36th Computational Material Design Workshop

Thursday, 20 February 2020
at Graduate School of Science and Technology, Osaka University

ABCAP: Beginners Course

ABCAP (**A**ll electron **B**and **CA**lculation **P**ackage): FLAPW code

Noriaki Hamada[1,2] and Hiroki Funashima[3]

[1]Department of Physics, Tokyo University of Science
[2]Center for Spintronics Research Network, Osaka University
[3]Department of Physics, Kyushu University

Email: hamada@rs.tus.ac.jp (Hamada), funashima.hiroki@phys.kyushu-u.ac.jp (Funashima)

Purpose in this course

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

②Study the symmetry of wavefunction (irreducible representations).

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

1-1. Environment variables

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

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


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

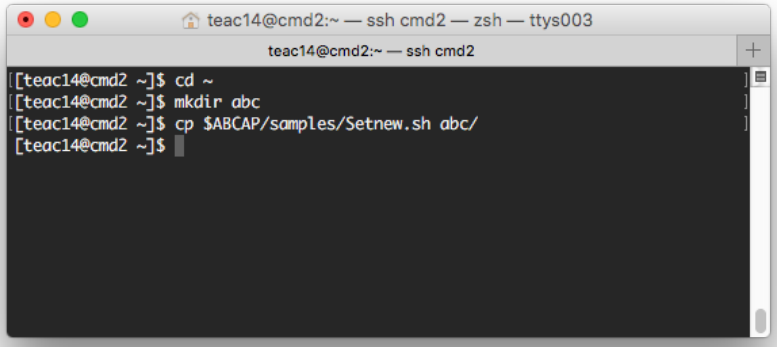
contents: /home/CMD/teac02/abcap1707/Bash_envs

1-2. Preparation

Make a directory, e.g., ***abc***, for the ABCAP calculation.

Copy a shell-script file, ***Setnew.sh*** to your directory, as follows:

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



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

Hands on DFT simulation

- Ferromagnetic Fe
- Nonmagnetic AlP

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

The procedure consists of

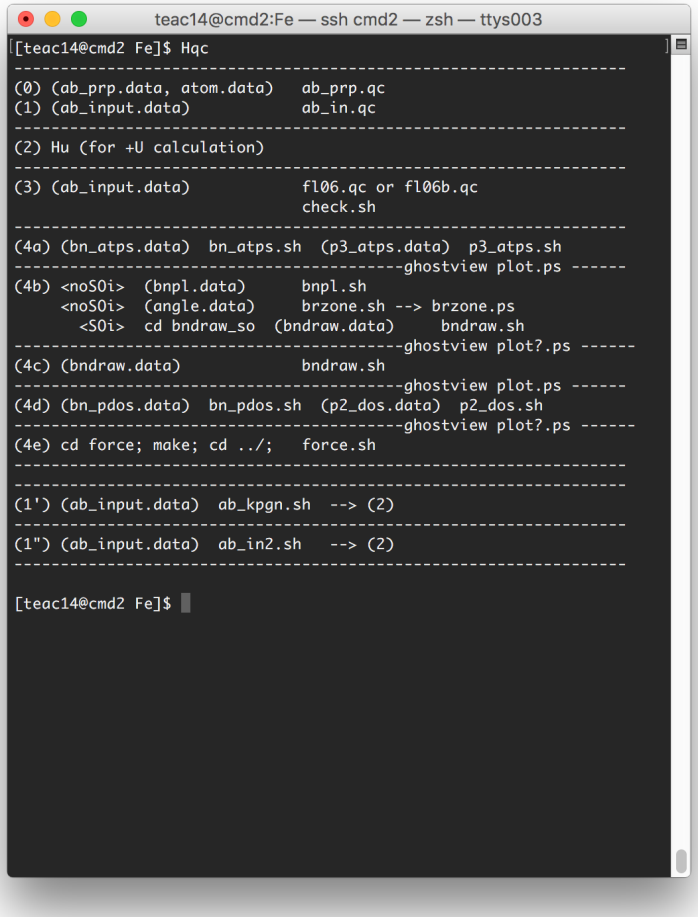
- Edit a file, ???.data.
- Execute a shell-script file, ???.sh/ ???.qsub

Attention

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

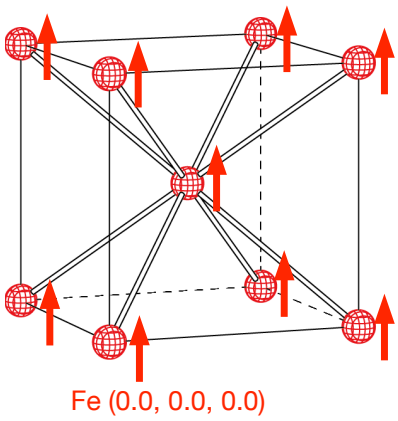
e.g.

ab_prp.qc -> ab_prp.qsub



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

Body Centered Cubic (BCC) Structure



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

Lattice Type

Point group O_h has full cubic symmetry.

3-fold rotation

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

Space Group

periodicity: 14 Bravais Lattice

point symmetry: 32 point group

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

7 crystal systems

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

Subgroup of O_h / D_{6h}

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

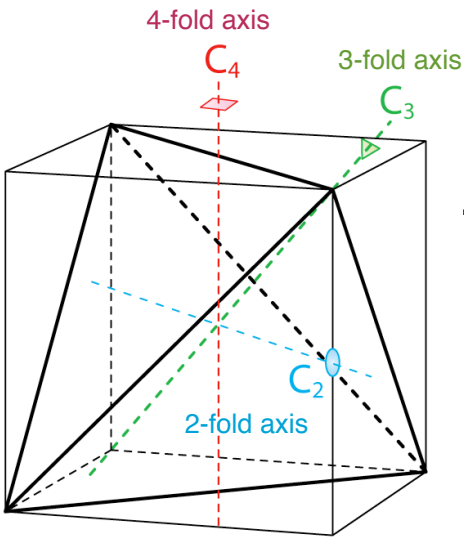
symmetry Operation

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

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

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

Point Group: O_h



Cubic Symmetry O_h

$E \cdots\cdots 1$ identity operation

$C_4 \cdots\cdots 6$

$C_4^2 \cdots\cdots 3$ $\pm\pi/2$

$C_2 \cdots\cdots 6$ $\pm\pi$

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

24 rotational operation

+ inversion, rotation inversion, reflection and rotational reflection

48 symmetry Operation

subgroup of O_h

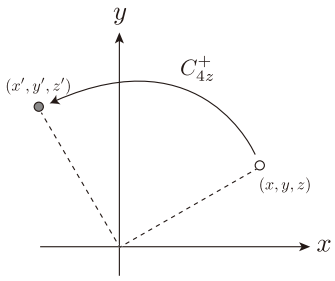
example

Tetrahedral Symmetry → T_d

$T_d \otimes C_4 = O_h$

Rotational Operation

example: C_{4z}^{+}

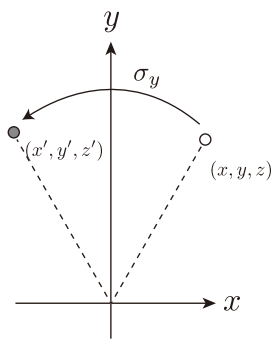


$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{matrix representation of } C_{4z}^{+}} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -y \\ x \\ z \end{bmatrix}$$

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

reflectional Operation

example: σ_{yz}



$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \underbrace{\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{matrix representation of } \sigma_{yz}} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ y \\ z \end{bmatrix}$$

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

$$= \underbrace{\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}}_{\text{space inversion(I)}} \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}}_{C_{2x}} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

C_{2x} ← x-axis is the normal direction of yz-plane

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

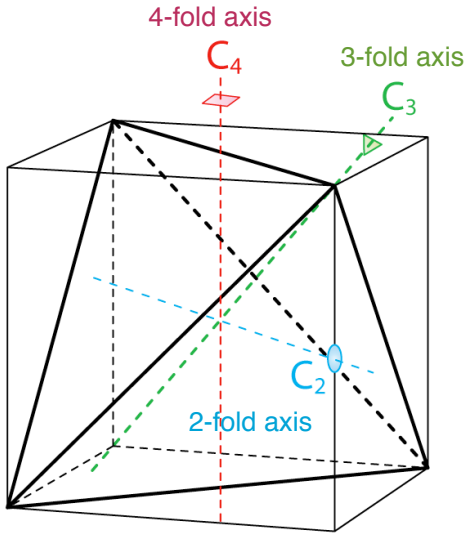
rotational operation code for O_h and subgroup in TSPACE

identity

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

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

space inversion



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

production between group elements

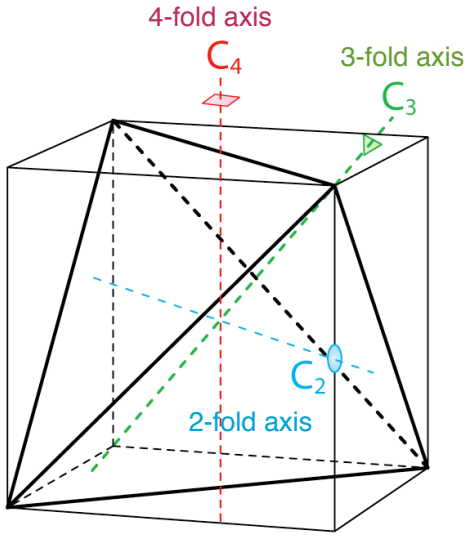
e.g. $C_{2b} \cdot C_{2x} = ?$

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

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

rotational operation code for O_h and subgroup in TSPACE

identity	(1)	E	(x, y, z)	(25)	IE	(-x, -y, -z)
C_4^2	(2)	C2x	(x, -y, -z)	(26)	IC2x	(-x, y, z)
	(3)	C2y	(-x, y, -z)	(27)	IC2y	(x, -y, z)
	(4)	C2z	(-x, -y, z)	(28)	IC2z	(x, y, -z)
$C_3^{\pm}$	(5)	C31+	(z, x, y)	(29)	IC31+	(-z, -x, -y)
	(6)	C32+	(-z, x, -y)	(30)	IC32+	(z, -x, y)
	(7)	C33+	(-z, -x, y)	(31)	IC33+	(z, x, -y)
	(8)	C34+	(z, -x, -y)	(32)	IC34+	(-z, x, y)
	(9)	C31-	(y, z, x)	(33)	IC31-	(-y, -z, -x)
	(10)	C32-	(y, -z, -x)	(34)	IC32-	(-y, z, x)
	(11)	C33-	(-y, z, -x)	(35)	IC33-	(y, -z, x)
	(12)	C34-	(-y, -z, x)	(36)	IC34-	(y, z, -x)
C_2	(13)	C2a	(y, x, -z)	(37)	IC2a	(-y, -x, z)
	(14)	C2b	(-y, -x, -z)	(38)	IC2b	(y, x, z)
	(15)	C2c	(z, -y, x)	(39)	IC2c	(-z, y, -x)
	(16)	C2d	(-x, z, y)	(40)	IC2d	(x, -z, -y)
	(17)	C2e	(-z, -y, -x)	(41)	IC2e	(z, y, x)
	(18)	C2f	(-x, -z, -y)	(42)	IC2f	(x, z, y)
$C_4^{\pm}$	(19)	C4x+	(x, -z, y)	(43)	IC4x+	(-x, z, -y)
	(20)	C4y+	(z, y, -x)	(44)	IC4y+	(-z, -y, x)
	(21)	C4z+	(-y, x, z)	(45)	IC4z+	(y, -x, -z)
	(22)	C4x-	(x, z, -y)	(46)	IC4x-	(-x, -z, y)
	(23)	C4y-	(-z, y, x)	(47)	IC4y-	(z, -y, -x)
	(24)	C4z-	(y, -x, z)	(48)	IC4z-	(-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
C_{2b} 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

e.g.

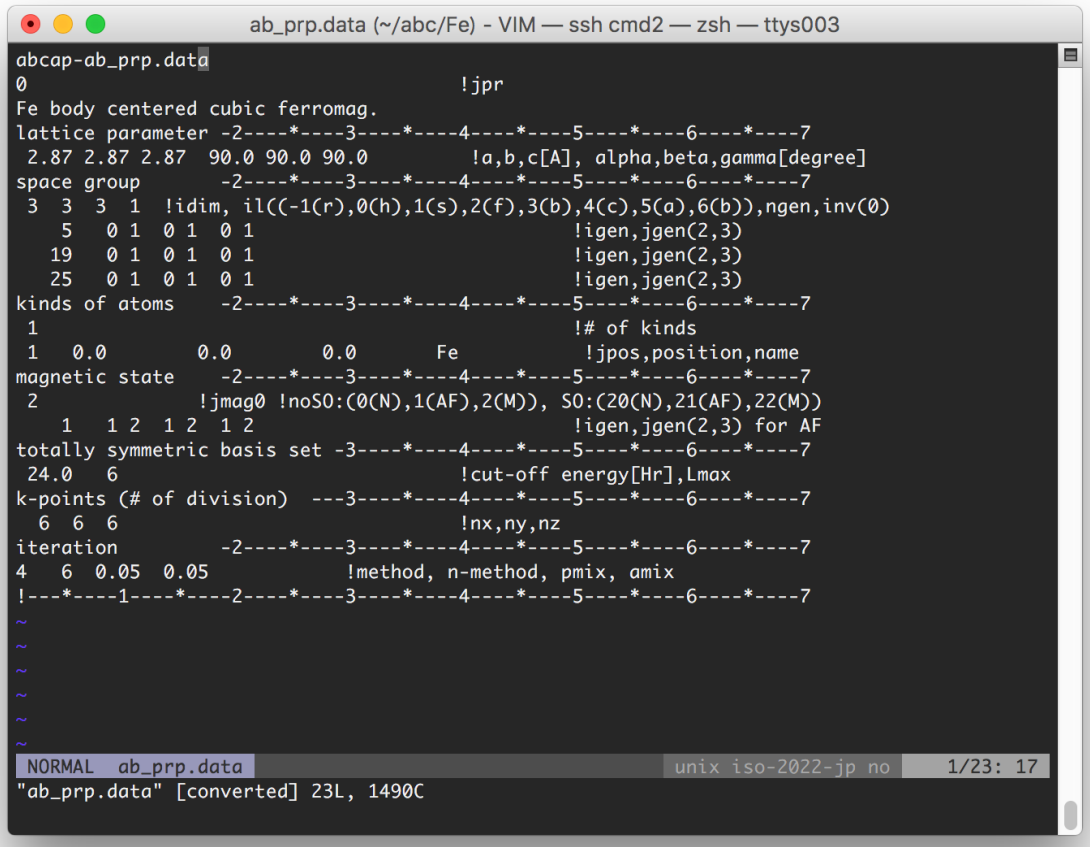
$C_{2b} \cdot C_{2x} = C_{4z}^{-}$

(14) (2) (24)

group multiplication table(including space inversion)

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

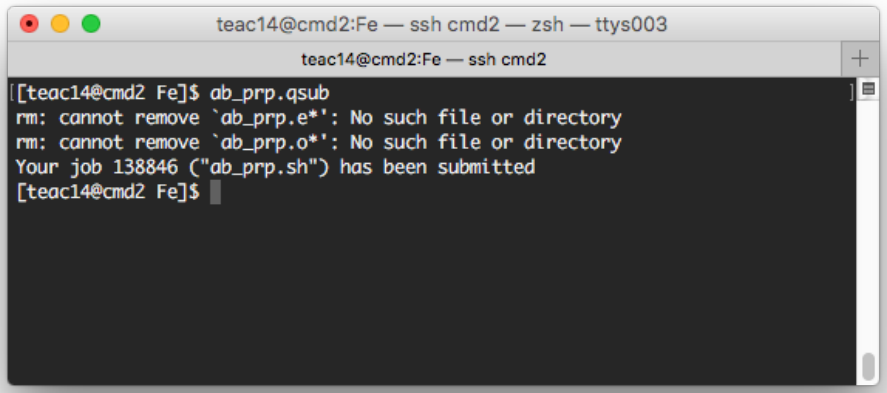
ab_prp.data for bcc ferromagnetic Iron



1. Crystal Structure

In this workshop, you execute *"ab_prp.qsub"* instead of *"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.



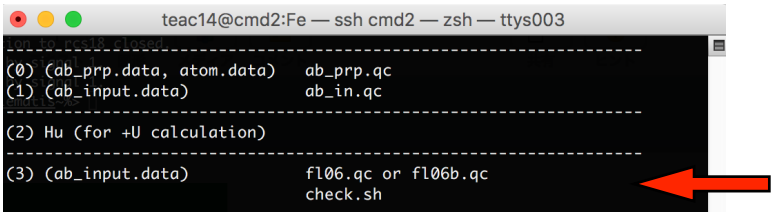
The file, ***ab_input.data***, is made from the informations of ***ab_prp.data*** and ***atom.data***.
The ***atom.data*** file is a data base for atoms from H(hydrogen) to U(uranium).

2. initial charge density, potential and etc…

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

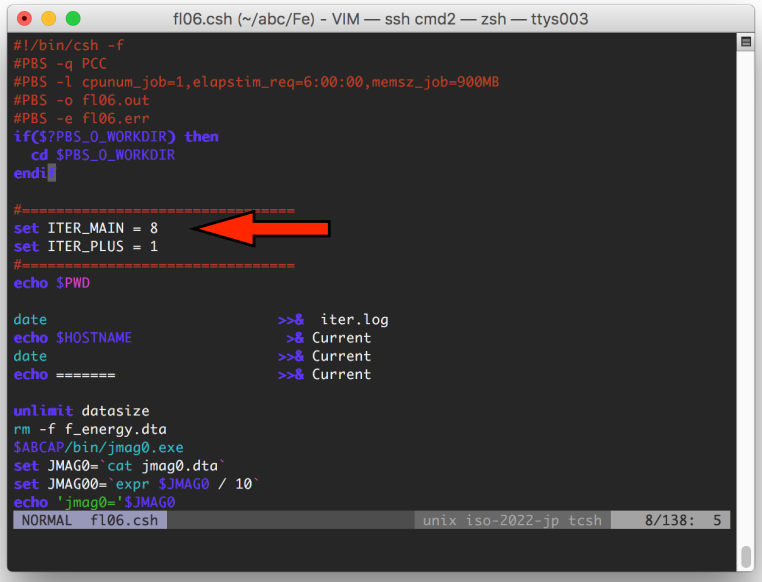
- ***ab_in.exe***: checks: the crystal structure, and makes totally-symmetric basis functions.
- ***ab_inch.exe***: makes the initial charge density as the superposition of atomic charge densities.
- ***ab_kpgn.exe***: generates the k points used in the calculation.
- ***ab_size.exe***: estimates the size of calculation.
- ***ab_ospw.exe***: calculates the overlap integral among the totally symmetric basis functions.
- ***fl_dm00.exe***: sets the initial value of the local density matrix. (diagonal elements are 1/2)

3. Self-Consistent Field(SCF) Calculation



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

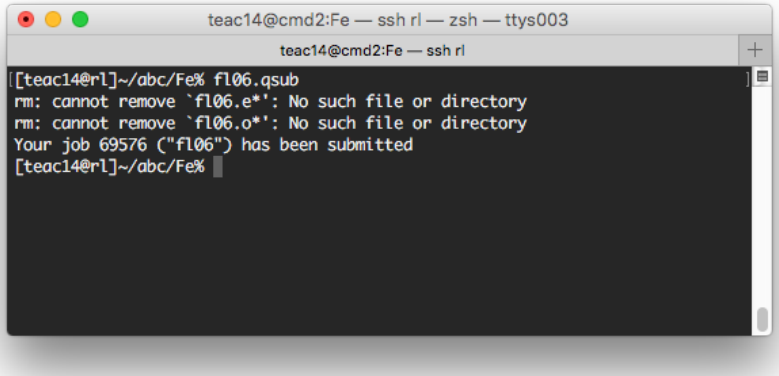
contents of ***"fl06.sh"***



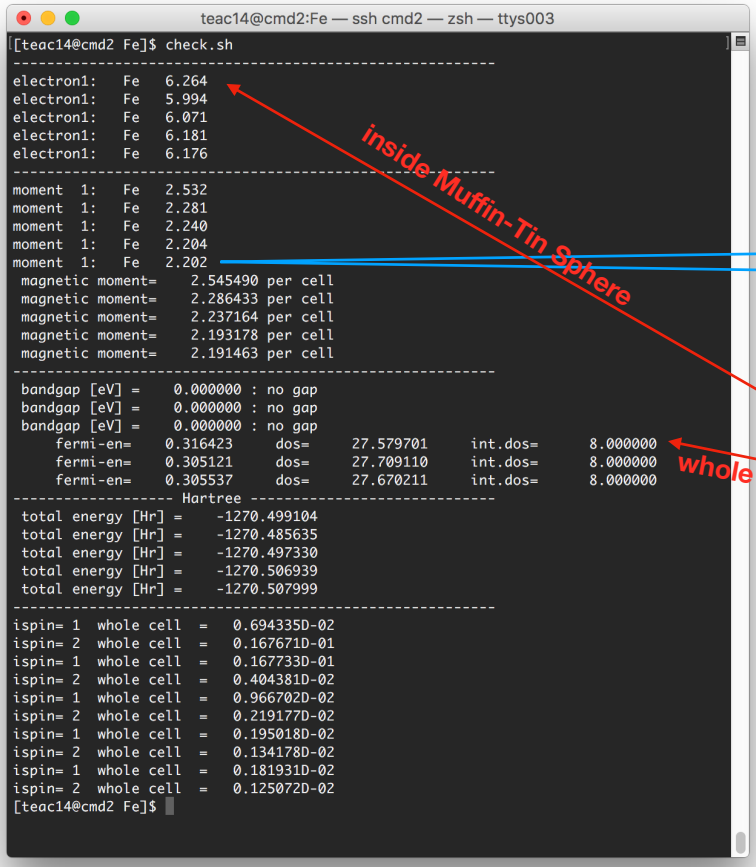
In ***fl06.qsub***, the following programs run:

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

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



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



Metal	M_s (μ_B / atom)
Iron	2.2
Cobalt	1.7
Nickel	0.6
Gd	6.8
Dy	10.2

magnetic moment per atom

atomic configuration for Fe

Fe: [Ar] $(3d)^6$ $(4s)^2$

core electron valence electron

total valence electrons: 6+2 = 8

character of valence electrons

3d electron: localized

4s electron: itinerant

4s electron is expanded at the interstitial region,

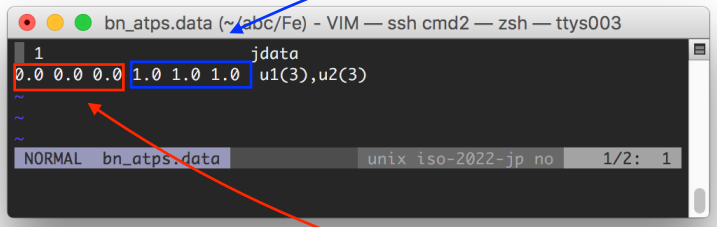
$$n_e = 6.0 + \delta$$

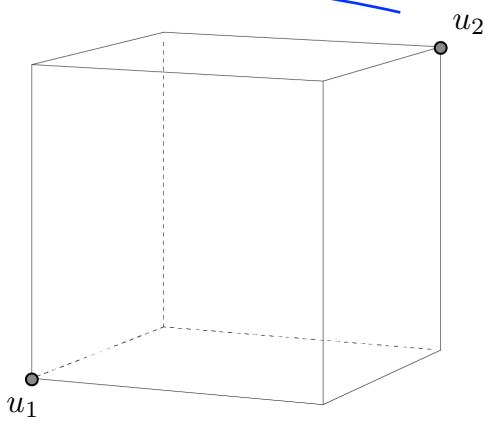
4-1. Drawing the Crystal Structure

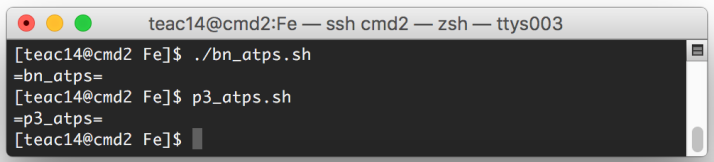
① Edit ***bn_atps.data***. Give the region of drawing in the file.

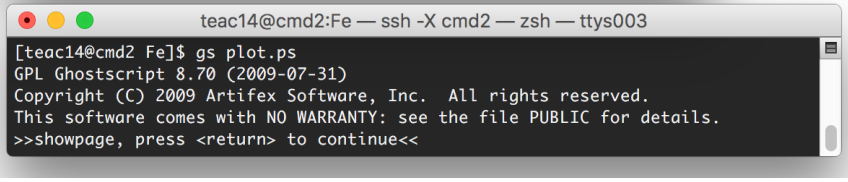
② Run ***bn_atps.sh*** and ***p3_atps.sh***.

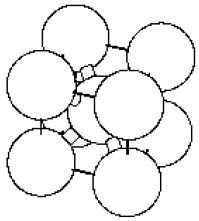
③ A postscript file, ***plot.ps***, is obtained.











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

① Edit ***bnpl.data*** and ***a_bnpl.data*** . Give paths in the k-space to be drawn.

② Run ***bnpl.sh***.

③ ***plot.ps*** is obtained for the nonmagnetic case (jmag=0) or the antiferromagnetic case (jmag=1); ***plot1.ps*** and ***plot2.ps*** are obtained for the magnetic case (jmag=2).

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

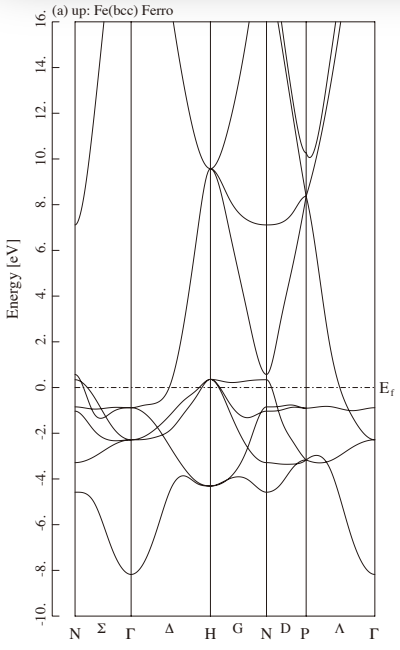
```
@bcap-a_bnpl.data

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 (rhobohedral)
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

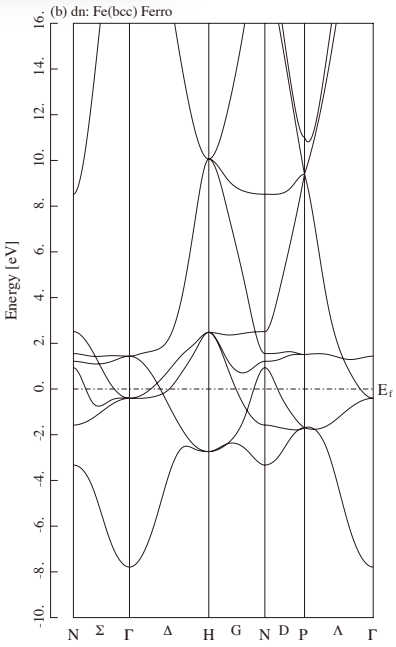
```
[teac14@cmd2 Fe]$ bnpl.sh
=reform_h=
=bnpl   =
[teac14@cmd2 Fe]$
```

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.
```



plot1.ps

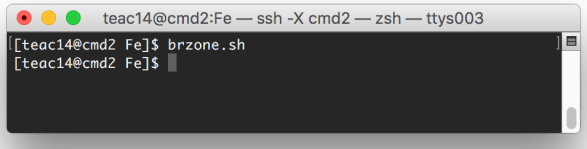


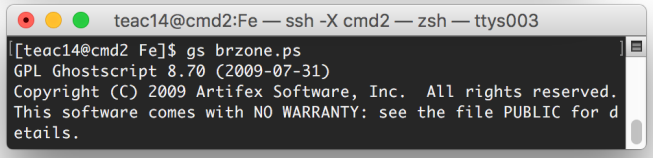
plot2.ps

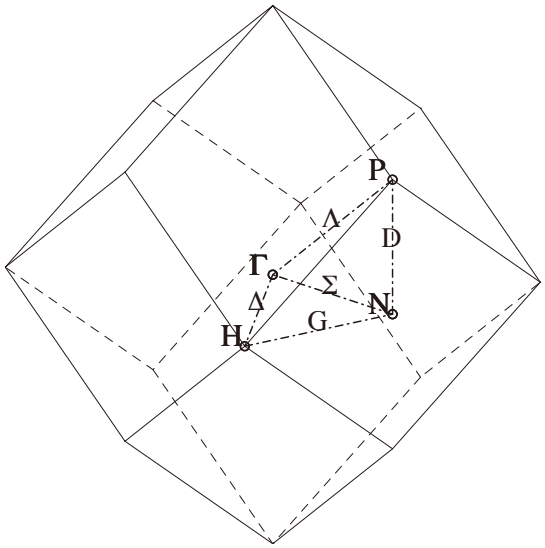
4-2. Drawing the k-space path and BZ

① Run ***brzone.sh***.

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







brzone.ps

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

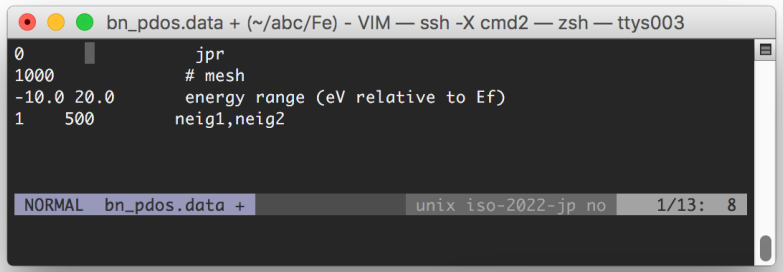
① Edit ***bn_pdos.data***. Give the energy region to be drawn.

② Run ***bn_pdos.sh***.

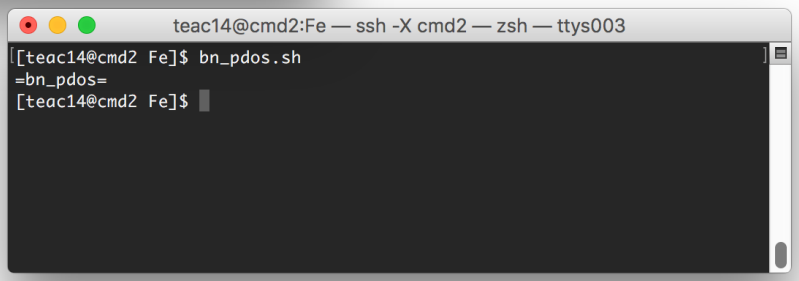
③ Edit ***p2_dos.data***. Select the total DOS, the s, p, d, and f partial DOS.

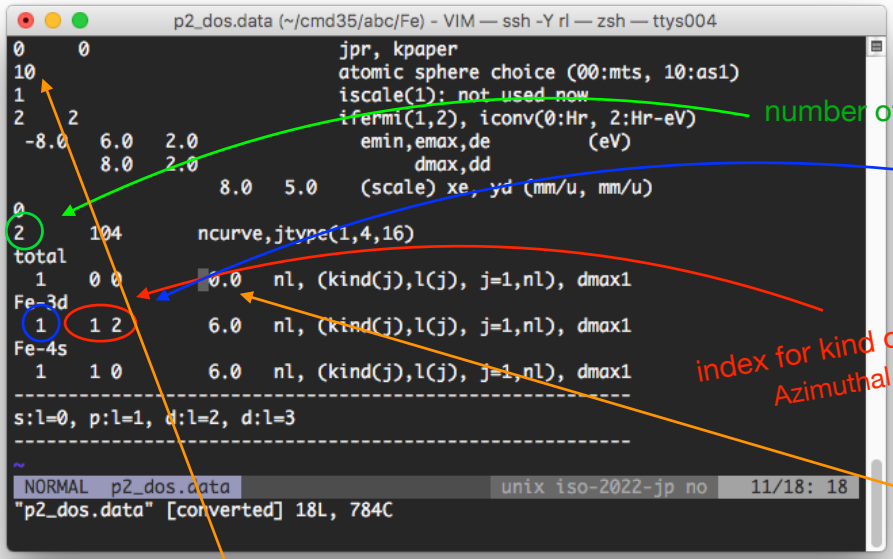
④ Run ***p2_dos.sh***

⑤ ***plot.ps*** is obtained for the nonmagnetic case (jmag=0) or the antiferromagnetic case (jmag=1); ***plot1.ps*** and ***plot2.ps*** are obtained for the magnetic case (jmag=2).



calculate DOS



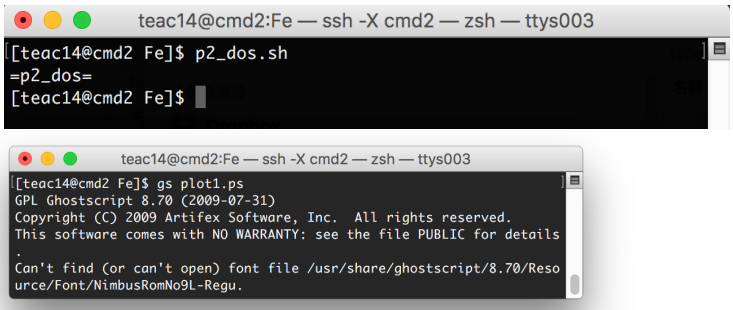


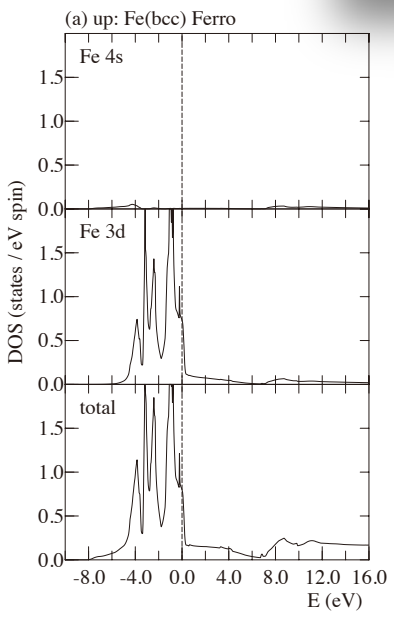
option for Partial density of states(PDOS)

00: only inside muffin-tin sphere, pdos is underestimated.
Because we should consider muffin-tin region and interstitial region.

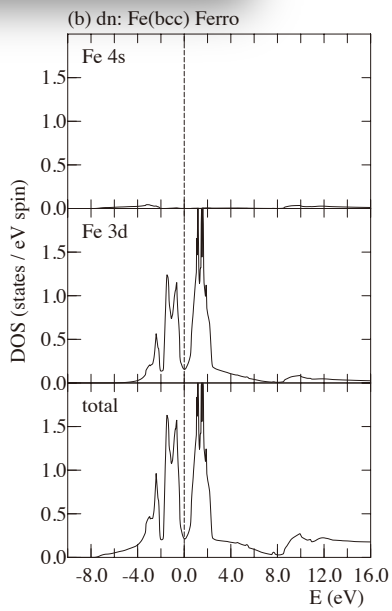
10: interpolated pdos, but sometimes pdos is overestimated.

drawing DOS curves





plot1.ps

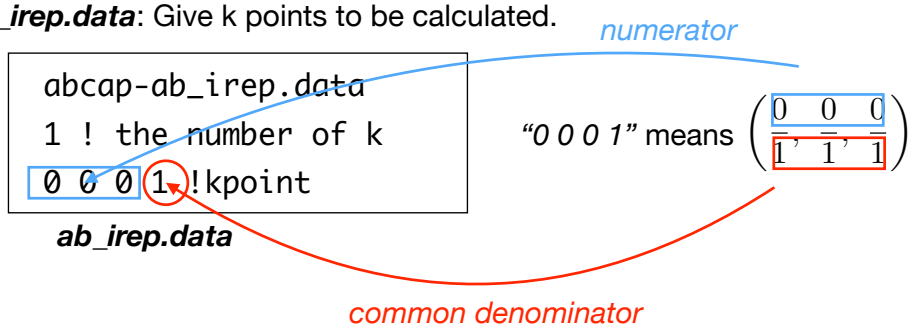


plot2.ps

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***.

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

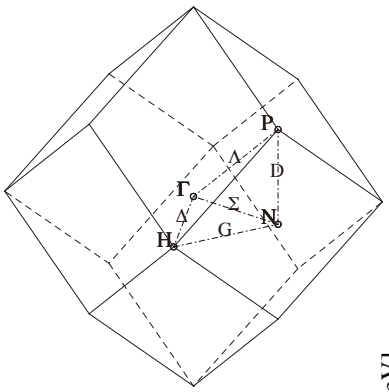
```
--- characters in (x,y,z) representation ---
jr3=  3 -1 -1 -1  0  0  0  0  0  0  0  0 -1 -1 -1 -1 -1 -1  1  1  1  1  1  1
     -3  1  1  1  0  0  0  0  0  0  0  0  1  1  1  1  1  1 -1 -1 -1 -1 -1 -1
order of the Gamma-point group = 48
no. of irreps=10  : dimension of irrep=  1  1  1  1  3  3  3 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

character of irreducible representation (case:Fe)

point group of k(case:Fe)

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

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



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

Irreducible representation at Γ(case:Fe)

1

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

7

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

9

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

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

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

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

Example: IR=9, symmetry operation index = 20

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

character table of Irreducible representation at Γ

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

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

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

1. 立方晶系の点群

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

1

9

7

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

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

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

Γ_6^+: $\{\alpha, \beta\}$

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

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

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

Γ_7^-: $\{xyz\alpha,\ xyz\beta\}$

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

A_{2u}: xyz

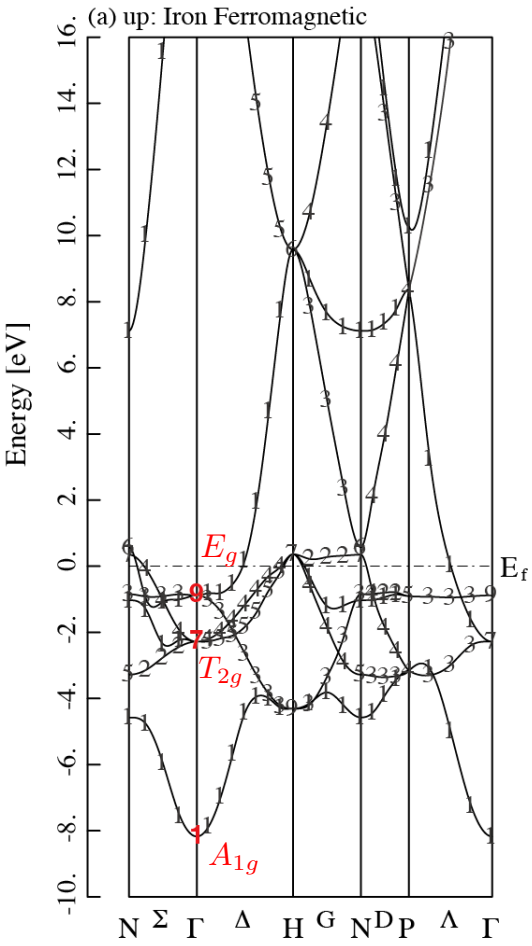
E_u : $\{xyzv, -xyzu\}$

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

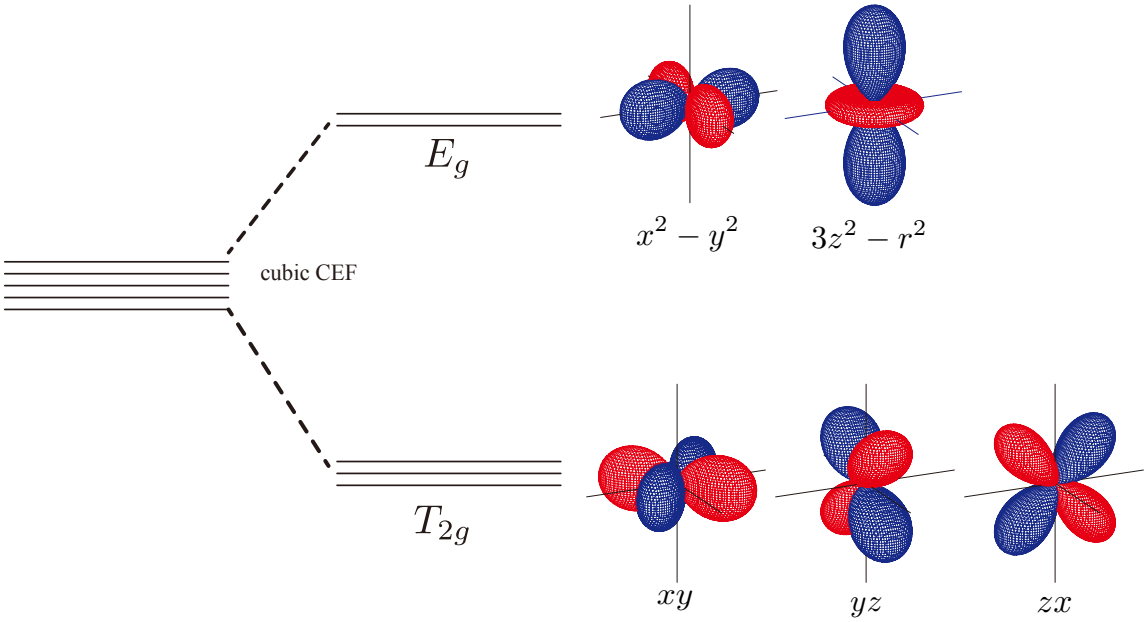
T_{2u}: $\{x(y^2-z^2),\ y(z^2-x^2),$
$z(x^2-y^2)\}$

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

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



Cubic Crystal Electric Field(CEF) for 3d



Optical property for semiconductor

- AIP

$$(\alpha|\vec{b})r = \alpha\vec{r} + \vec{b}$$ ⟸ lattice invariant

rotational operator

translation vector

$$\left(\alpha\left|\vec{b}\right.\right) = \left(\alpha\left|\vec{R_n} + \vec{b}'\right.\right) = \left(\epsilon\left|\vec{R_n}\right.\right)\left(\alpha\left|\vec{b}'\right.\right)$$

general vector of the Bravais lattice

zero vector or not primitive translation vector

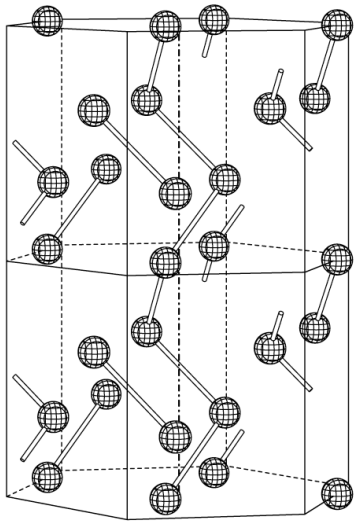
With a suitable choice of origin...

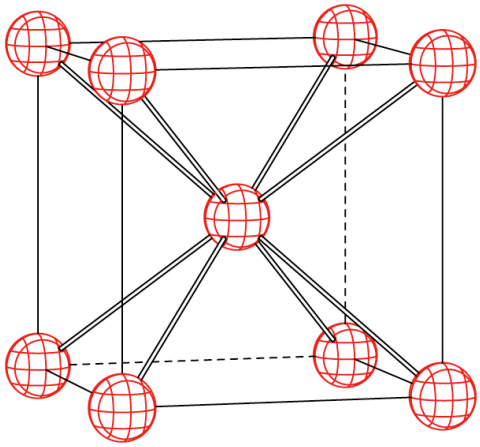
Do we find all the element of the symmetry operation in the form

$$\left(\alpha\left|\vec{b}\right.\right) = \left(\alpha\left|\vec{R_n}\right.\right) = \left(\epsilon\left|\vec{R_n}\right.\right)\left(\alpha\left|\vec{0}\right.\right) \quad ?$$

Yes ⇒ **symmorphic(共型)**

No ⇒ **non-symmorphic(非共型)**





non-symmorphic(非共型)

157(screw:らせん and glide:映進 + 2)

symmorphic(共型)

73 space group

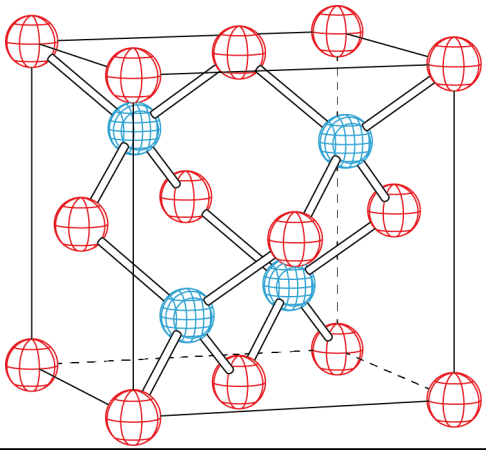
In symmorphic case, most of $\left(\alpha \mid \vec{b}'\right)$

are screw operation or glide operation

Example: non-symmorphic crystals

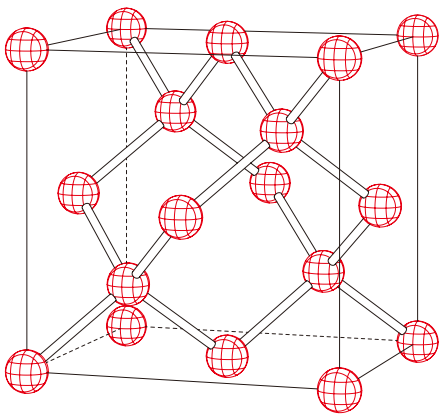
AlP(Aluminum Phosphide)

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



Si(Sillicon)

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



5.Optical property

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

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

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

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

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

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

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

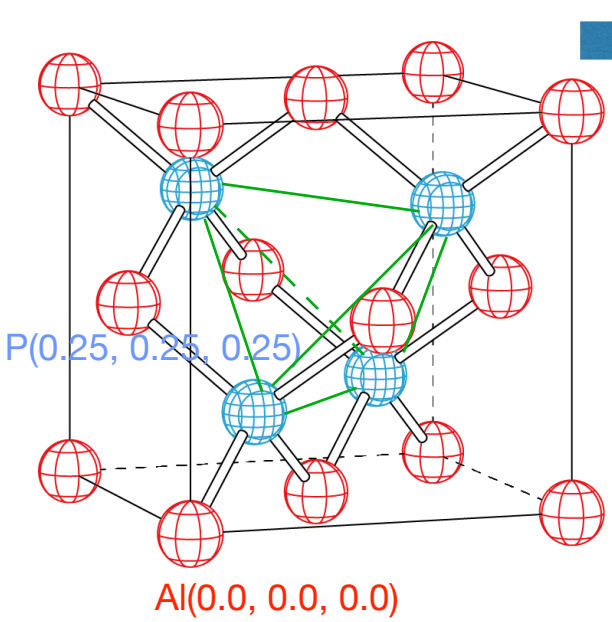
$$v_{\boldsymbol{k},n} = \left\langle \psi_{\boldsymbol{k},n} \left| \frac{\boldsymbol{p}}{m} \right| \psi_{\boldsymbol{k},n} \right\rangle$$

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

AlP

Zincblende Structure

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



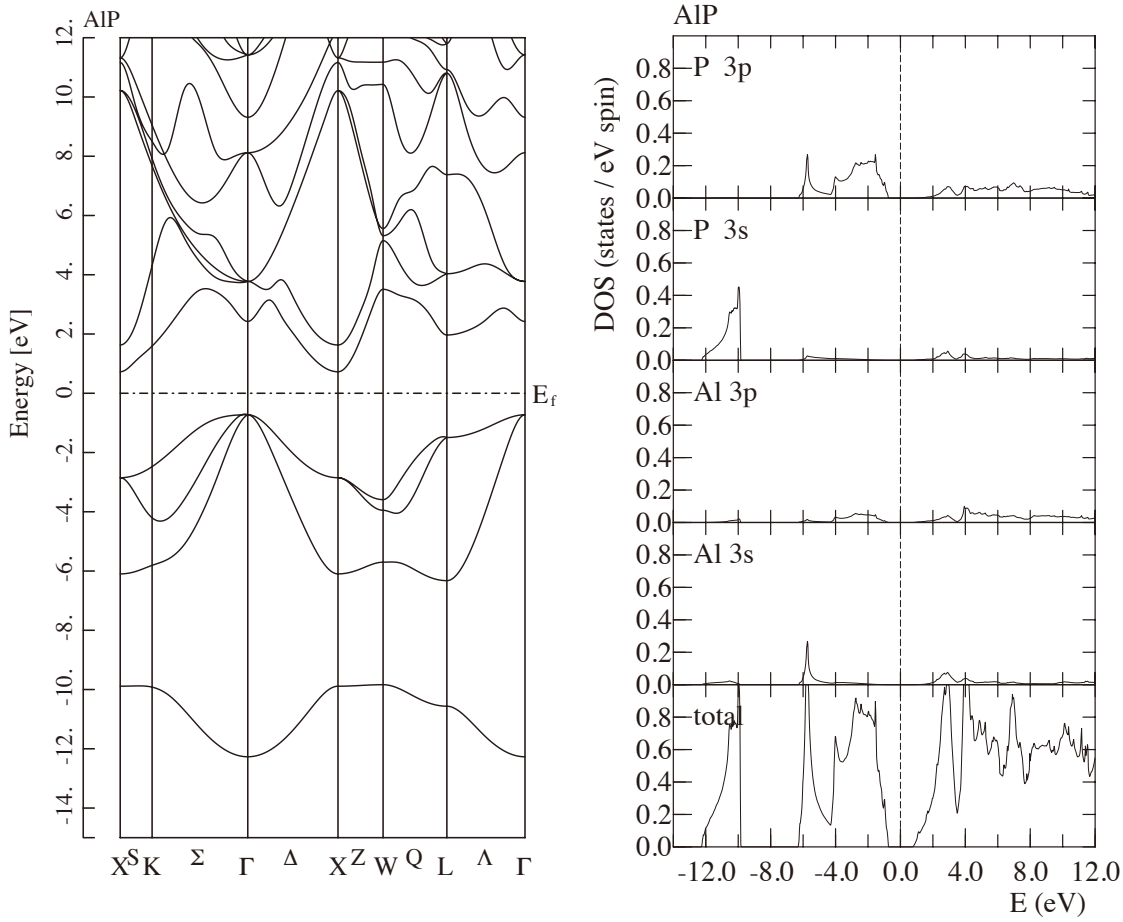
Point group T_d has full tetrahedral symmetry.

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

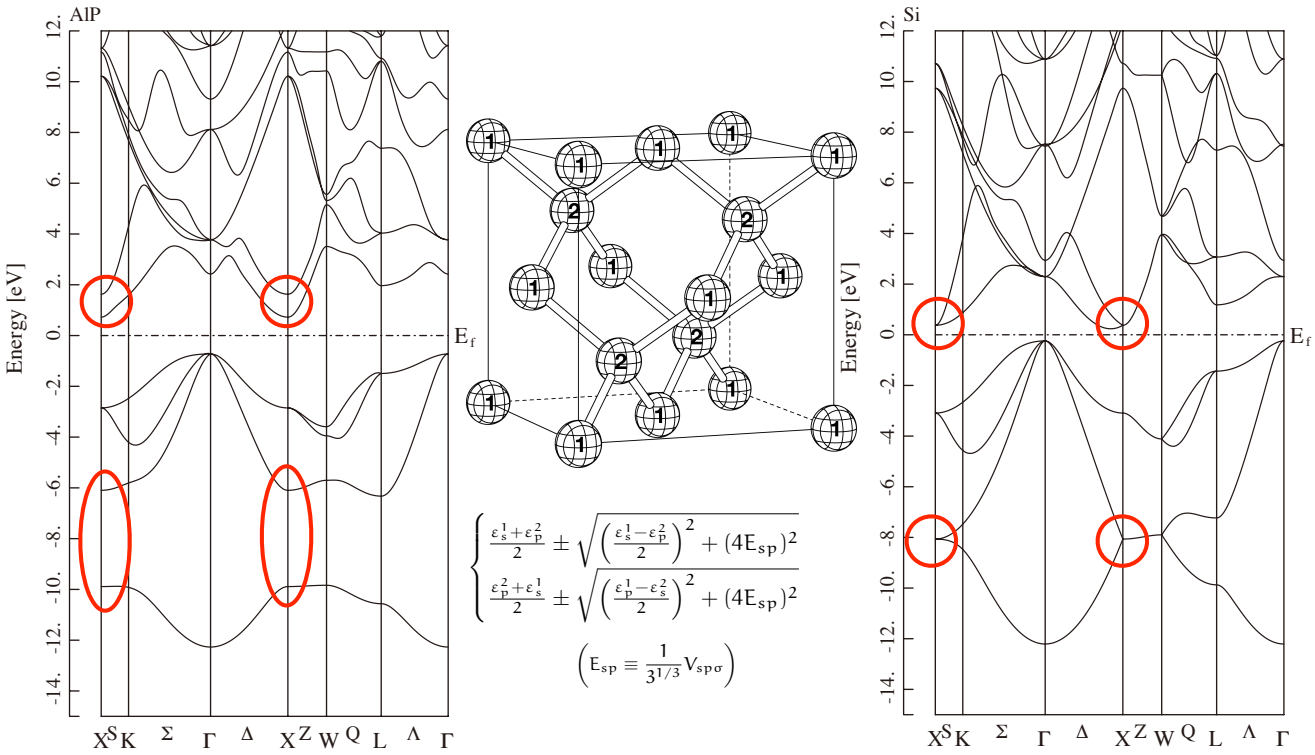
“*ab_prp.data*” for AlP

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

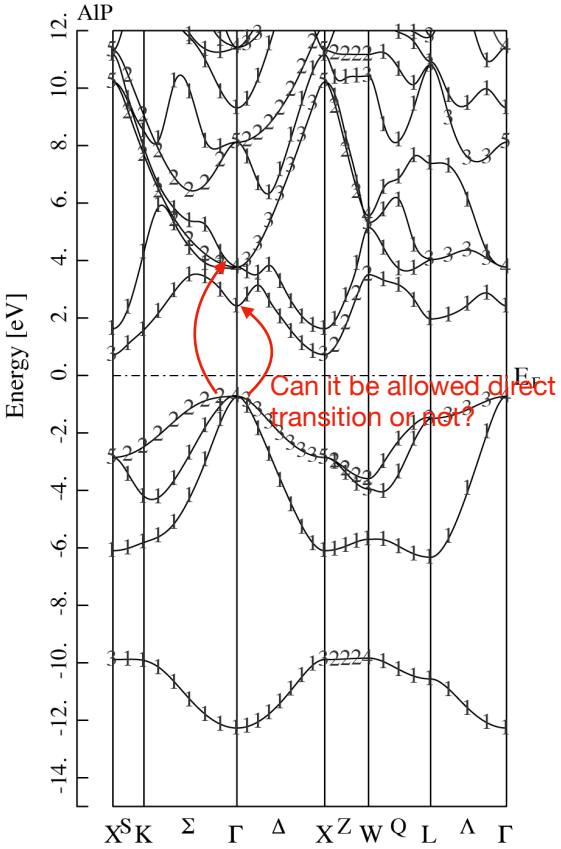
```
abcap-ab_prp.data
0                                       !jpr
AlN
lattice parameter -2----*----3----*----4----*----5----*----6----*----7
 5.45 5.45 5.45  90.0 90.0 90.0          !a,b,c[A], alpha,beta,gamma[degree]
space group       -2----*----3----*----4----*----5----*----6----*----7
 3  2  2  0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



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



5.1 preparation to check for optical transition(dipole allowed)



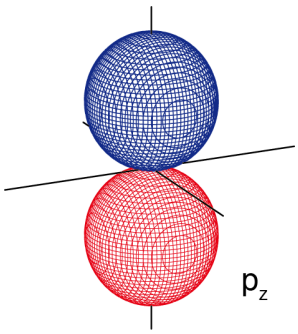
In quantum mechanics, the basis for an optical selection rule is the value of follow transition momentum integral

$$\int \psi_i^* \mu \psi_f \mathrm{d}\mathbf{r}$$

transition momentum operator

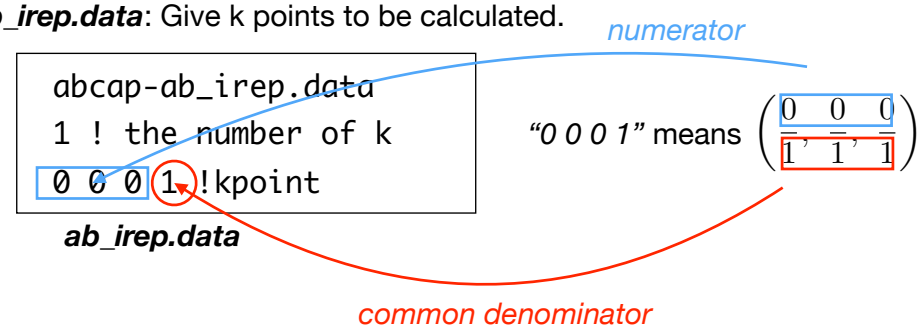
for z direction, μ="z".

Operator "z" has same symmetry which p_z has.



1: calculate Jones faithful representation

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



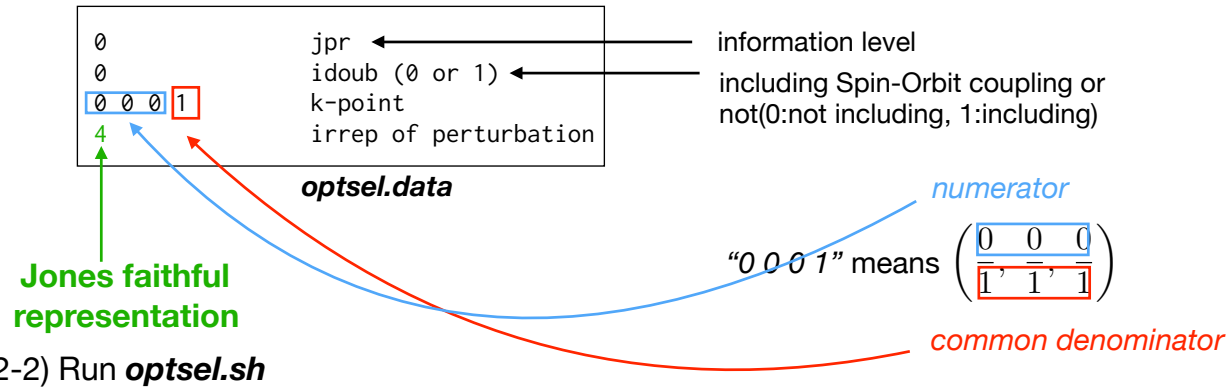
(2) Run ***ab_irep.sh***.

```
order of the Gamma-point group = 24
no. of irreps= 5  : dimension of irrep=  1  1  3  3  2
nkg,ir1=   24    1     nd(ir1)=    1
nkg,ir1=   24    2     nd(ir1)=    1
nkg,ir1=   24    3     nd(ir1)=    3
nkg,ir1=   24    4     nd(ir1)=    3
nkg,ir1=   24    5     nd(ir1)=    2
irrep=    4   nint(abs(qr(ir1)))=   24
--- irredusible decomposition of Jones faithful rep.---
irrep= 4 :  ndim= 3
```

check

2: check optical dielectric transition

(2-1) Edit ***optsel.data***: Give k points to be calculated.



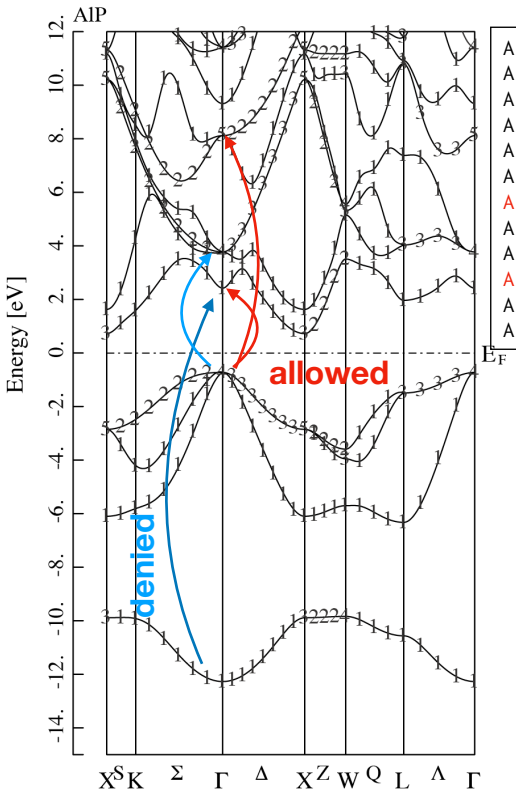
(2-2) Run ***optsel.sh***

(2-3) See ***optsel.txt***

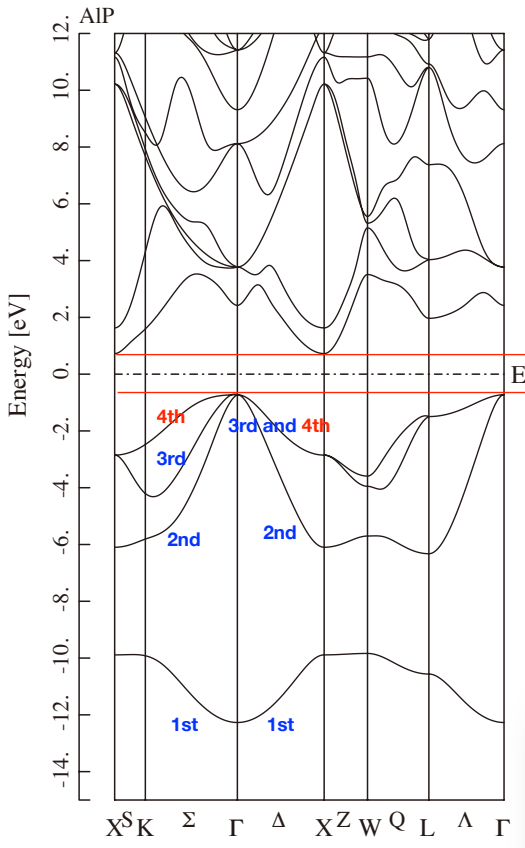
```
 Allowed transition : irrep  1 --> irrep  4   by irrep(  4 )-perturbation
 Allowed transition : irrep  2 --> irrep  3   by irrep(  4 )-perturbation
 Allowed transition : irrep  3 --> irrep  2   by irrep(  4 )-perturbation
 Allowed transition : irrep  3 --> irrep  3   by irrep(  4 )-perturbation
 Allowed transition : irrep  3 --> irrep  4   by irrep(  4 )-perturbation
 Allowed transition : irrep  3 --> irrep  5   by irrep(  4 )-perturbation
 Allowed transition : irrep  4 --> irrep  1   by irrep(  4 )-perturbation
 Allowed transition : irrep  4 --> irrep  3   by irrep(  4 )-perturbation
 Allowed transition : irrep  4 --> irrep  4   by irrep(  4 )-perturbation
 Allowed transition : irrep  4 --> irrep  5   by irrep(  4 )-perturbation
 Allowed transition : irrep  5 --> irrep  3   by irrep(  4 )-perturbation
 Allowed transition : irrep  5 --> irrep  4   by irrep(  4 )-perturbation
```

optsel.txt

summary for transition




```
Allowed transition : irrep  1 --> irrep  4   by irrep(  4 )-perturbation
Allowed transition : irrep  2 --> irrep  3   by irrep(  4 )-perturbation
Allowed transition : irrep  3 --> irrep  2   by irrep(  4 )-perturbation
Allowed transition : irrep  3 --> irrep  3   by irrep(  4 )-perturbation
Allowed transition : irrep  3 --> irrep  4   by irrep(  4 )-perturbation
Allowed transition : irrep  3 --> irrep  5   by irrep(  4 )-perturbation
Allowed transition : irrep  4 --> irrep  1   by irrep(  4 )-perturbation
Allowed transition : irrep  4 --> irrep  3   by irrep(  4 )-perturbation
Allowed transition : irrep  4 --> irrep  4   by irrep(  4 )-perturbation
Allowed transition : irrep  4 --> irrep  5   by irrep(  4 )-perturbation
Allowed transition : irrep  5 --> irrep  3   by irrep(  4 )-perturbation
Allowed transition : irrep  5 --> irrep  4   by irrep(  4 )-perturbation
```



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

```
teac14@cmd2:AlP — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 AlP]$ 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
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
```

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***"

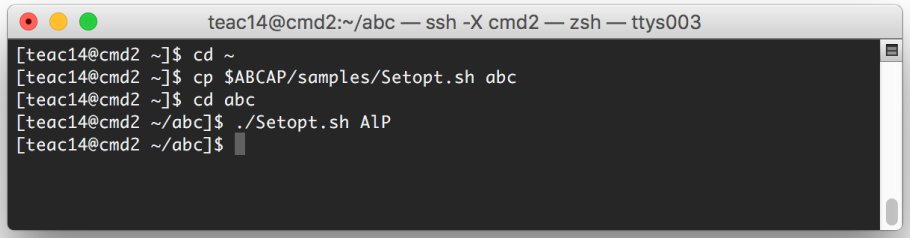
```
f_ef.dta (~/abc/AlP) - VIM — ssh -X cmd2 — zsh — ttys002
@bcap-ef[Hr]:   Fermi-level, dos, vale, band-E (/spin)
  0.1768167130061111E+00          1   40
         4         4        40     # of fully-occ. bands, # of occ. bands
  0.0000000000000000E+00  0.4000000000000000E+01 -0.5711363479187916E-01 spin=1
~
~
~
~
NORMAL  f_ef.dta                                  unix iso-2022-jp no    1/4:  1
```

5.2 preparation to calculation for optical properties

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

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

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



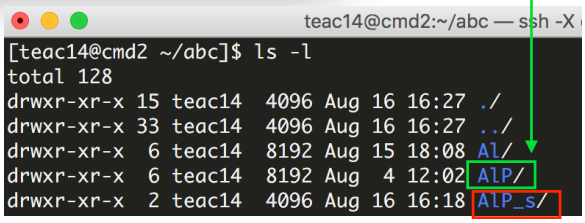
working directory for SCF calc.

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

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

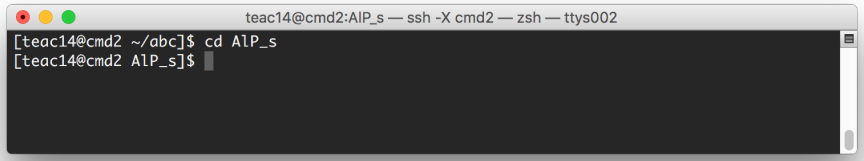
② results for SCF calculation for "AlP" is copied from "AlP" to "AlP_s"

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

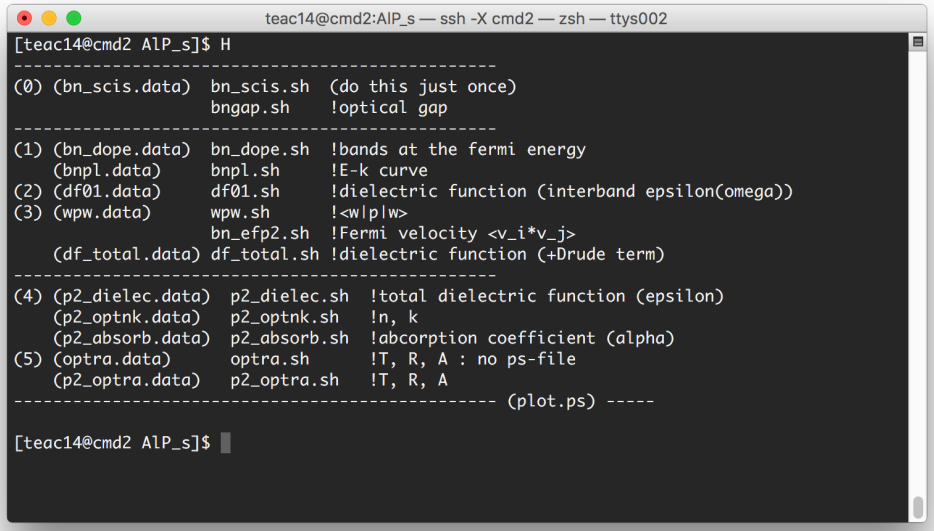


working directory for the calculation for optical properties (script makes).

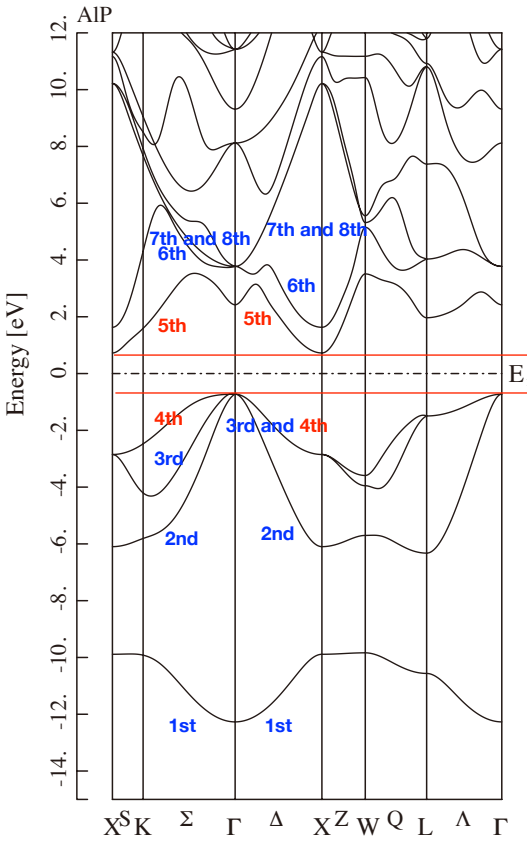
Firstly, we enter the working directory, *"AlP_s"*



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



5.2.1 correct to optical band gap (Scissors Operator)



1.449960[ev] (indirect)

underestimated band gap(~1.0eV)

experimental data:

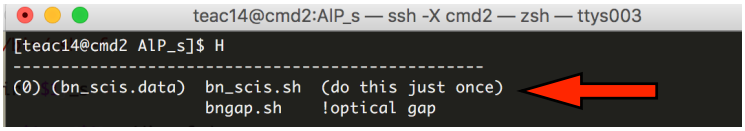
2.45[ev](indirect)

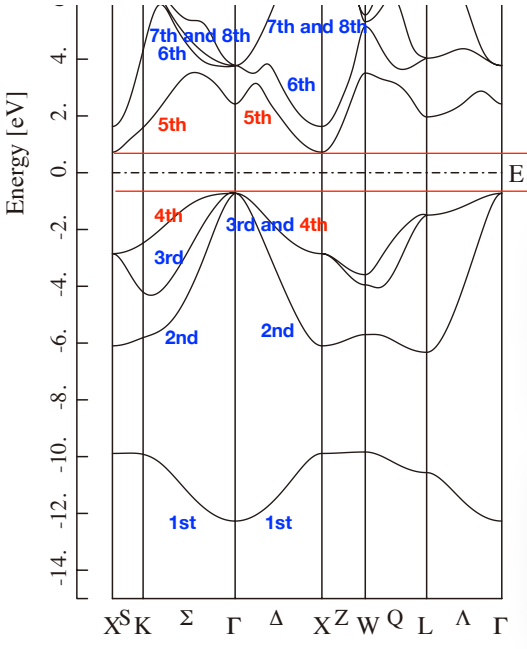
L. I. Berger, *"Semiconductor Materials"* (1996). CRC Press.

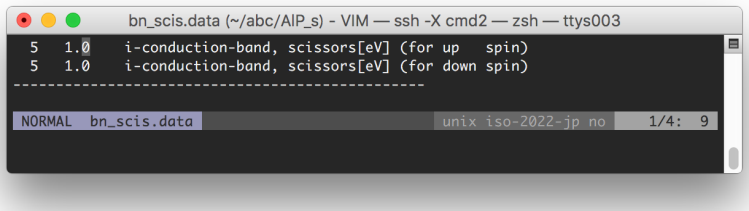
① Edit ***bn_scis.data*** Set band indexes which Scissors operator operate.

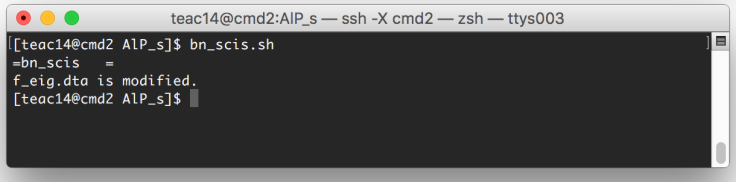
② Run ***bn_scis.sh***.

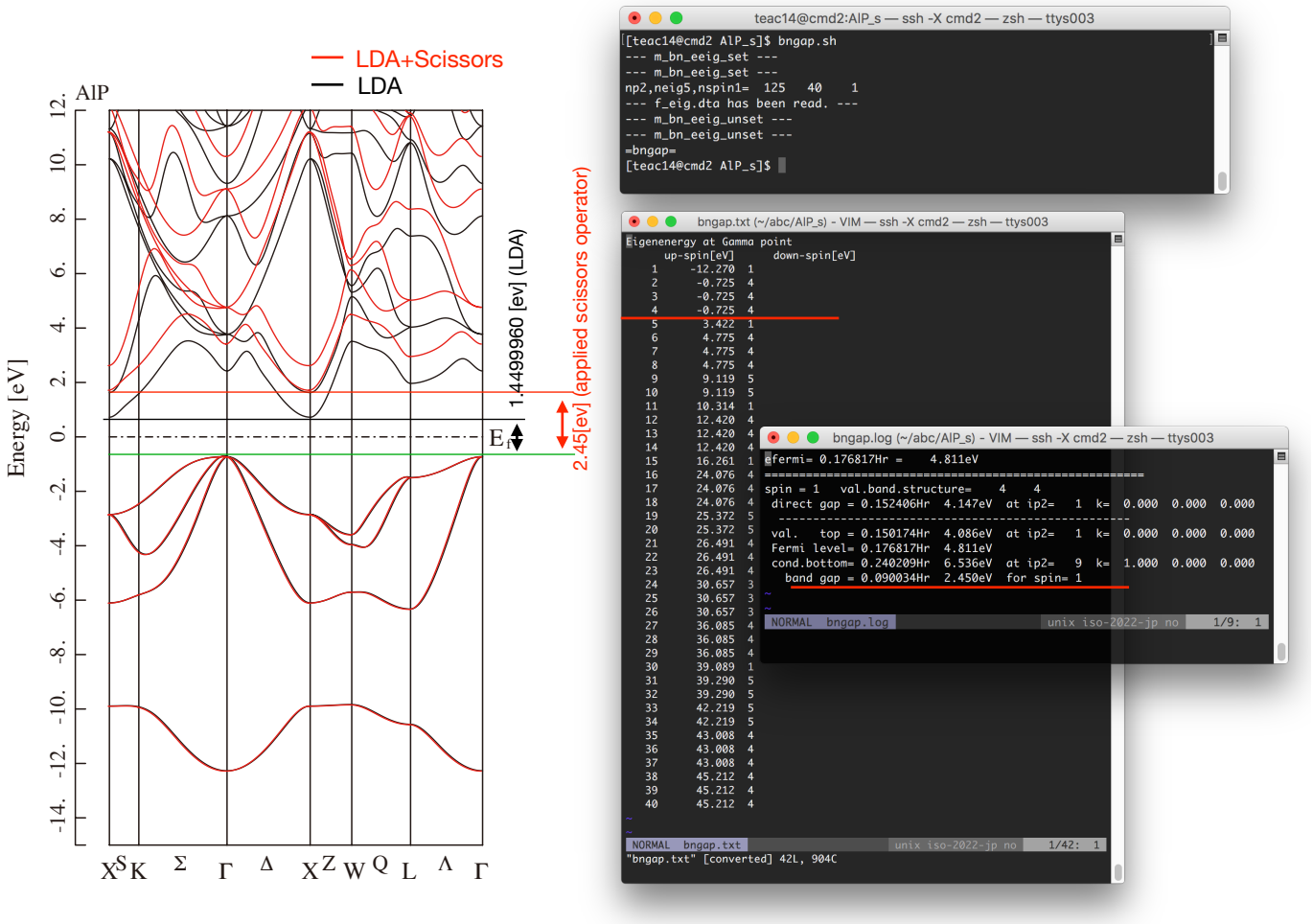
③ ***bngap.sh*** show the information about optical band gap

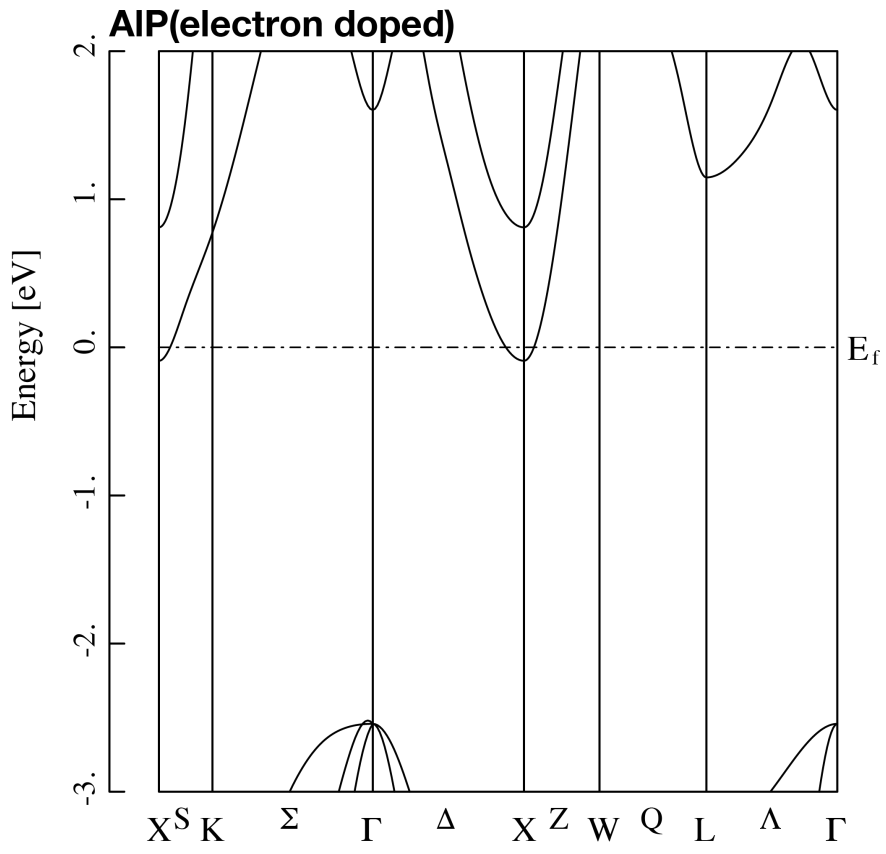









LDA+Scissors
LDA
AlP
Energy [eV]
12.
10.
8.
6.
4.
2.
0.
-2.
-4.
-6.
-8.
-10.
-12.
-14.
1.4499960 [ev] (LDA)
2.45[ev] (applied scissors operator)
E_f
X^S K Σ Γ Δ X^Z W Q L Λ Γ
teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys003
[teac14@cmd2 AlP_s]$ bngap.sh
--- m_bn_eeig_set ---
--- m_bn_eeig_set ---
np2,neig5,nspin1= 125 40 1
--- f_eig.dta has been read. ---
--- m_bn_eeig_unset ---
--- m_bn_eeig_unset ---
=bngap=
[teac14@cmd2 AlP_s]$
bngap.txt (~/abc/AlP_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
NORMAL bngap.txt unix iso-2022-jp no 1/42: 1
"bngap.txt" [converted] 42L, 904C
bngap.log (~/abc/AlP_s) - VIM — ssh -X cmd2 — zsh — ttys003
efermi= 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


AlP(electron doped)
Energy [eV]
2.
1.
0.
-1.
-2.
-3.
E_f
X^S K Σ Γ Δ X^Z W Q L Λ Γ

5.2.2 calculation for dielectric function

Here we calculate the dielectric function, $\epsilon_{ij}(\omega)$

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

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

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

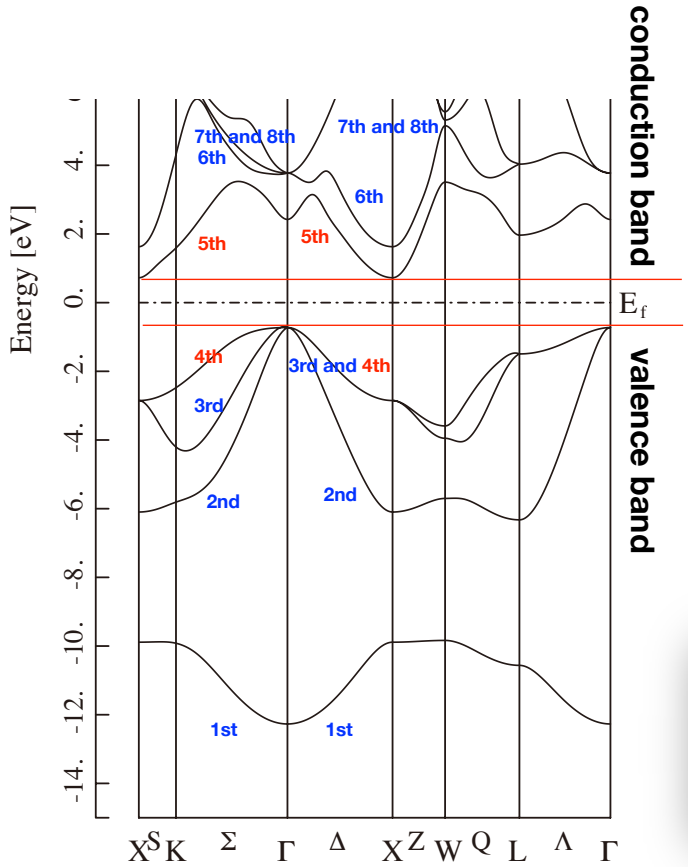
```
teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys002
[teac14@cmd2 AlP_s]$ H
-----------------------------------------------
(0) (bn_scis.data)  bn_scis.sh  (do this just once)
                    bngap.sh    !optical gap
-----------------------------------------------
(1) (bn_dope.data)  bn_dope.sh  !bands at the fermi energy
    (bnpl.data)     bnpl.sh     !E-k curve
(2) (df01.data)     df01.sh     !dielectric function (interband epsilon(omega))
(3) (wpw.data)      wpw.sh      !<w|p|w>
                    bn_efp2.sh  !Fermi velocity <v_i*v_j>
```

① Edit ***df01.data***. Give the energy region to be drawn.

② Run ***df01.qsub***.

```
df01.data (~/abc/AlP_s) - VIM — ssh -X cmd2 — zsh — ttys008
0               jpr
200             ne  # mesh
0.0  10.0       emin,emax [eV]
0.000005 1 0    eshift[Hr],ipath,matopt
2   4           nv1,nv2  : valence bands
5   8           nw1,nw2  : conduction bands
=====================================
 3 18    3 16    nv1,nv2(up), nv1,nv2(down) : valence bands
19 26   17 25    nw1,nw2(up), nw1,nw2(down) : conduction bands
=====================================
10   18         nv1,nv2  : valence bands
17   25         nw1,nw2  : conduction bands
=====================================
0               jpr
1000            ne  # mesh
0.0  10.0       emin,emax [eV]
0.000005 1 0    esift,ipath,matopt
 1   18         nv1,nv2
19   48         nw1,nw2
c-------------------------------------------------------------------
c     jpr    i4 (O) : print option
c     ne     i4 (O) : number of mesh for complex energy parameter z
c     emin   r8 (O) : min. value of Re(z)   ( when ipath=1 )
c                     min. value of Im(z)   ( when ipath=2 )
c     emax   r8 (O) : max. value of Re(z)   ( when ipath=1 )
c                     max. value of Im(z)   ( when ipath=2 )
c     esift  r8 (O) : imaginary part of z   ( when ipath=1 )
c                     real      part of z   ( when ipath=2 )
c     ipath  i4 (O) : integral path index
c                     =1 : along real axis
c                     =2 : along imaginary axis
c     matopt i4 (O) : matrix element option
c                     = 0 : F(n'sigma'k,n sigma k)
c                     = 1 : 1.0
c     nv1    i4 (O) : min. band index for valence band
c     nv2    i4 (O) : max. band index for valence band
c     nw1    i4 (O) : min. band index for conduction band
c     nw2    i4 (O) : max. band index for conduction band
~
~
~
~
NORMAL  df01.data                          unix iso-2022-jp no    6/39:  5
"df01.data" [converted] 39L, 1738C
```

df01.data




```
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
```

df01.data

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

5.2.3 calculation for velocity

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

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

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

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

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

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

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

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

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

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

calculate fermi velocity

teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys002

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

[teac14@cmd2 AlP_s]$
```

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

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

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

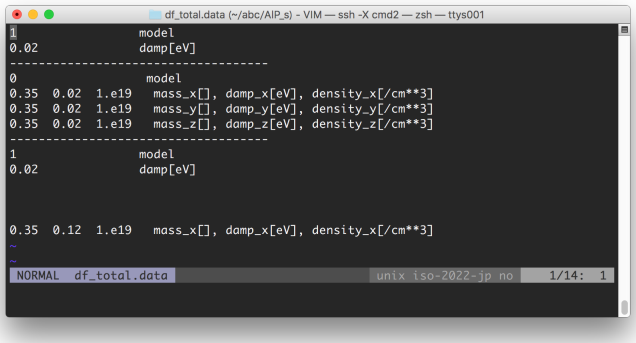
```
isp,ibn,ieig=    1    6    7
isp,ibn,ieig=    1    7    8

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

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

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

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

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



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



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

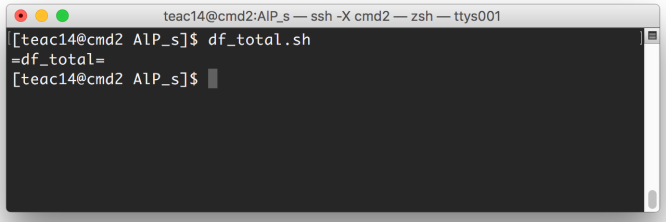
5.2.4 calculation for the Drude term and total dielectric function

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

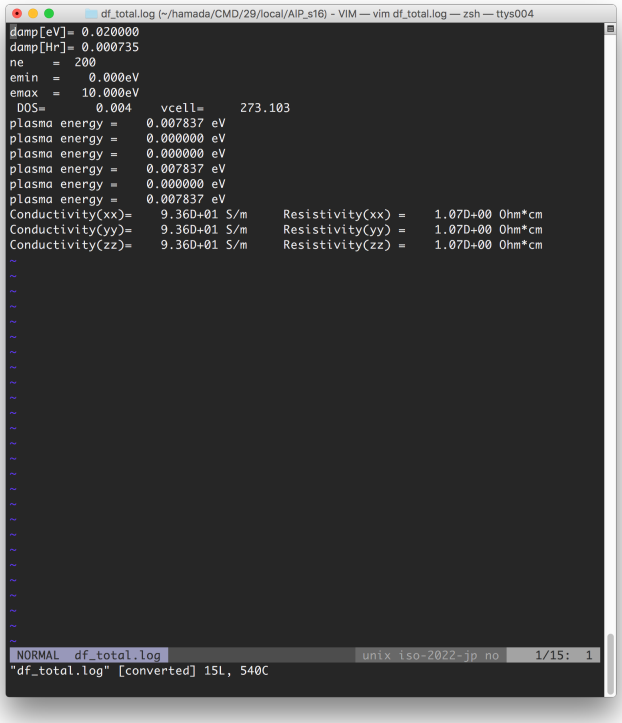
$$\frac{i}{\omega}\frac{\sigma_{ij}(0)}{1-i\omega\tau} = \frac{-1}{\omega}\frac{\sigma_{ij}(0)/\tau}{\omega + i/\tau}$$

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





result for total dielectric function



5.2.5 check results

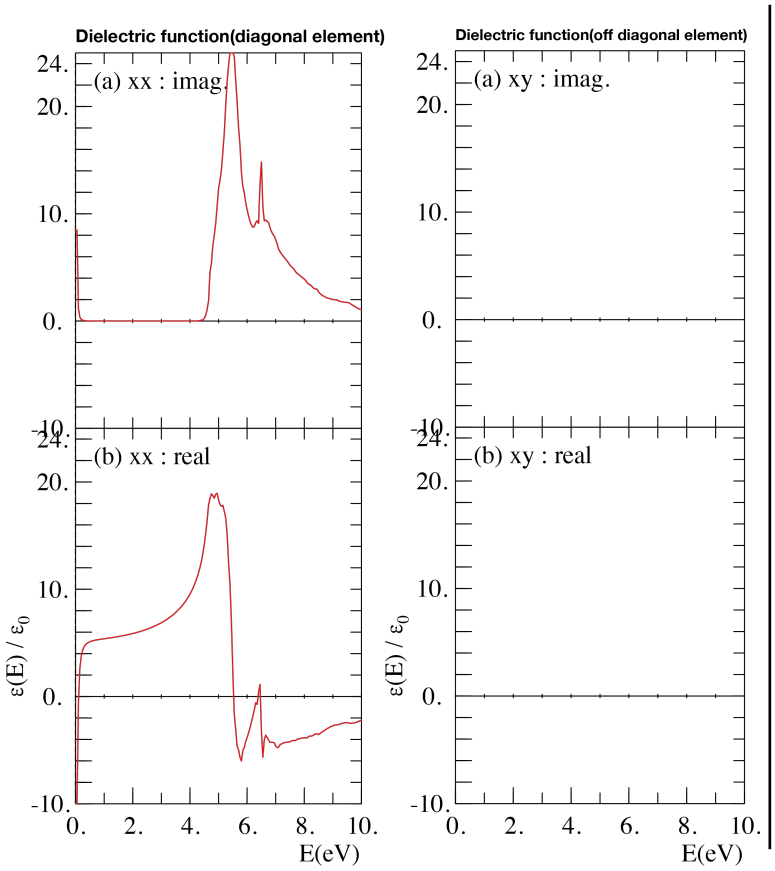
Index of the component for the dielectric function

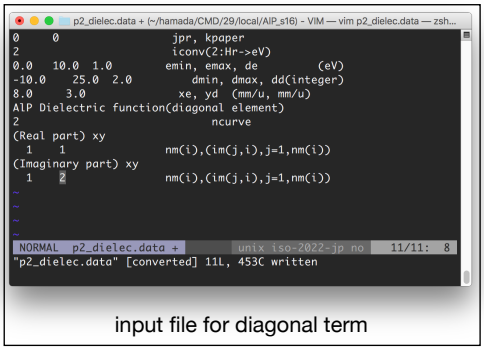
$$\epsilon = \begin{bmatrix} \underset{(1)}{\mathrm{Re}(\epsilon_{xx})} & \underset{(2)}{\mathrm{Im}(\epsilon_{xx})} & \underset{(3)}{\mathrm{Re}(\epsilon_{xy})} & \underset{(4)}{\mathrm{Im}(\epsilon_{xy})} & \underset{(5)}{\mathrm{Re}(\epsilon_{xz})} & \underset{(6)}{\mathrm{Im}(\epsilon_{xz})} \\ \mathrm{Re}(\epsilon_{yx})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

In this case, this crystal has a cubic symmetry,

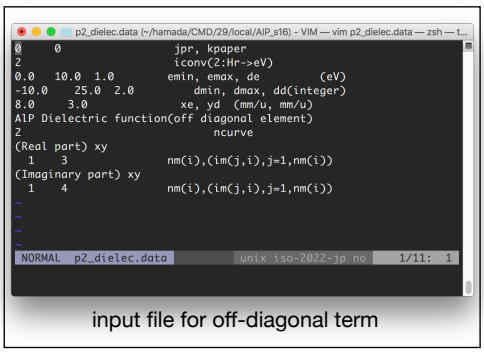
$$\begin{cases} \epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz} & \text{diagonal element} \\ \epsilon_{xy} = \epsilon_{yz} = \epsilon_{zx} & \text{off-diagonal element} \end{cases}$$

diagonal and off diagonal element of dielectric function tensor

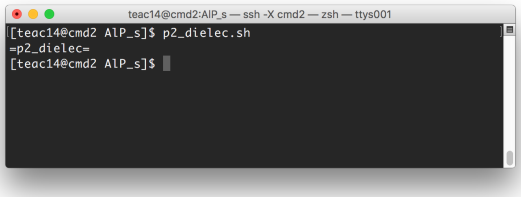




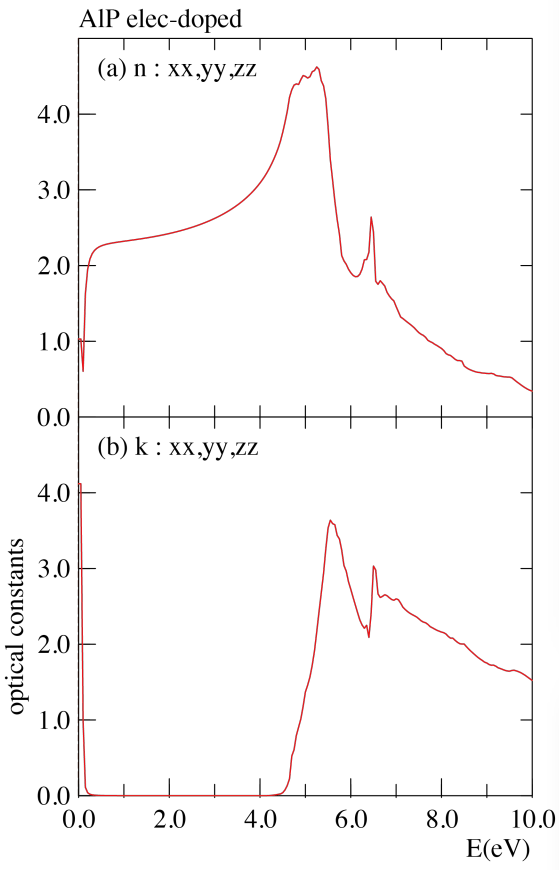
input file for diagonal term

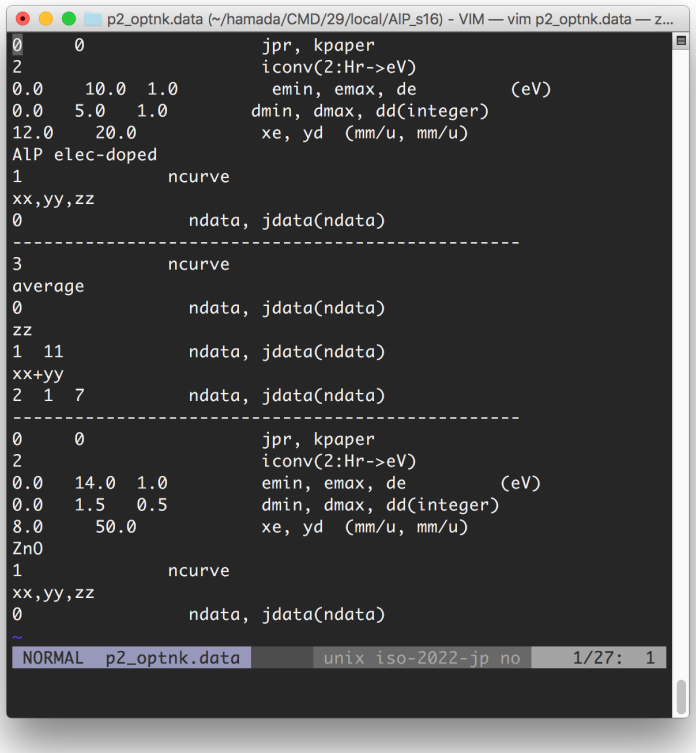


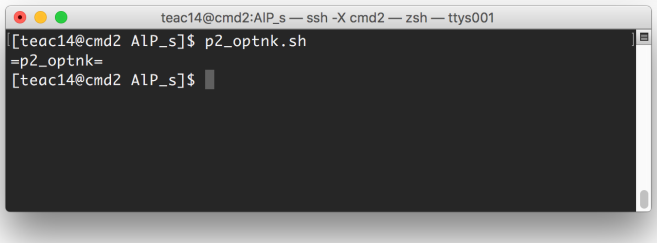
input file for off-diagonal term



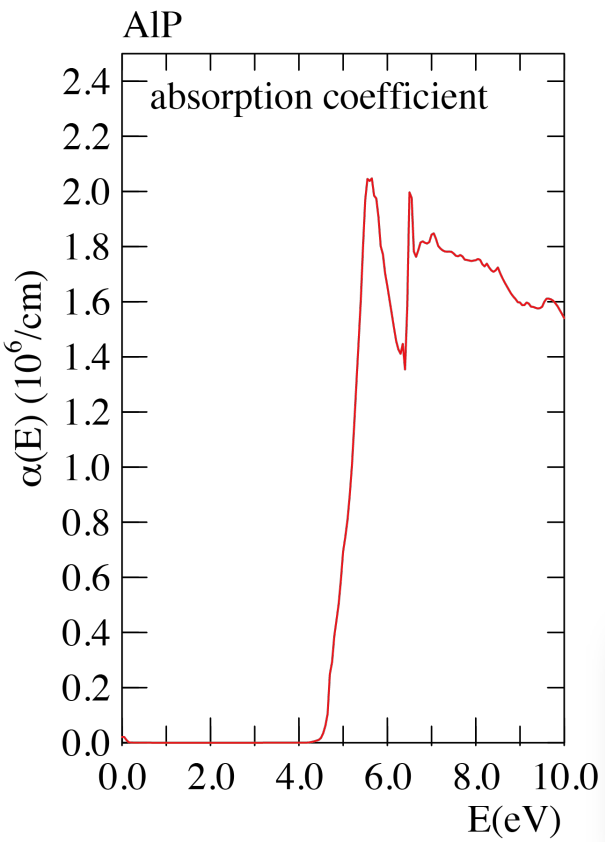
optical constant







absorb constant

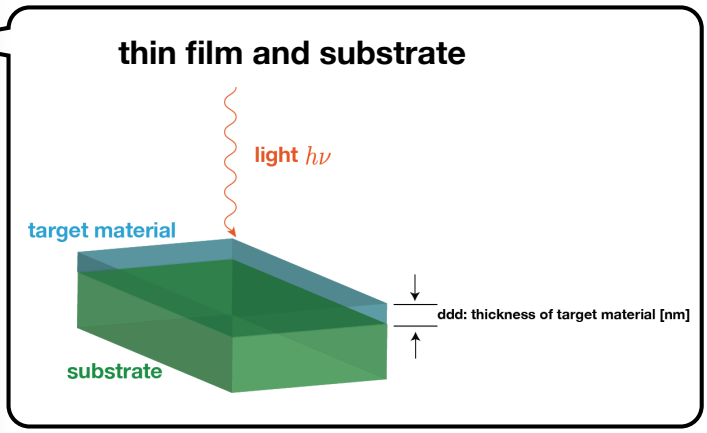



```
p2_absorb.data (~/hamada/CMD/29/local/AlP_s16) - VIM — vim p2_absorb.data —...
0     0                jpr, kpaper
2                      iconv(2:Hr->eV)
0.0   10.0  1.0        emin, emax, de          (eV)
0.0   2.5   0.2        dmin, dmax, dd(integer)
8.0     50.0           xe, yd  (mm/u, mm/u)
AlP
1              ncurve
xx,yy,zz
0                ndata, jdata(ndata)
-------------------------------------------------
3              ncurve
average
0                ndata, jdata(ndata)
zz
1  11            ndata, jdata(ndata)
xx+yy
2  1  7          ndata, jdata(ndata)
-------------------------------------------------
~
~
~
~
~
~
~
~
~
~
NORMAL  p2_absorb.data      unix iso-2022-jp no      1/18:  1
"p2_absorb.data" [converted] 18L, 561C
```

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

device simulation

```
optra.data (~/hamada/CMD/29/local/AlP_s16) - VIM — vim optra.data — zsh — tty...
 1                          ij_epsilon(1:xx,4:yy,6:zz)
 200.0                      ddd [nm]
 1.0d0    1.53d0            n-incident, n-substrate
-------------------------------------------------------
 ij_epsilon: tensor component of the dielectric constant
           (direction of the incident beam)
 ddd  : thickness of the material [nm]
 n-incident  : refractive index in front of the material
 n-substrate : refractive index of substrate


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



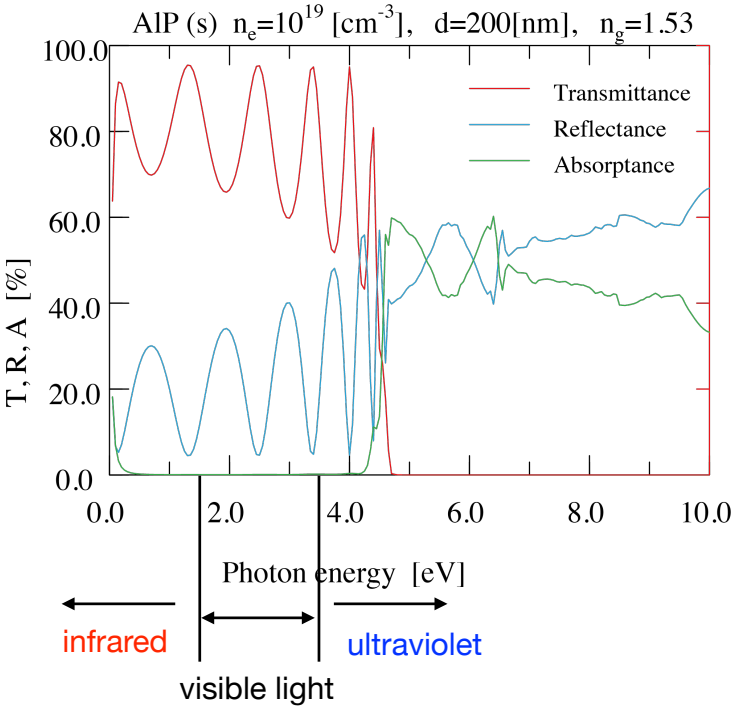

```
teac14@cmd2:AlP_s — ssh -X cmd2 — zsh — ttys001
[teac14@cmd2 AlP_s]$ optra.sh
=optra =
[teac14@cmd2 AlP_s]$
```

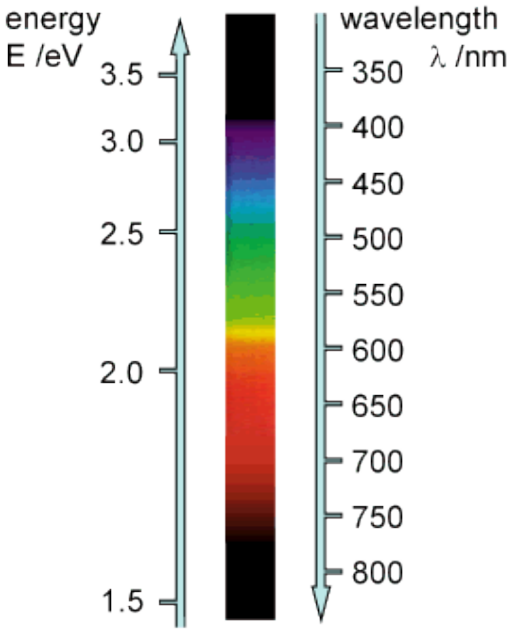
Indices of Refraction

Substance	Index of Refraction	Substance	Index of Refraction
Solids at 20°C		*Liquids at 20°C*	
Cubic zirconia	2.20	Benzene	1.501
Diamond (C)	2.419	Carbon disulfide	1.628
Fluorite (CaF_2)	1.434	Carbon tetrachloride	1.461
Fused quartz (SiO_2)	1.458	Ethyl alcohol	1.361
Gallium phosphide	3.50	Glycerin	1.473
Glass, crown	1.52	Water	1.333
Glass, flint	1.66		
Ice (H_2O)	1.309	*Gases at 0°C, 1 atm*	
Polystyrene	1.49	Air	1.000 293
Sodium chloride (NaCl)	1.544	Carbon dioxide	1.000 45

Note: All values are for light having a wavelength of 589 nm in vacuum.

Result of Optical Properties for AlP





Additional Information

Other Examples

Al(Aluminum)

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

Ni(Nickel)

```
>>>>>>>>> ab_prp.data >>>>>>>>>>>
Ni (225, Oh5, Fm-3m) fcc
  a=3.53 A
  face-centered (il=2) cubic lattice
  generators    5   (0, 0, 0)
               19   (0, 0, 0)
               25   (0, 0, 0)
  atomic position (0.0, 0.0, 0.0)
  magnetic (jmag=1)
>>>>>>>>> ab_prp.data >>>>>>>>>>>
```

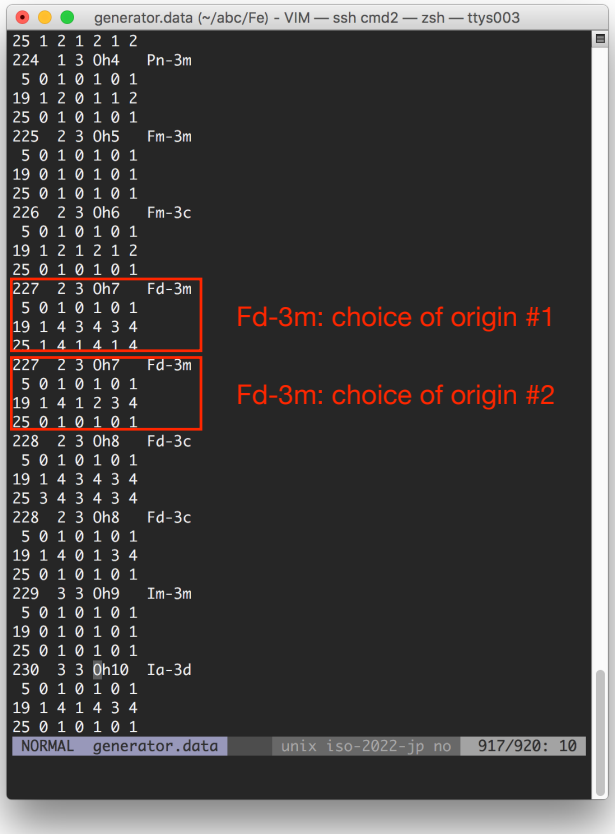
Cr(Chromium)

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

Cu(Copper)

```
>>>>>>>>> ab_prp.data >>>>>>>>>>>
Cu (225, Oh5, Fm-3m) fcc
  a=3.53 A
  face-centered (il=2) cubic lattice
  generators    5   (0, 0, 0)
               19   (0, 0, 0)
               25   (0, 0, 0)
  atomic position (0.0, 0.0, 0.0)
  nonmagnetic (jmag=0)
>>>>>>>>> ab_prp.data >>>>>>>>>>>
```

Space group information



Generator of the space group

File: **generator.data**

---

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

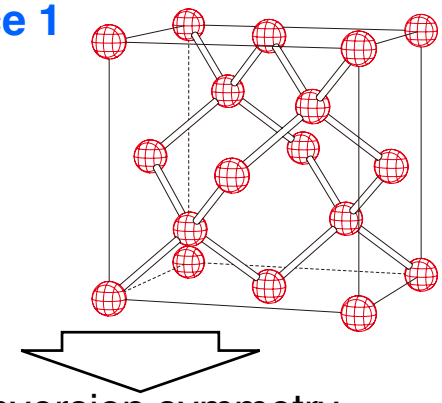
```
227  2 3 Oh7  Fd-3m
  5  0 1 0 1 0 1
 19  1 4 3 4 3 4
 25  1 4 1 4 1 4
```

rotation translation

How do you define the origin of Nonsymmorphic Crystal?

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

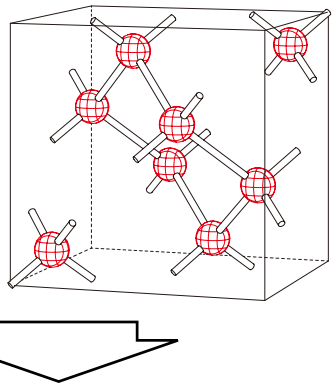
choice 1



× inversion symmetry

○ atom on origin

choice 2



○ inversion symmetry

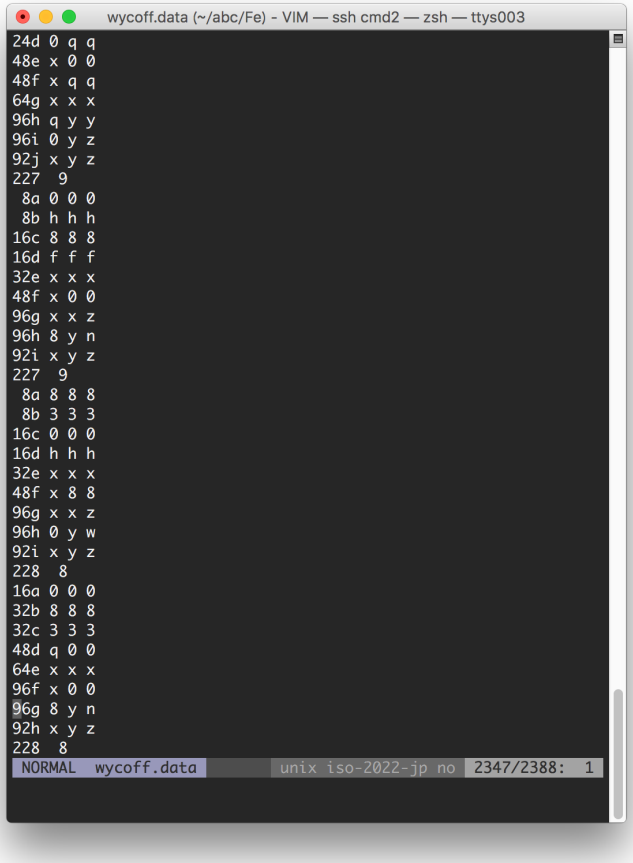
× atom on origin

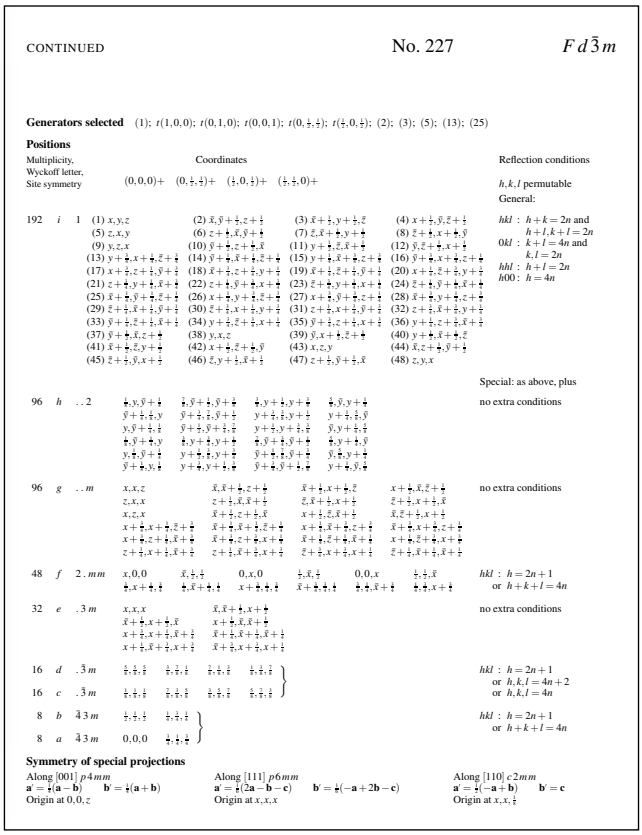
	atomic position	inversion center
choice 1	(0,0,0) and (1/4,1/4,1/4)	No
choice 2	(±1/8,±1/8,±1/8)	Yes

which is better?

Generator of the space group

File: **wycoff.data**





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

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

Positions

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

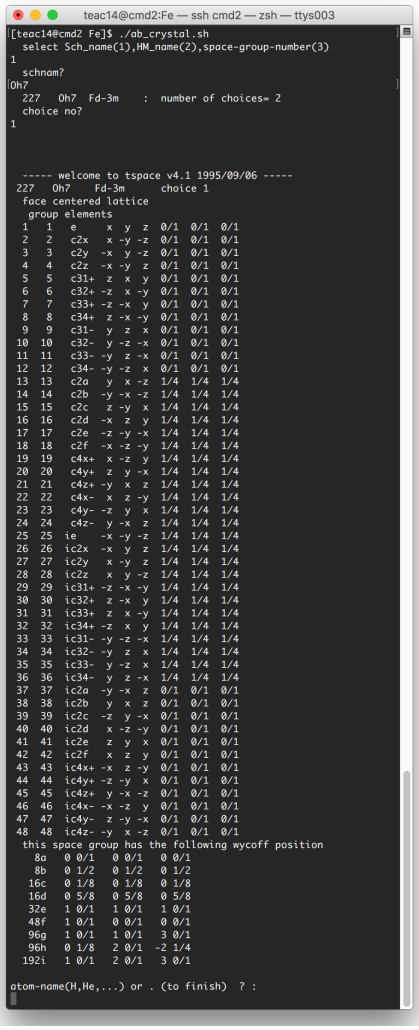
Symmetry of special projections

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

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

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

International Table of Crystallography A



How to make “ab_prp.data”

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).