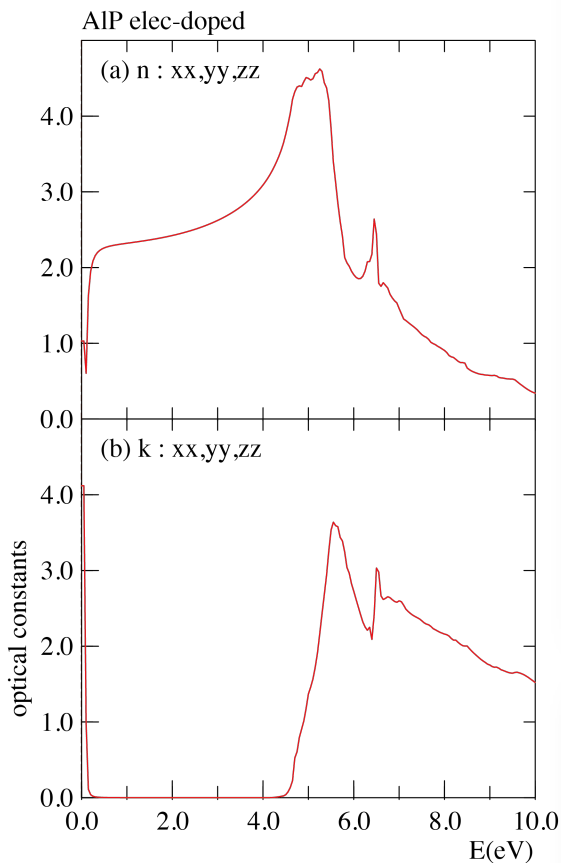
input file for diagonal term

```
p2_dielec.data (~/hamada/CMD/29/local/AIP_s16) - VIM - vim p2_dielec.data - zsh - L...
0 0 jpr, kpaper
2 iconv(2:Hr->eV)
0.0 10.0 1.0 emin, emax, de (eV)
-10.0 25.0 2.0 dmin, dmax, dd(integer)
8.0 3.0 xe, yd (mm/u, mm/u)
AIP Dielectric function(off diagonal element)
2 ncurve
(Real part) xy
1 3 nm(i),(im(j,i),j=1,nm(i))
(Imaginary part) xy
1 4 nm(i),(im(j,i),j=1,nm(i))
~
~
NORMAL p2_dielec.data unix iso-2022-jp no 1/11: 1
```

input file for off-diagonal term

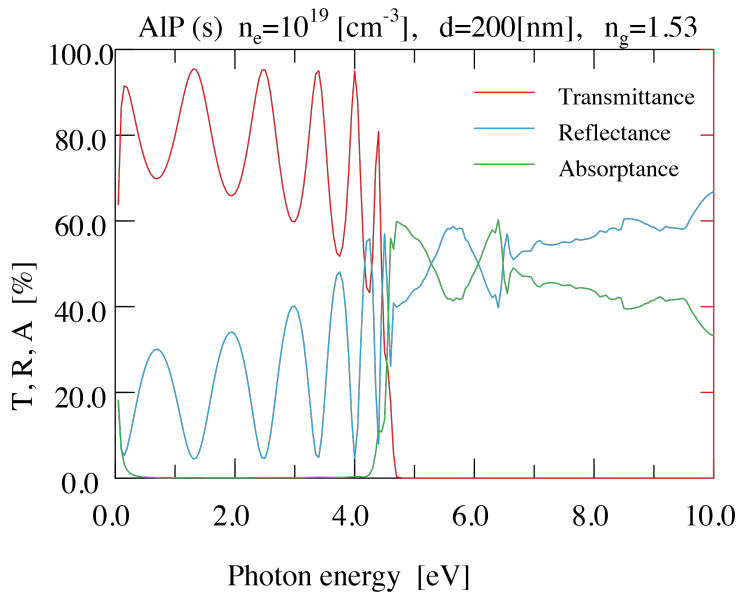
```
teac14@cmd2:AIP_s - ssh -X cmd2 - zsh - ttys001
[teac14@cmd2 AIP_s]$ p2_dielec.sh
=p2_dielec=
[teac14@cmd2 AIP_s]$
```

optical constant

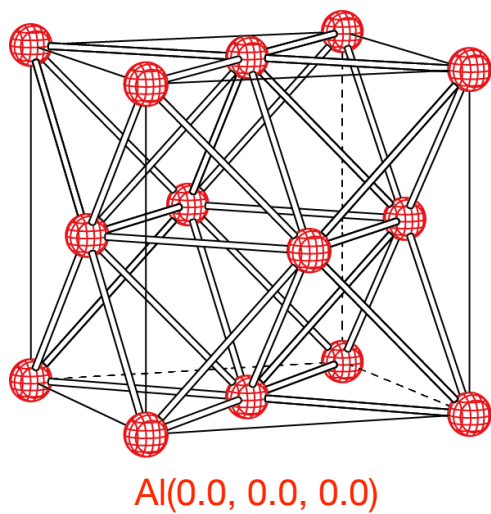


```
p2_optnk.data (~/hamada/CMD/29/local/AIP_s16) - VIM - vim p2_optnk.data - z...
0 0 jpr, kpaper
2 iconv(2:Hr->eV)
0.0 10.0 1.0 emin, emax, de (eV)
0.0 5.0 1.0 dmin, dmax, dd(integer)
12.0 20.0 xe, yd (mm/u, mm/u)
AIP elec-doped
1 ncurve
xx,yy,zz
0 ndata, jdata(ndata)
-----
3 ncurve
average
0 ndata, 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)
Zn0
1 ncurve
xx,yy,zz
0 ndata, jdata(ndata)
~
~
NORMAL p2_optnk.data unix iso-2022-jp no 1/27: 1
```

```
teac14@cmd2:AIP_s - ssh -X cmd2 - zsh - ttys001
[teac14@cmd2 AIP_s]$ p2_optnk.sh
=p2_optnk=
[teac14@cmd2 AIP_s]$
```

4-2. Al



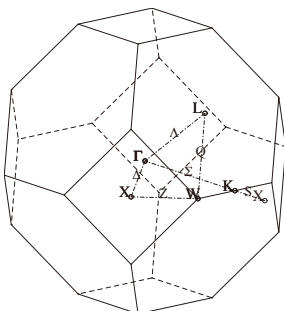
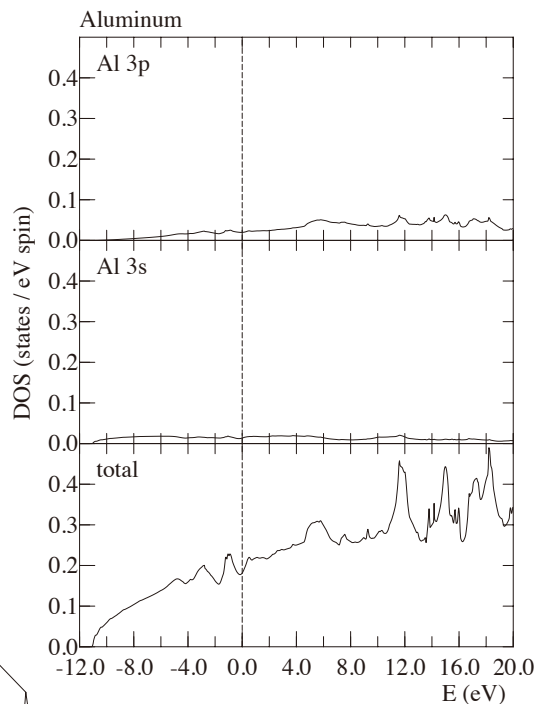
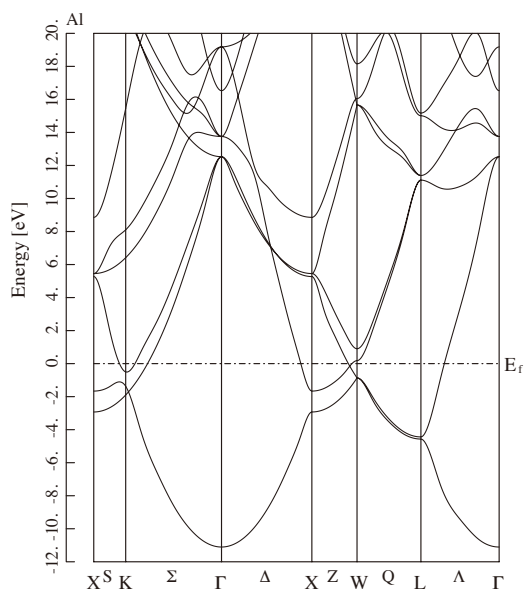
$Fm\bar{3}m(O_h^5, \#225)$

```
>>>>>>> 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

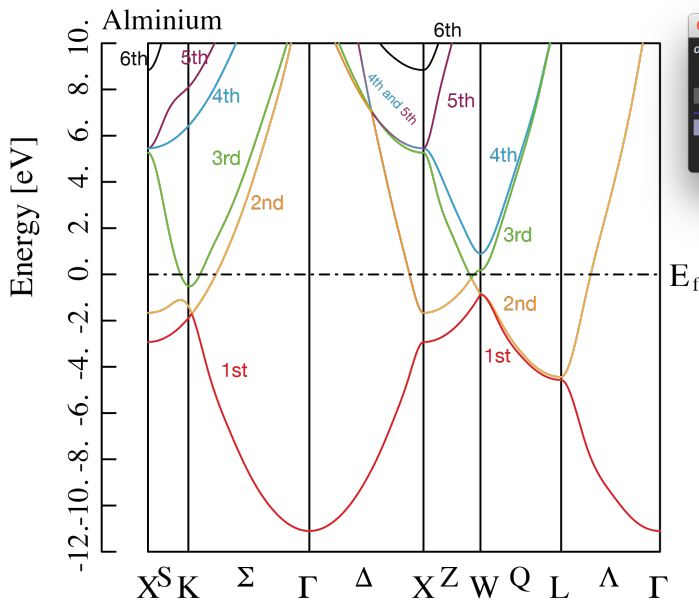
```
ab_prp.data (~/abc/Al) - VIM — ssh -X cmd2 — zsh — ttys003
abcap-ab_prp.data
0                               !jpr
aluminum
lattice parameter -2---*---3---*---4---*---5---*---6---*---7
4.05 4.05 4.05 90.0 90.0 90.0      !a,b,c[A], alpha,beta,gamma[degree]
space group        -2---*---3---*---4---*---5---*---6---*---7
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 !noS0:(0(N),1(AF),2(M)), S0:(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**"



```
f_ef.dta (~|abc/Al) - VIM - ssh -X cmd2 - zsh - ttys003
abcp-ef[Hr]: Fermi-level, dos, vde, band-E (/spin)
0.2537158569163260E+00 1 25
1 3 25 # of fully-occ. bands, # of occ. bands
0.4937232019982947E+01 0.1499999997388030E+01 0.1380323016921401E+00 spin=1
NORMAL f_ef.dta unix iso-2022-jp no 4/4: 1
```

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
```

```
teac14@cmd2:~/abc - ssh -X cmd2 - zsh - ttys001
[teac14@cmd2 ~]$ cd ~/abc
[teac14@cmd2 ~/abc]$ ./Setopt.sh Al
[teac14@cmd2 ~/abc]$
```

working directory for SCF calc.

```
teac14@cmd2:~/abc - ssh -X cmd2 - zsh -
[teac14@cmd2 ~/abc]$ ls -l
total 128
drwxr-xr-x 16 teac14 4096 Aug 25 16:23 ./
drwxr-xr-x 33 teac14 4096 Aug 25 16:19 ../
drwxr-xr-x 6 teac14 8192 Aug 15 18:08 AL/
drwxr-xr-x 6 teac14 8192 Aug 16 20:07 ALP/
drwxr-xr-x 2 teac14 4096 Aug 19 14:53 ALP_s/
drwxr-xr-x 2 teac14 4096 Aug 25 16:23 AL_s/
```

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

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]$
```

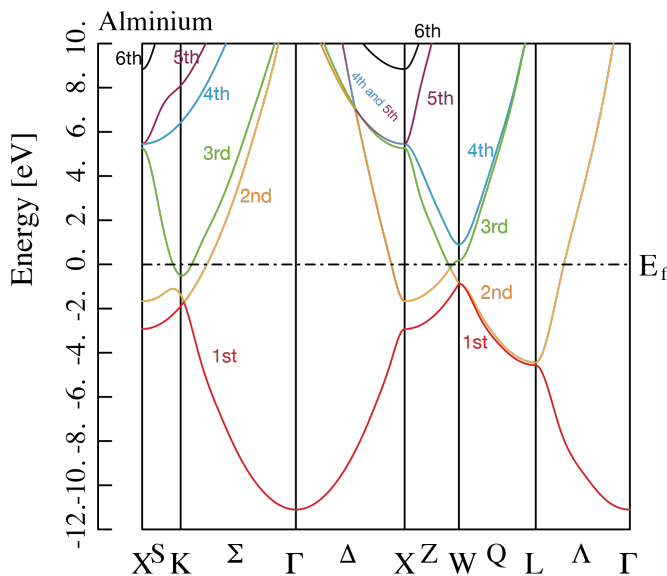
Enter a command, **H**, which shows a procedure of the calculation.

```
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)   bnp1.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 !absorption 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
jpr
ne # mesh
0.0 10.0
0.000005 1 0
eshift[Hr], ipath, matopt
1 3
2 6
nv1,nv2 : valence bands
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
ne # mesh
1000
0.0 10.0
0.000005 1 0
esift, ipath, matopt
1 18
19 48
nv1,nv2 : valence bands
nw1,nw2 : conduction bands
-----
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 emax r8 (0) : max. value of Re(z) (when ipath=1)
c esift r8 (0) : imaginary part of z (when ipath=1)
c ipath i4 (0) : integral path index
c matopt i4 (0) : matrix element option
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
```

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

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

$$\chi_{ij}^{cv}(z) = -\frac{1}{N} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}v} (1 - f_{\mathbf{k}c}) \langle v | p_i | c \rangle \langle c | p_j | v \rangle}{z - (\epsilon_{\mathbf{k}c} - \epsilon_{\mathbf{k}v})}$$

```
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]$
```

Calculation for the velocity

```
wpw.data (~/.abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys000
-3 3  bnbgn+, bndend+ (spin up)
-3 3  bnbgn+, bndend+ (spin down)
~
NORMAL wpw.data          unix iso-2022-jp no    1/2: 2
"wpw.data" [converted] 2L, 76C
```

```
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys000
[teac14@cmd2 Al_s]$ wpw.sh
=wpw =
[teac14@cmd2 Al_s]$
```

```
wpw.log (~/.abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys000
prw9= 75  neig9= 25
prw9= 80  neig9= 25
prw9= 76  neig9= 25
prw9= 80  neig9= 25
prw9= 76  neig9= 25

ispin = 1
1 band      <px>      <py>      <pz>
2 -0.000000000000 0.000000000000 0.000000000000
3 0.100636988982 0.000000000000 -0.000000000000
4 0.200570861504 0.000000000000 0.000000000000
5 0.399433647141 0.000000000000 0.000000000000
6 0.396541917292 -0.000000000000 -0.000000000000
7 0.490946878300 -0.000000000000 0.000000000000
8 0.580175253538 -0.000000000000 -0.000000000000
9 0.648483623132 0.000000000000 0.000000000000
10 -0.000000000000 0.000000000000 -0.000000000000
11 0.100524109777 0.100524109777 0.000000000000
12 0.200415006225 0.100219826087 0.000000000000
13 0.299106638849 0.099725407522 0.000000000000
14 0.396117457351 0.09905817226 0.000000000000
15 0.490415443991 0.098210870077 0.000000000000
16 0.579528470242 0.097134941195 0.000000000000
17 0.647422841080 0.095605025712 0.000000000000
18 -0.000000000000 0.092234056018 0.000000000000
19 -0.199817471080 0.199817471080 -0.000000000000

NORMAL wpw.log          unix iso-2022-jp no    859/1372: 4
85 band      <px>      <py>      <pz>
86 -0.000000000000 0.000000000000 0.000000000000
87 0.000000000000 0.000000000000 -0.000000000000
88 -0.509982680923 -0.000000000000 0.000000000000
89 -0.542891094248 0.000000000000 0.000000000000
90 -0.477585941887 0.000000000000 0.000000000000
91 -0.390160871060 -0.000000000000 0.000000000000
92 -0.258165704225 -0.000000000000 0.000000000000
93 -0.171885494869 -0.000000000000 0.000000000000
94 -0.085802970334 -0.000000000000 -0.000000000000
95 0.000000000000 -0.000000000000 0.000000000000
96 0.098005054181 0.098005054181 0.000000000000
97 -0.457414810637 0.740846227276 0.000000000000
98 -0.437971500355 0.811696331142 0.000000000000
99 -1.070799975370 0.088456417740 -0.000000000000
100 -0.360562614663 -0.374918904709 -0.000000000000
101 -0.179534256261 -0.47838463589 -0.000000000000
102 -0.089107433676 -0.487803593529 -0.000000000000
103 0.000000000000 -0.49050887856 0.000000000000
104 0.195054465557 0.195054465557 -0.000000000000
105 -1.028572176931 0.099982009629 -0.000000000000
106 -1.056325495941 0.164582758170 -0.000000000000
107 -0.984203301655 0.170428379287 0.000000000000
108 -0.266785404534 -0.423225954073 0.000000000000
109 -0.096616747652 -0.511403468027 0.000000000000
110 0.000000000000 -0.51687528196 -0.000000000000

NORMAL wpw.log          unix iso-2022-jp no    1112/1372: 5
```

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

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

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

```
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys000
[teac14@cmd2 Al_s]$ ./bn_efp2.sh
=bn_efp2 =
[teac14@cmd2 Al_s]$
```

```
bn_efp2.log (~/.abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys000
isp,ibn,ieig= 1 5 5
isp,ibn,ieig= 1 6 6

--- p**2 (atomic unit) --- (each band)
1 2 4.373574
0.178658
0.000000 0.178658
0.000000 0.000000 0.178658
1 3 0.561716
0.061821
0.000000 0.061821
0.000000 -0.000000 0.061821

--- p**2 (anisotropy) --- (each band)
1 2 (vxx+vyy)/vzz= 1.000000
1 3 (vxx+vyy)/vzz= 1.000000

--- DOS[/Hr], v [m/s] (SI unit) --- (each band)
1 2 4.373574 924691. 924691. 924691.
1 3 0.561716 543946. 543946. 543946.

--- p**2 (atomic unit) --- (each spin)
1 4.937232 0.165295 0.000000 0.000000 0.165295 0.000000 0.165295
--- DOS[/Hr], v [m/s] (SI unit) --- (each spin)
1 4.937232 889437. 889437. 889437.

--- DOS, xx, yx,yy, zx,zy,zz --- (whole bands)=
DOS[/Hr]= 0.874464
--- p**2 (atomic unit) ---
0.165295
0.000000 0.165295
0.000000 0.000000 0.165295
--- v [m/s] (SI unit) ---
889437. 889437. 889437.

--- 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= 2.927193E+02 2.927193E+02 2.927193E+02 A
conductivity= 1.642787E+07 1.642787E+07 1.642787E+07 [/Ohm*m]
conductivity= 1.642787E+05 1.642787E+05 1.642787E+05 [/Ohm*cm]

--- m_bn_eieg_unset ---
--- m_bn_kp_unset ---
--- end_m_input_unset ---
NORMAL bn_efp2.log          unix iso-2022-jp no    12982/12982: 1
```

Calculation for the Drude term and total dielectric function

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

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

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

result for total dielectric function

```
df_total.data (~/.abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys001
1
model
0.02
damp[eV]
-----
model
0.35 0.02 1.e19 mass_x[], damp_x[eV], density_x[cm**3]
0.35 0.02 1.e19 mass_y[], damp_y[eV], density_y[cm**3]
0.35 0.02 1.e19 mass_z[], damp_z[eV], density_z[cm**3]
-----
1
model
0.02
damp[eV]
-----
0.35 0.12 1.e19 mass_x[], damp_x[eV], density_x[cm**3]
~
~
~
NORMAL df_total.data
"df_total.data" [converted] 14L, 445C
```

```
df_total.log (~/.abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys001
damp[eV]= 0.020000
damp[Hr]= 0.000735
ne = 200
emin = 0.000eV
emax = 10.000eV
DOS= 9.874 vcell= 112.073
plasma energy = 11.636147 eV
plasma energy = 0.000000 eV
plasma energy = 0.000000 eV
plasma energy = 11.636147 eV
plasma energy = 0.000000 eV
plasma energy = 11.636147 eV
Conductivity(xx)= 2.060+08 S/m Resistivity(xx) = 4.840-07 Ohm*cm
Conductivity(yy)= 2.060+08 S/m Resistivity(yy) = 4.840-07 Ohm*cm
Conductivity(zz)= 2.060+08 S/m Resistivity(zz) = 4.840-07 Ohm*cm
~
~
~
NORMAL df_total.log
unix iso-2022-jp no 1/15: 1
```

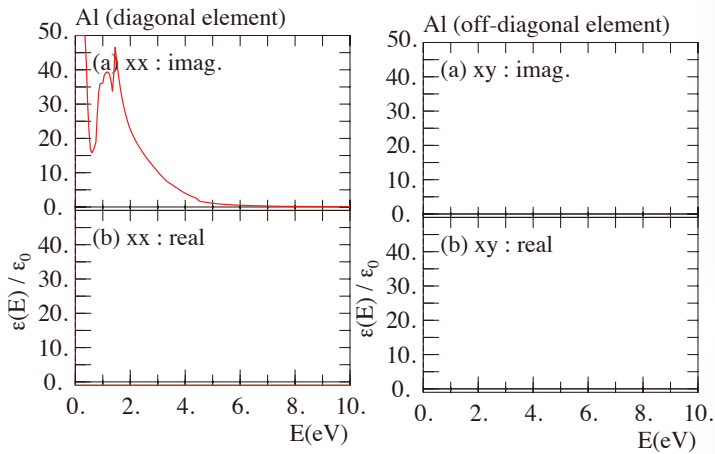
```
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys001
[teac14@cmd2 Al_s]$ df_total.sh
=df_total=
[teac14@cmd2 Al_s]$
```

Index of the component for the dielectric function

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

In this case, this crystal has a cubic symmetry,

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



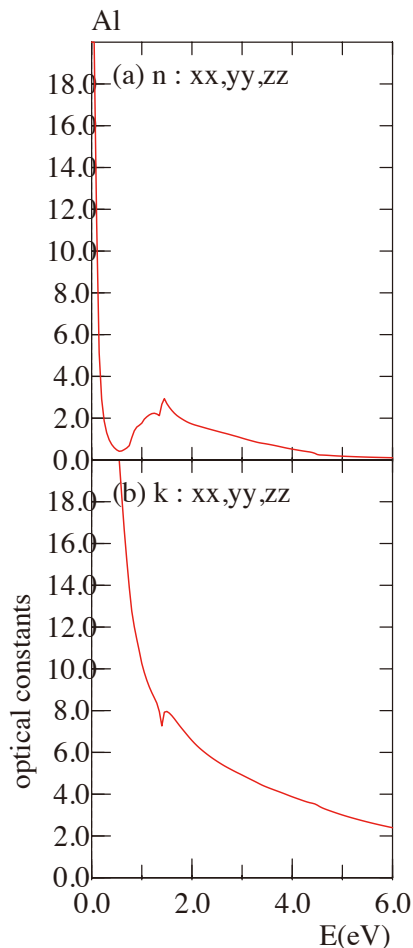
```
teac14@cmd2:Al_s — ssh -X cmd2 — zsh — ttys001
[teac14@cmd2 Al_s]$ p2_dielec.sh
=p2_dielec=
[teac14@cmd2 Al_s]$
```

```
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
```

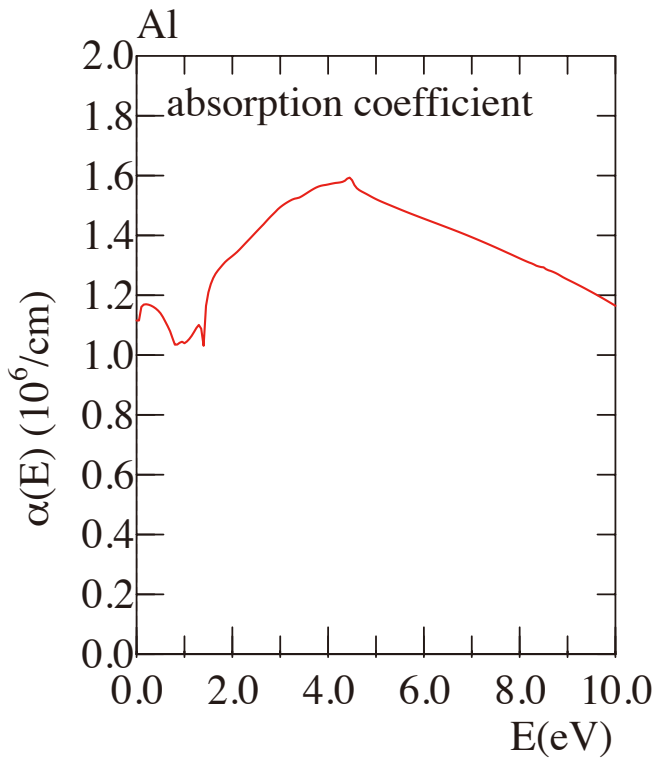
```
p2_dielec.data (~/.abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys001
0 0 jpr, kpaper
2 iconv(2:Hr->eV)
0.0 10.0 1.0 emin, emax, de (eV)
-1.0 50.0 5.0 dmin, dmax, dd(integer)
8.0 1.0 xe, yd (mm/u, mm/u)
Al (off-diagonal element)
2 ncurve
(real part) xx,yy,zz
1 3 nm(i),(im(j,i),j=1,nm(i))
(imaginary part) 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
```



```
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)
Zn0
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]$
```

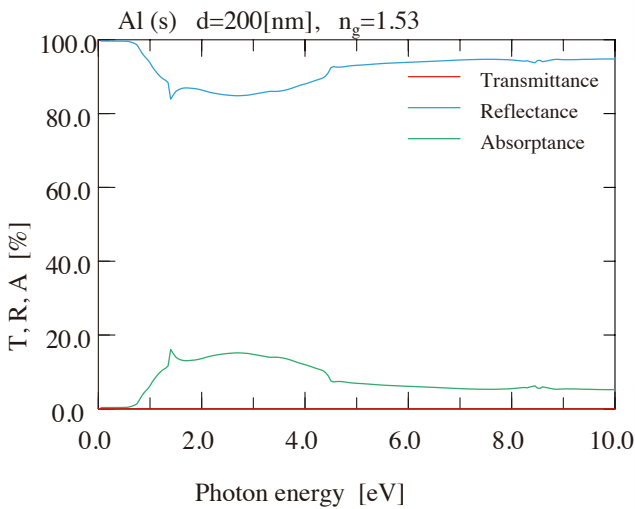



```
p2_absorb.data (~:/abc/Al_s) - VIM — ssh -X cmd2 — zsh — ttys001
0 0 jpr, kpaper
2 lconv(2:Hr->eV)
0.0 10.0 1.0 emin, emax, de (eV)
0.0 2.0 0.2 dmin, dmax, dd(integer)
8.0 50.0 xe, yd (mm/u, mm/u)
Al
1 ncurve
xx,yy,zz ndata, jdata(ndata)
-----
3 ncurve
average ndata, jdata(ndata)
0
zz
1 11 ndata, 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,iyy,type of line
'f_TRAeV.dta',1 3 2 'Reflectance' iix,iyy,type of line
'f_TRAeV.dta',1 4 3 'Absorptance' iix,iyy,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.data (~/.abc/Fe) - VIM — ssh cmd2 — zsh — ttys003
25 1 2 1 2 1 2
224 1 3 0h4 Pn-3m
5 0 1 0 1 0 1
19 1 2 0 1 1 2
25 0 1 0 1 0 1
225 2 3 0h5 Fm-3m
5 0 1 0 1 0 1
19 0 1 0 1 0 1
25 0 1 0 1 0 1
226 2 3 0h6 Fm-3c
5 0 1 0 1 0 1
19 1 2 1 2 1 2
25 0 1 0 1 0 1
227 2 3 0h7 Fd-3m
5 0 1 0 1 0 1
19 1 4 3 4 3 4
25 1 4 1 4 1 4
227 2 3 0h7 Fd-3m
5 0 1 0 1 0 1
19 1 4 1 2 3 4
25 0 1 0 1 0 1
228 2 3 0h8 Fd-3c
5 0 1 0 1 0 1
19 1 4 3 4 3 4
25 3 4 3 4 3 4
228 2 3 0h8 Fd-3c
5 0 1 0 1 0 1
19 1 4 0 1 3 4
25 0 1 0 1 0 1
229 3 3 0h9 Im-3m
5 0 1 0 1 0 1
19 0 1 0 1 0 1
25 0 1 0 1 0 1
230 3 3 0h10 Ia-3d
5 0 1 0 1 0 1
19 1 4 1 4 3 4
25 0 1 0 1 0 1
NORMAL generator.data unix iso-2022-jp no 917/920: 10
    
```

Fd-3m: choice of origin #1

Fd-3m: choice of origin #2

Generator of the space group

File: **generator.data**

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

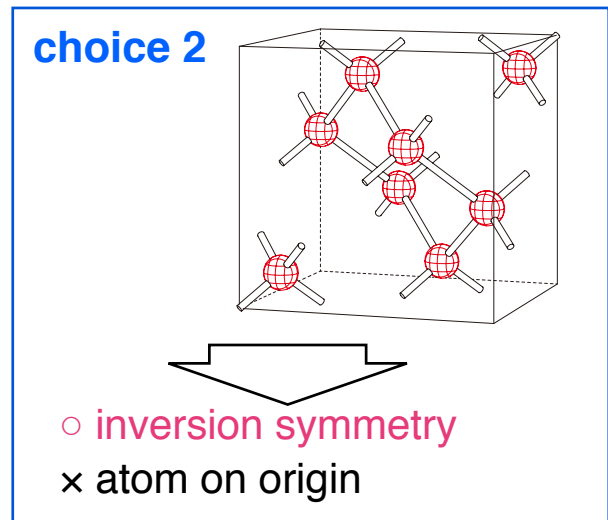
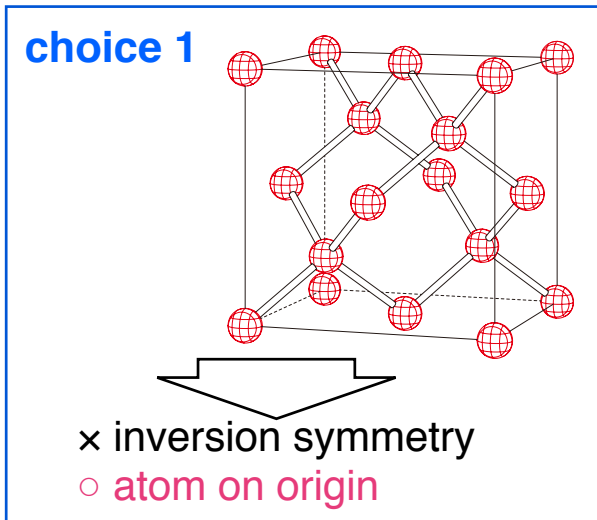
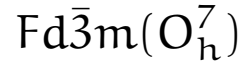
227 2 3 0h7 Fd-3m

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



	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**

```
wycoff.data (~/abc/Fe) - VIM - ssh cmd2 - zsh - tty003
24d 0 q q
48e x 0 0
48f x q q
64g x x x
96h q y y
96i 0 y z
92j x y z
227 9
8a 0 0 0
8b h h h
16c 8 8 8
16d f f f
32e x x x
48f x 0 0
96g x x z
96h 8 y n
92i x y z
227 9
8a 8 8 8
8b 3 3 3
16c 0 0 0
16d h h h
32e x x x
48f x 8 8
96g x x z
96h 0 y w
92i x y z
228 8
16a 0 0 0
32b 8 8 8
32c 3 3 3
48d q 0 0
64e x x x
96f x 0 0
96g 8 y n
92h x y z
228 8
NORMAL wycoff.data unix iso-2022-jp no 2347/2388: 1
```

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

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

Multiplicity	Wyckoff letter	Coordinates	Reflection conditions
192	i 1	(1) x, y, z (2) $\bar{x}, \bar{y}, \bar{z} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ (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) $\bar{z}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$ (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) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (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) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (19) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (20) $x + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (21) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (22) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (23) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (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) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (28) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (29) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (30) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (31) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (32) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (33) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (34) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (35) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (36) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (37) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (38) y, z, x (39) $\bar{y}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (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) $\bar{x} + \frac{1}{2}, \bar{z}, y + \frac{1}{2}$ (43) x, z, y (44) $\bar{x}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (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, x, y	$hkl : h+k=2n$ and $h+l, k+l=2n$ $0kl : k+l=4n$ and $hkl : h+l=2n$ $h00 : h=4n$
96	h ..2	$\frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, y + \frac{1}{2}, \bar{z}$ $\bar{y} + \frac{1}{2}, \bar{z}, y$ $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ $\bar{y}, \bar{z} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ $\bar{y}, \bar{z} + \frac{1}{2}, y$ $\bar{y}, \bar{z} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ $\bar{y}, \bar{z} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{z}, y$ $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$	Special: as above, plus no extra conditions
96	g ..m	x, x, z $\bar{x}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ z, x, x $z + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$ $z, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x}$ x, z, x $x + \frac{1}{2}, \bar{z}, z + \frac{1}{2}$ $x + \frac{1}{2}, \bar{z}, z + \frac{1}{2}$ $x, z + \frac{1}{2}, x + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	no extra conditions
48	f 2..mm	$x, 0, 0$ $\bar{x}, \frac{1}{2}, \frac{1}{2}$ $0, x, 0$ $\frac{1}{2}, \bar{x}, \frac{1}{2}$ $0, 0, x$ $\frac{1}{2}, \bar{x}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$	$hkl : h=2n+1$ or $h+k+l=4n$
32	e ..3m	x, x, x $\bar{x}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ $x + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	no extra conditions
16	d ..3m	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ }	$hkl : h=2n+1$ or $h, k, l=4n+2$ or $h, k, l=4n$
8	b ..3m	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ }	$hkl : h=2n+1$ or $h+k+l=4n$
8	a ..3m	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ }	

Symmetry of special projections
 Along [001] $p4mm$ $a = \frac{1}{2}(a-b)$ $b = \frac{1}{2}(a+b)$ $c = c$
 Along [111] $p6mm$ $a = \frac{1}{2}(2a-b-c)$ $b = \frac{1}{2}(-a+2b-c)$ $c = c$
 Origin at $0, 0, c$
 Origin at x, x, z
 Origin at x, x, z

```

[teac14@cmd2 Fe] ssh cmd2 -- zsh -- ttys003
[teac14@cmd2 Fe]$ ./ab_crystal.sh
select Sch_name(1),HM_name(2),space-group-number(3)
1
schname?
0h7
227 0h7 Fd-3m : number of choices= 2
choice no.?
1

----- welcome to tspace v4.1 1995/09/06 -----
227 0h7 Fd-3m choice 1
Face centered lattice
group elements
1 1 e x y z 0/1 0/1 0/1
2 2 c2x x -y -z 0/1 0/1 0/1
3 3 c2y -x y -z 0/1 0/1 0/1
4 4 c2z -x -y z 0/1 0/1 0/1
5 5 c31+ z x y 0/1 0/1 0/1
6 6 c32+ -z x -y 0/1 0/1 0/1
7 7 c33+ -z -x -y 0/1 0/1 0/1
8 8 c34+ z -x -y 0/1 0/1 0/1
9 9 c31- y z x 0/1 0/1 0/1
10 10 c32- y -z -x 0/1 0/1 0/1
11 11 c33- y z -x 0/1 0/1 0/1
12 12 c34- -y -z x 0/1 0/1 0/1
13 13 c2a y x -z 1/4 1/4 1/4
14 14 c2b -y -x -z 1/4 1/4 1/4
15 15 c2c z -y x 1/4 1/4 1/4
16 16 c2d -x z y 1/4 1/4 1/4
17 17 c2e -z -y -x 1/4 1/4 1/4
18 18 c2f -x -z -y 1/4 1/4 1/4
19 19 c4x+ x -z y 1/4 1/4 1/4
20 20 c4y+ z y -x 1/4 1/4 1/4
21 21 c4z+ -y x z 1/4 1/4 1/4
22 22 c4x- x z -y 1/4 1/4 1/4
23 23 c4y- -z y x 1/4 1/4 1/4
24 24 c4z- y -x z 1/4 1/4 1/4
25 25 ie -x -y -z 1/4 1/4 1/4
26 26 ic2x -x y z 1/4 1/4 1/4
27 27 ic2y x -y z 1/4 1/4 1/4
28 28 ic2z x y -z 1/4 1/4 1/4
29 29 ic31+ -z -x -y 1/4 1/4 1/4
30 30 ic32+ z -x y 1/4 1/4 1/4
31 31 ic33+ z x -y 1/4 1/4 1/4
32 32 ic34+ -z x y 1/4 1/4 1/4
33 33 ic31- -y -z x 1/4 1/4 1/4
34 34 ic32- -y z x 1/4 1/4 1/4
35 35 ic33- y -z x 1/4 1/4 1/4
36 36 ic34- y z -x 1/4 1/4 1/4
37 37 ic2a -y -x z 0/1 0/1 0/1
38 38 ic2b y x z 0/1 0/1 0/1
39 39 ic2c -z y -x 0/1 0/1 0/1
40 40 ic2d x -z -y 0/1 0/1 0/1
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 0/1 0/1 0/1
44 44 ic4y+ -z -y x 0/1 0/1 0/1
45 45 ic4z+ y -x -z 0/1 0/1 0/1
46 46 ic4x- -x -z y 0/1 0/1 0/1
47 47 ic4y- z -y -x 0/1 0/1 0/1
48 48 ic4z- -y x -z 0/1 0/1 0/1

this space group has the following wycoff position
8a 0 0/1 0 0/1 0 0/1
8b 0 1/2 0 1/2 0 1/2
16c 0 1/3 0 1/3 0 1/3
16d 0 5/8 0 5/8 0 5/8
32e 1 0/1 1 0/1 1 0/1
48f 1 0/1 0 0/1 0 0/1
96g 1 0/1 1 0/1 3 0/1
96h 0 1/3 2 0/1 -2 1/4
192i 1 0/1 2 0/1 3 0/1

atom-name(H,He,...) or . (to finish) ? :

```

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).

