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All electron Band structure CAlculation Package
— ABCAP —

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DFT (Density functional theory)

LAPW basis function

Crystal structure

Translational symmetry $\otimes$ Rotational symmetry

Space group — ”TSPACE” package by Yanase

1 Density Functional Theory (DFT)

Kohn-Sham equations

To understand the many-electron system

in terms of one-electron states

Iteration process of Kohn-Sham equations

$$
\begin{aligned}
& n^{\mathrm{in}}(\boldsymbol{r}) \\
& \quad \Downarrow \\
& v_{\mathrm{eff}}(\boldsymbol{r}) = v_{\mathrm{H}}(\boldsymbol{r}) + v_{\mathrm{xc}}(\boldsymbol{r}) + v(\boldsymbol{r}) \\
& \quad \Downarrow \\
& \left[-\frac{\hbar^2}{2m} \nabla^2 + v_{\mathrm{eff}}(\boldsymbol{r}) \right] \psi_i(\boldsymbol{r}) = \epsilon_i \psi_i(\boldsymbol{r}) \\
& \quad \Downarrow \\
& n^{\mathrm{out}}(\boldsymbol{r}) = \sum_{i=1}^{N} |\psi_i(\boldsymbol{r})|^2 \\
& \quad \Downarrow \\
& (1-\delta) \cdot n^{\mathrm{in}}(\boldsymbol{r}) + \delta \cdot n^{\mathrm{out}}(\boldsymbol{r}) \quad \Rightarrow n^{\mathrm{in}}(\boldsymbol{r})
\end{aligned}
$$

2 FLAPW method

Full-Potential
Linearized Augmented Plane Wave Method

Muffin-Tin spheres

Takeda-Kübler scheme (linearization)

Totally symmetric basis functions

Crystal Structure

Lattice :

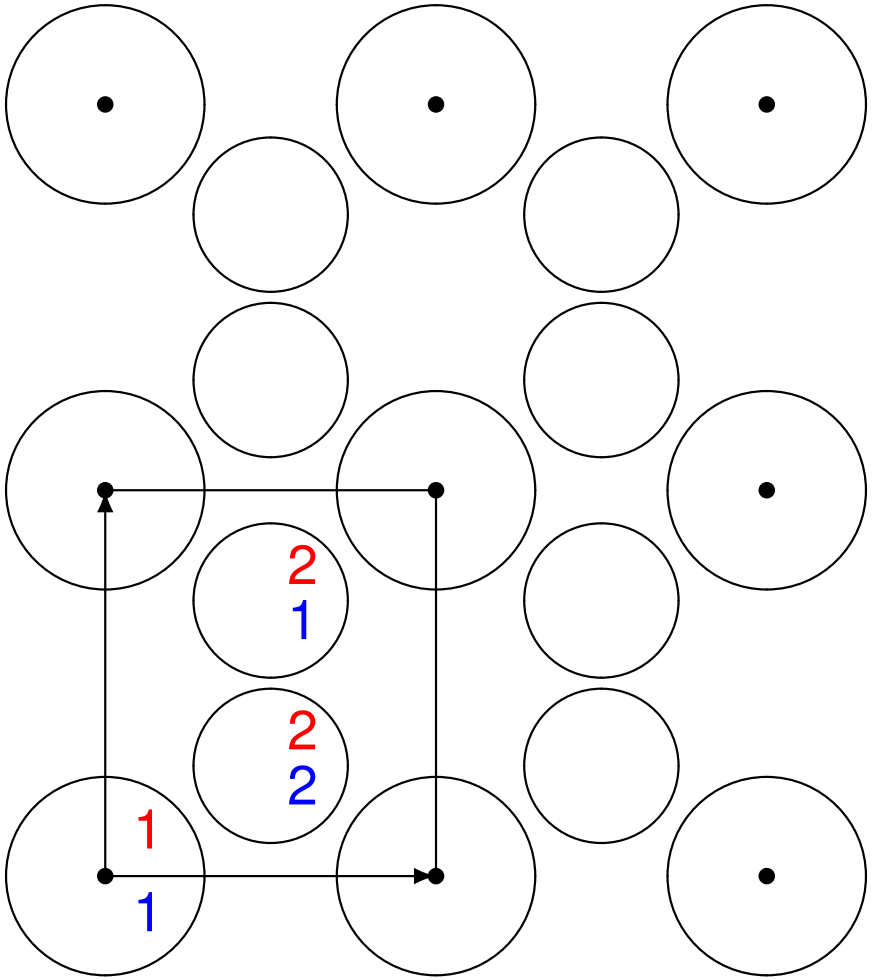
- a, b, c
- α, β, γ

Primitive cell :

- ν : kind of atom
- α : atom no.

Two regions in APW method

- Muffin-Tin (MT) Sphere
- Interstitial



C_2

Linearized Augmented Plane Wave Method

Muffin-Tin sphere (MT sphere)

MT-sphere mask function of the $\nu\alpha$ atom (ν:kind) :

$$\Theta_{\nu\alpha}(\boldsymbol{r}) = \begin{cases} 1 & \text{if } |\boldsymbol{r} - \boldsymbol{R}_{\nu\alpha}| \leq S_\nu \\ 0 & \text{otherwise} \end{cases}$$

$$\Theta(\boldsymbol{r}) = \sum_{\nu\alpha} \Theta_{\nu\alpha}(\boldsymbol{r})$$

Fe_3O_4 magnetite

	ν	α
Fe	1	1
		2
Fe	2	1
		2
		3
		4
O	3	1
		⋮
		8

LAPW : Basis function

$\boldsymbol{K} = \boldsymbol{k} + \boldsymbol{G}$: wave vector

$\boldsymbol{k}$: inside the Brillouin zone

$\boldsymbol{G}$: Reciprocal lattice vector

$$\chi^{\boldsymbol{K}}(\boldsymbol{r}) = [1 - \Theta(\boldsymbol{r})]e^{i\boldsymbol{K}\cdot\boldsymbol{r}} + \sum_{\nu\alpha} \Theta_{\nu\alpha}(\boldsymbol{r})\chi^{\boldsymbol{K}}_{\nu\alpha}(\boldsymbol{r})$$

$\chi^{\boldsymbol{K}}_{\nu\alpha}(\boldsymbol{r})$: 'atomic' wavefunction

(1) Interstitial

Plane wave cut-off energy $E_{k\max 1}$[Hr] : $\frac{1}{2}K^2 \leq E_{k\max 1}$

ABCAP	
$ekmax1$	cut-off energy

(2) Inside MT sphere ($\boldsymbol{r}_{\nu\alpha} = \boldsymbol{r} - \boldsymbol{R}_{\nu\alpha}$)

$$\chi^{\boldsymbol{K}}_{\nu\alpha}(\boldsymbol{r}) = 4\pi e^{i\boldsymbol{K}\cdot\boldsymbol{R}_{\nu\alpha}} \sum_{lm} i^l Y^*_{lm}(\hat{\boldsymbol{K}}) Y_{lm}(\hat{\boldsymbol{r}}_{\nu\alpha}) \Phi^K_{\nu l}(r_{\nu\alpha})$$

$$\Phi^K_{\nu l}(r) = \sum_{\beta=1}^{2} \phi_{\nu l\beta}(r) a^K_{\nu l\beta}$$

ABCAP	
$lmax1$	maximum value of l

Schrödinger equation

$$H\psi_{\boldsymbol{k}n}(\boldsymbol{r}) = E_{\boldsymbol{k}n}\psi_{\boldsymbol{k}n}(\boldsymbol{r})$$

Eigenfunction expanded by LAPW basis

$$\psi_{\boldsymbol{k}n}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} \chi_{\boldsymbol{k}+\boldsymbol{G}}(\boldsymbol{r})\ c^{\boldsymbol{G}}_{\boldsymbol{k}n}$$

Schrödinger equation (matrix form)

$$\sum_{G'} H^{\boldsymbol{G},\boldsymbol{G'}}_{\boldsymbol{k}}\, c^{\boldsymbol{G'}}_{\boldsymbol{k}n} = E_{\boldsymbol{k}n} \sum_{G'} S^{\boldsymbol{G},\boldsymbol{G'}}_{\boldsymbol{k}}\, c^{\boldsymbol{G'}}_{\boldsymbol{k}n}$$

$$H^{\boldsymbol{G},\boldsymbol{G'}}_{\boldsymbol{k}} = \left\langle \chi_{\boldsymbol{k}+\boldsymbol{G}} \middle| H \middle| \chi_{\boldsymbol{k}+\boldsymbol{G'}} \right\rangle$$

$$S^{\boldsymbol{G},\boldsymbol{G'}}_{\boldsymbol{k}} = \left\langle \chi_{\boldsymbol{k}+\boldsymbol{G}} \middle| \chi_{\boldsymbol{k}+\boldsymbol{G'}} \right\rangle$$

Full potential

$$v(\boldsymbol{r}) = [1 - \Theta(\boldsymbol{r})] \sum_p G_p(\boldsymbol{r}) v_p + \Theta(\boldsymbol{r}) \sum_{\nu s} \int \mathrm{d}\rho F_{\nu s}(\rho; \boldsymbol{r}) v_{\nu s}(\rho)$$

(SPW) Totally symmetric basis function in the interstitial:

$$G_p(\boldsymbol{r}) = \left\langle \boldsymbol{r} \middle| G_p \right\rangle = \sum_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}} c_{\boldsymbol{G}p} \tag{1}$$

(SSW) Totally symmetric basis function in the MT sphere: ($\boldsymbol{r}_{\nu\alpha} = \boldsymbol{r} - \boldsymbol{R}_{\nu\alpha}$)

$$\begin{aligned} F_{\nu s}(\rho; \boldsymbol{r}) &= \left\langle \boldsymbol{r} \middle| F_{\nu s}(\rho) \right\rangle \\ &= \sum_{\alpha} \Theta_{\nu\alpha}(\boldsymbol{r}) \delta(\rho - r_{\nu\alpha}) \sum_m Y_{lm}(\boldsymbol{r}_{\nu\alpha}) d_{\alpha m \nu s} \end{aligned} \tag{2}$$

ABCAP	
$egmax0$	cut-off energy
$lmax0$	maximum value of l

Totally symmetric plane-wave basis (SPW)

Orthogonality:

$$\int_\Omega \mathrm{d}^3 r G_p^*(\boldsymbol{r}) G_{p'}(\boldsymbol{r}) = \Omega \sum_{\boldsymbol{G}} c^*_{\boldsymbol{G}p} c_{\boldsymbol{G}p'} = \frac{\Omega}{N_p} \delta_{pp'} \tag{3}$$

Overlap integrals in the interstitial: (OSPW matrix)

$$O^{\mathrm{SPW}}_{pp'} = \int_\Omega \mathrm{d}^3 r G_p^*(\boldsymbol{r}) G_{p'}(\boldsymbol{r}) [1 - \Theta(\boldsymbol{r})] \tag{4}$$

3 Example : Si

Two important input files

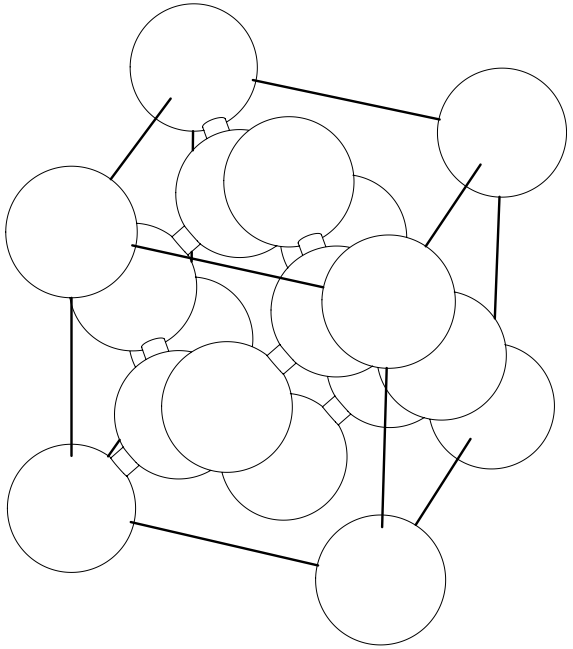
ab_prp.data
Crystal structure

ab_atom.data
Electron configulation of atom

Parameters on the calculational scheme

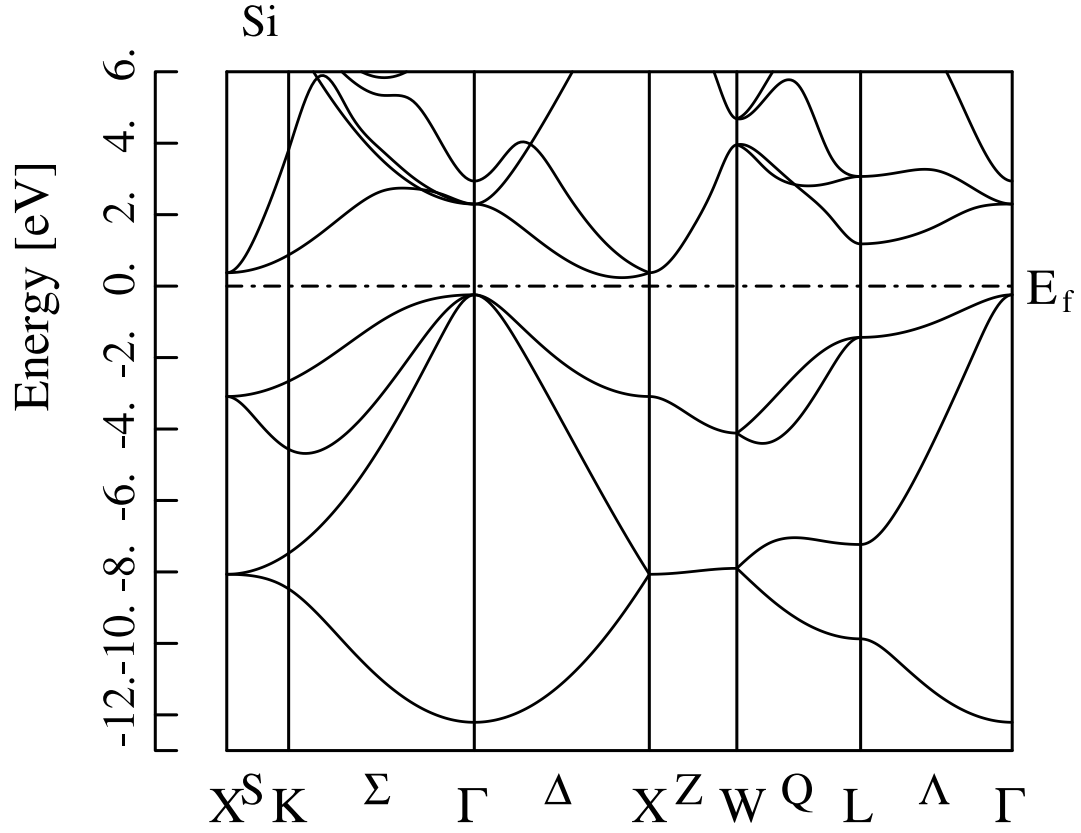
Silicon (Si)

Crystal structure



Band structure : $\epsilon(\boldsymbol{k})$

$\hbar\boldsymbol{k}$: crystal momentum ($\boldsymbol{k}$: crystal wave number)



```
Input for Si (diamond)  ---ab_prp.data---
lattice parameter -2----*----3----*----4----*----5----*----6----*---
5.4296 5.4296 5.4296  90.0 90.0 90.0 !a,b,c[A], alpha,beta,gamma
space group       -2----*----3----*----4----*----5----*----6----*---
 3   2   3   0                !idim, il(R,H,P(1),F,I,C,A,B),ngen,inv
    5   0 1  0 1  0 1                              !igen,jgen(2,3)
   19   1 4  1 4  1 4                              !igen,jgen(2,3)
   25   1 4  1 4  1 4                              !igen,jgen(2,3)
kinds of atoms    -2----*----3----*----4----*----5----*----6----*---
 1                                                 !# of kinds
 1   0.0        0.0        0.0       Si            !jpos,position,name
magnetic state    -2----*----3----*----4----*----5----*----6----*---
 0                                                 !jmag(0,1,2)
k-points (# of division)  ---3----*----4----*----5----*----6----*---
  8  8  8                              !nx,ny,nz
!---*----1----*----2----*----3----*----4----*----5----*----6----*---
```

```
Atomic data ---atom.data---
-----------------------------------
H
 1.0   1    1.0079  1.0
105
0.5
0.5
-----------------------------------
Si
14.0   5   28.086   2.0
100 200 210 305 315
1.0 1.0 3.0 1.0 1.0
1.0 1.0 3.0 1.0 1.0
-----------------------------------
```

4 Crystal structure

”TSPACE”

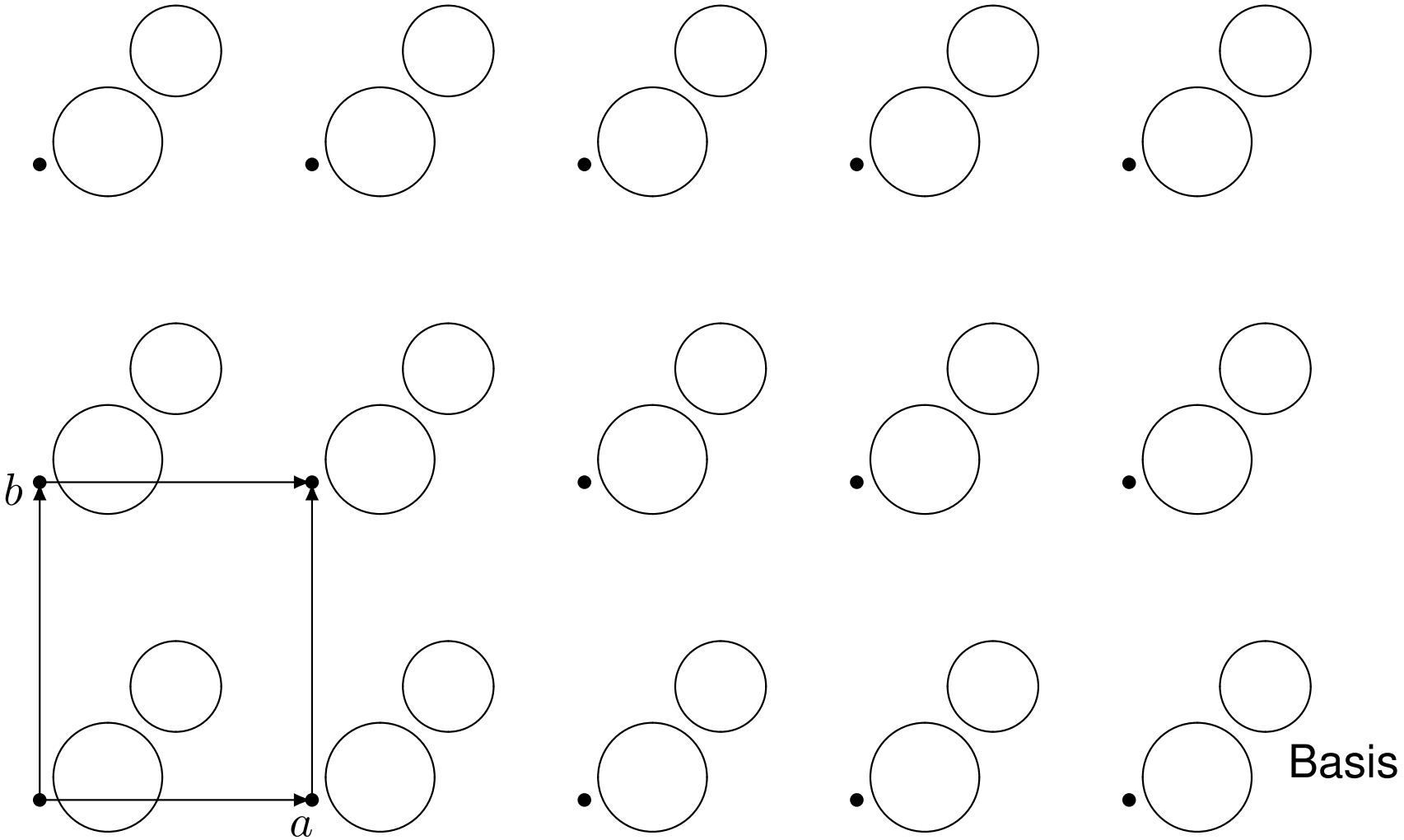
Translational symmetry
Bravais lattice

Rotational symmetry

Crystal point group
with non-primitive translation

”International Tables for Crystallography”

Crystal $=$ Lattice $\otimes$ Basis



Lattice (14 Bravais lattices)

Crystal System	Lattice Parameter	Bravais lattice
Triclinic		P
Monoclinic	$\beta = \gamma = 90^\circ$	P C
Orthorhombic	$\alpha = \beta = \gamma = 90^\circ$	P C I F
Tetragonal	$a = b$	P I
Cubic	$a = b = c$	P I F
Hexagonal, Trigonal	$a = b,\ \gamma = 120^\circ$	P R

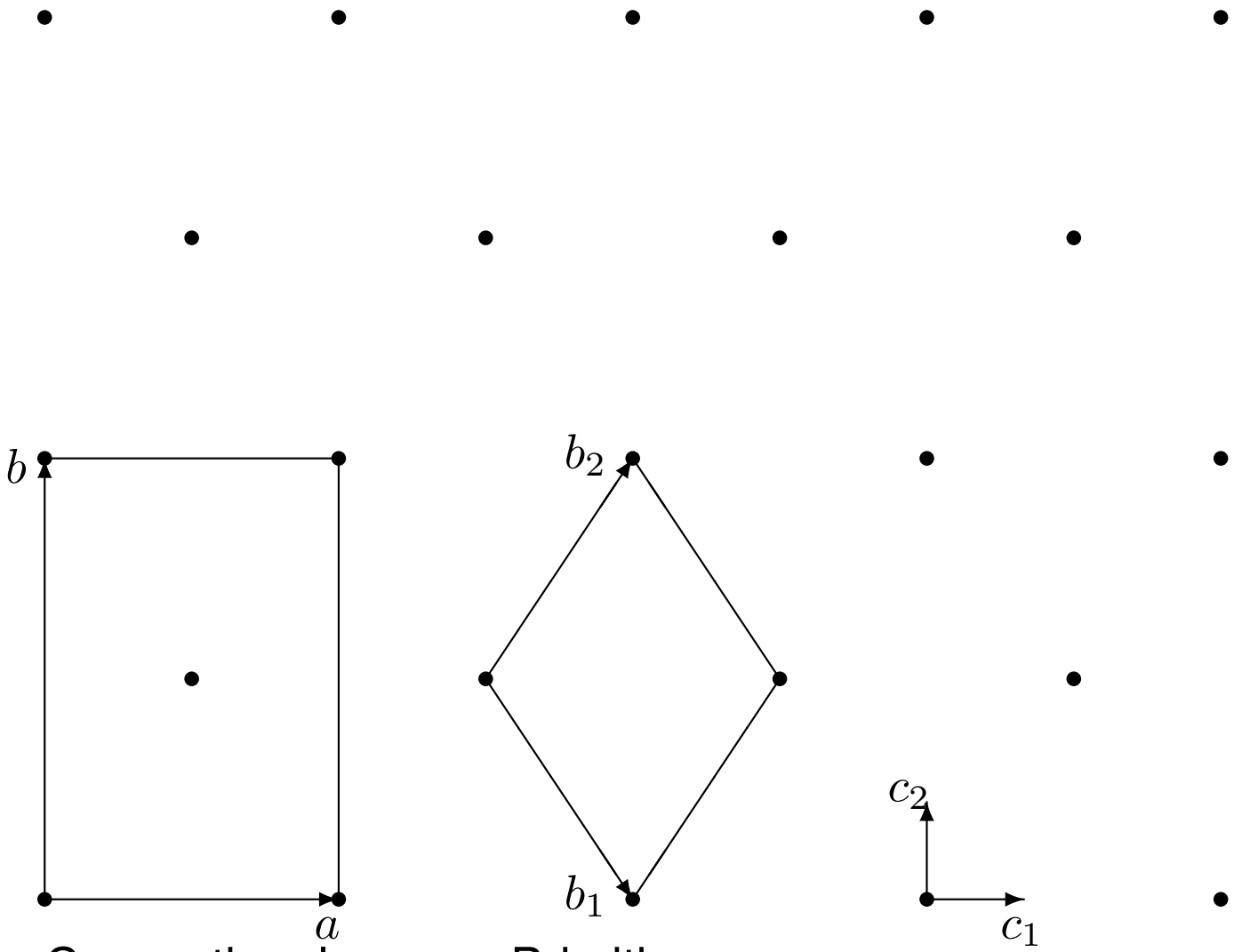
P: primitive, C: C-centered, I: body-centered, F: face-centered

---

P : hexagonal lattice, R : rhombohedral lattice

Hexagonal system : P6, Trigonal system : P3, R

Face-centered rectangular lattice（2 dimensional）



Conventional u.c.

A coordinate

Primitive u.c.

B coordinate

C coordinate

Conventional unit cell $=$ Multiply primitive cell

Lattice points are added to a primitive cell

Lattice type		Added lattice points
TSPACE	International	
-1	R	$(2/3, 1/3, 1/3)$, $(1/3, 2/3, 2/3)$
0	P6, P3	
1	P	
2	F	$(0, 1/2, 1/2)$, $(1/2, 0, 1/2)$, $(1/2, 1/2, 0)$
3	I	$(1/2, 1/2, 1/2)$
4	C	$(1/2, 1/2, 0)$
	A	$(0, 1/2, 1/2)$
	B	$(1/2, 0, 1/2)$

Conventional coordinate system : $\{\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}\}$ **(A coordinate system)**

Lattice translation vector:

$$\boldsymbol{T} = p_1\boldsymbol{a} + p_2\boldsymbol{b} + p_3\boldsymbol{c}$$
$$p_1,\ p_2,\ p_3 \quad : \quad \text{integers and fractions} \tag{5}$$

Positions in a cell:

$$\boldsymbol{x} = x_1\boldsymbol{a} + x_2\boldsymbol{b} + x_3\boldsymbol{c}$$
$$x_1,\ x_2,\ x_3 \quad : \quad \text{real numbers} \tag{6}$$

ABCAP	
il	lattice type (TSPACE code)
a, b, c	axes
α, β, γ	angles
x_1, x_2, x_3	atomic positions

Primitive coordinate system $\{\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3\}$: **B coordinate system**

$$(\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3) = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) T_{ab}$$

Primitive lattice（P）:

$$T_{ab}^{P} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Body-centered lattice（I）:

$$T_{ab}^{I} = \begin{pmatrix} -1/2 & 1/2 & 1/2 \\ 1/2 & -1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{pmatrix}$$

C-centered lattice（C）:

$$T_{ab}^{C} = \begin{pmatrix} 1/2 & 1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Face-centered lattice（F）:

$$T_{ab}^{F} = \begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \\ 1/2 & 1/2 & 0 \end{pmatrix}$$

A-centered lattice（A）:

$$T_{ab}^{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 1/2 \\ 0 & -1/2 & 1/2 \end{pmatrix}$$

Rhombohedral lattice（R）:

$$T_{ab}^{R} = \begin{pmatrix} 2/3 & -1/3 & -1/3 \\ 1/3 & 1/3 & -2/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}$$

Translational symmetry

Lattice translation vector

$$\boldsymbol{T} = p_1\boldsymbol{a} + p_2\boldsymbol{b} + p_3\boldsymbol{c} \quad (p_1,\ p_2,\ p_3 \ : \ \text{integers and fractions}) \tag{7}$$

$$= n_1\boldsymbol{b}_1 + n_2\boldsymbol{b}_2 + n_3\boldsymbol{b}_3 \quad (n_1,\ n_2,\ n_3 \ : \ \text{integer}) \tag{8}$$

Lattice translation operator : T

Lattice translation group $\{T\}$

(i) Closure: $T_2T_1 \in \{T\}$

(ii) Associativity: $(T_3T_2)T_1 = T_3(T_2T_1)$

(iii) Identity element: $\boldsymbol{T} = 0$

(iv) Inverse element: $-\boldsymbol{T}$

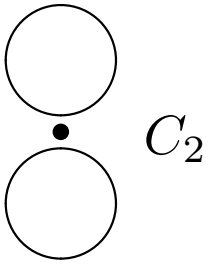
$\{T\}$: Abelian group **($T_2T_1 = T_1T_2$)**

(1) Irreducible representation (irrep.): 1 dimentional

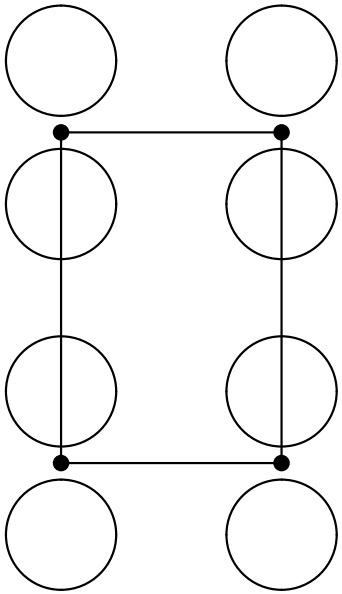
(2) Bloch's theorem ($\boldsymbol{k}$: label of irrep.)

Rotational symmetry

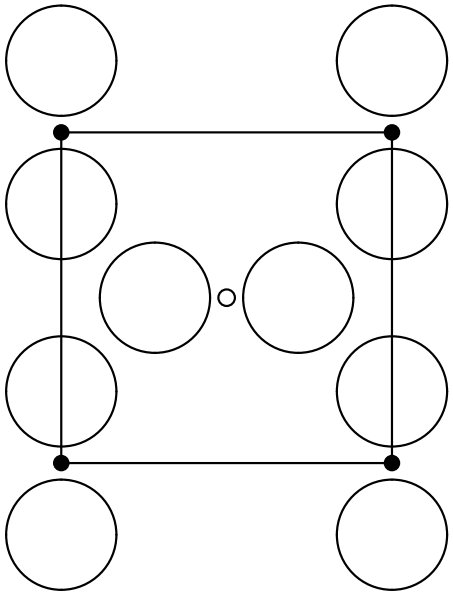
Example of rotation :



C_2



C_2



C_4
or
$\left(C_4 \middle| (1/2,\ 1/2)\right)$

Point group $\{E, C_2\}$, Crystal point group $\{E, C_2\}$, $\{E, C_2, C_4\}$

symmorphic

Space group

Group element (Seitz notation): $(R|\boldsymbol{T}+\boldsymbol{t}_R)$

- R : $E,\ C_2,\ C_3,\ C_4,\ C_6,\quad I$
- $\boldsymbol{T}$: lattice translation vector

  $\boldsymbol{t}_R$: nonprimitive translation vector

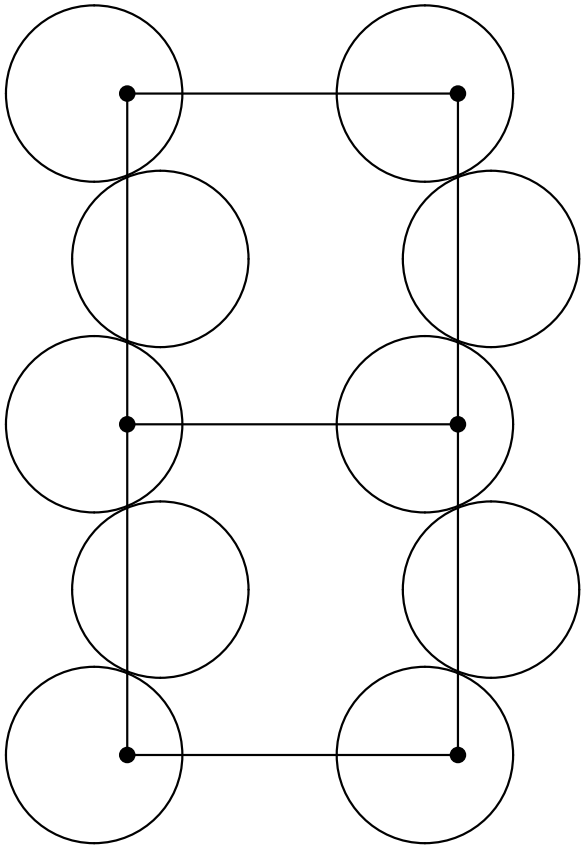
230 space groups

- $\boldsymbol{t}_R = 0$

  symmorphic : 73

- $\boldsymbol{t}_R \neq 0$ (screw, glide)

  nonsymmorphic : 157



$\big(\sigma\big|(0,\ 1/2)\big)$ glide

nonsymmorphic

TSPACE convention

Rotations

"TSPACE" symmetry operation code (Hexagonal and Trigonal)

```
(il=-1,0)  ----- hexagonal rotation (w=x-y: A coordinate) -------
   ( 1)  E      ( x, y, z)      (13) I       (-x,-y,-z)
   ( 2)  C6+    ( w, x, z)      (14) IC6+    (-w,-x,-z)
   ( 3)  C3+    (-y, w, z)      (15) IC3+    ( y,-w,-z)
   ( 4)  C2     (-x,-y, z)      (16) IC2     ( x, y,-z)
   ( 5)  C3-    (-w,-x, z)      (17) IC3-    ( w, x,-z)
   ( 6)  C6-    ( y,-w, z)      (18) IC6-    (-y, w,-z)
   ( 7)  C211   (-w, y,-z)      (19) IC211   ( w,-y, z)
   ( 8)  C221   ( x, w,-z)      (20) IC221   (-x,-w, z)
   ( 9)  C231   (-y,-x,-z)      (21) IC231   ( y, x, z)
   (10)  C212   ( w,-y,-z)      (22) IC212   (-w, y, z)
   (11)  C222   (-x,-w,-z)      (23) IC222   ( x, w, z)
   (12)  C232   ( y, x,-z)      (24) IC232   (-y,-x, z)
```

"TSPACE" symmetry operation code

(Cubic, Tetragonal, Orthorhombic, Monoclinic, Triclinic)

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

Generator

Rhombohedral lattice

146	C_3^4	R3	
	3	0 1 0 1 0 1	

167	D_{3d}^6	$R\bar{3}c$	
	3	0 1 0 1 0 1	
	10	0 1 0 1 1 2	
	13	0 1 0 1 0 1	

Hexagonal lattice

194	D_{6h}^4	$P6_3/mmc$	hcp
	2	0 1 0 1 1 2	
	7	0 1 0 1 1 2	
	13	0 1 0 1 0 1	

Cubic lattice

221	O_h^1	$Pm\bar{3}m$	sc
	5	0 1 0 1 0 1	
	19	0 1 0 1 0 1	
	25	0 1 0 1 0 1	

225	O_h^5	$Fm\bar{3}m$	fcc
	5	0 1 0 1 0 1	
	19	0 1 0 1 0 1	
	25	0 1 0 1 0 1	

227	O_h^7	$Fd\bar{3}m$	diamond
	5	0 1 0 1 0 1	
	19	1 4 1 4 1 4	
	25	1 4 1 4 1 4	

227	O_h^7	$Fd\bar{3}m$	diamond
	5	0 1 0 1 0 1	
	19	1 4 0 1 1 4	
	25	0 1 0 1 0 1	

229	O_h^9	$Im\bar{3}m$	bcc
	5	0 1 0 1 0 1	
	19	0 1 0 1 0 1	
	25	0 1 0 1 0 1	

ABCAP

$ngen$	Number of generators
$igen$, $jgen$	Rotation, Nonprim. tr.
$nkat$	Number of atom kinds
xat	position of atom

” ”

Reciprocal Space

Definition of reciprocal lattice

The B coordinate system in the reciprocal space

$$\{\boldsymbol{b}_1^*,\ \boldsymbol{b}_2^*,\ \boldsymbol{b}_3^*\}$$

Reciprocal (lattice) space

Primitive reciprocal lattice vectors: $\{\boldsymbol{b}_1^*,\ \boldsymbol{b}_2^*,\ \boldsymbol{b}_3^*\}$

$$\begin{aligned}
&\boldsymbol{b}_1^* \cdot \boldsymbol{b}_1 = 2\pi, \quad &&\boldsymbol{b}_1^* \cdot \boldsymbol{b}_2 = 0, \quad &&\boldsymbol{b}_1^* \cdot \boldsymbol{b}_3 = 0, \\
&\boldsymbol{b}_2^* \cdot \boldsymbol{b}_1 = 0, \quad &&\boldsymbol{b}_2^* \cdot \boldsymbol{b}_2 = 2\pi, \quad &&\boldsymbol{b}_2^* \cdot \boldsymbol{b}_3 = 0, \\
&\boldsymbol{b}_3^* \cdot \boldsymbol{b}_1 = 0, \quad &&\boldsymbol{b}_3^* \cdot \boldsymbol{b}_2 = 0, \quad &&\boldsymbol{b}_3^* \cdot \boldsymbol{b}_3 = 2\pi
\end{aligned}$$

Reciprocal lattice vector

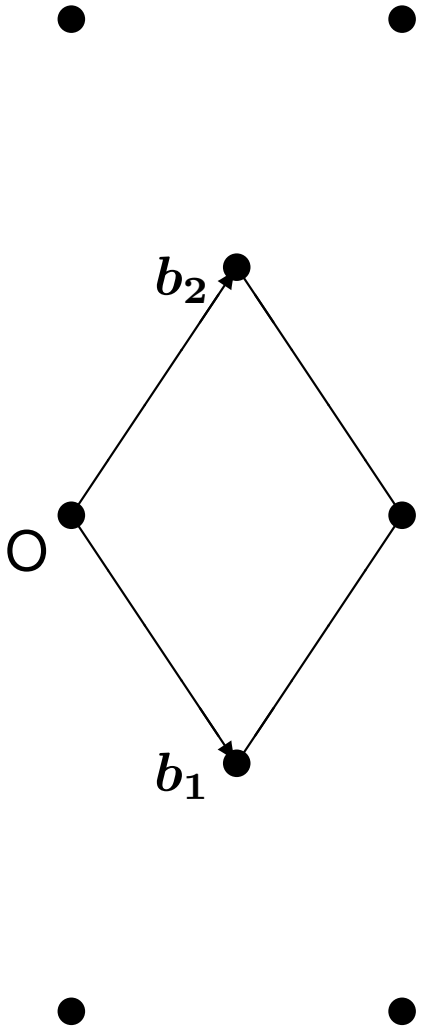
$$\begin{aligned}
\boldsymbol{G} &= m_1\boldsymbol{b}_1^* + m_2\boldsymbol{b}_2^* + m_3\boldsymbol{b}_3^* \\
m_1,\ m_2,\ m_3 &= \text{integer}
\end{aligned}$$

$\boldsymbol{G}$ and $\boldsymbol{T}$

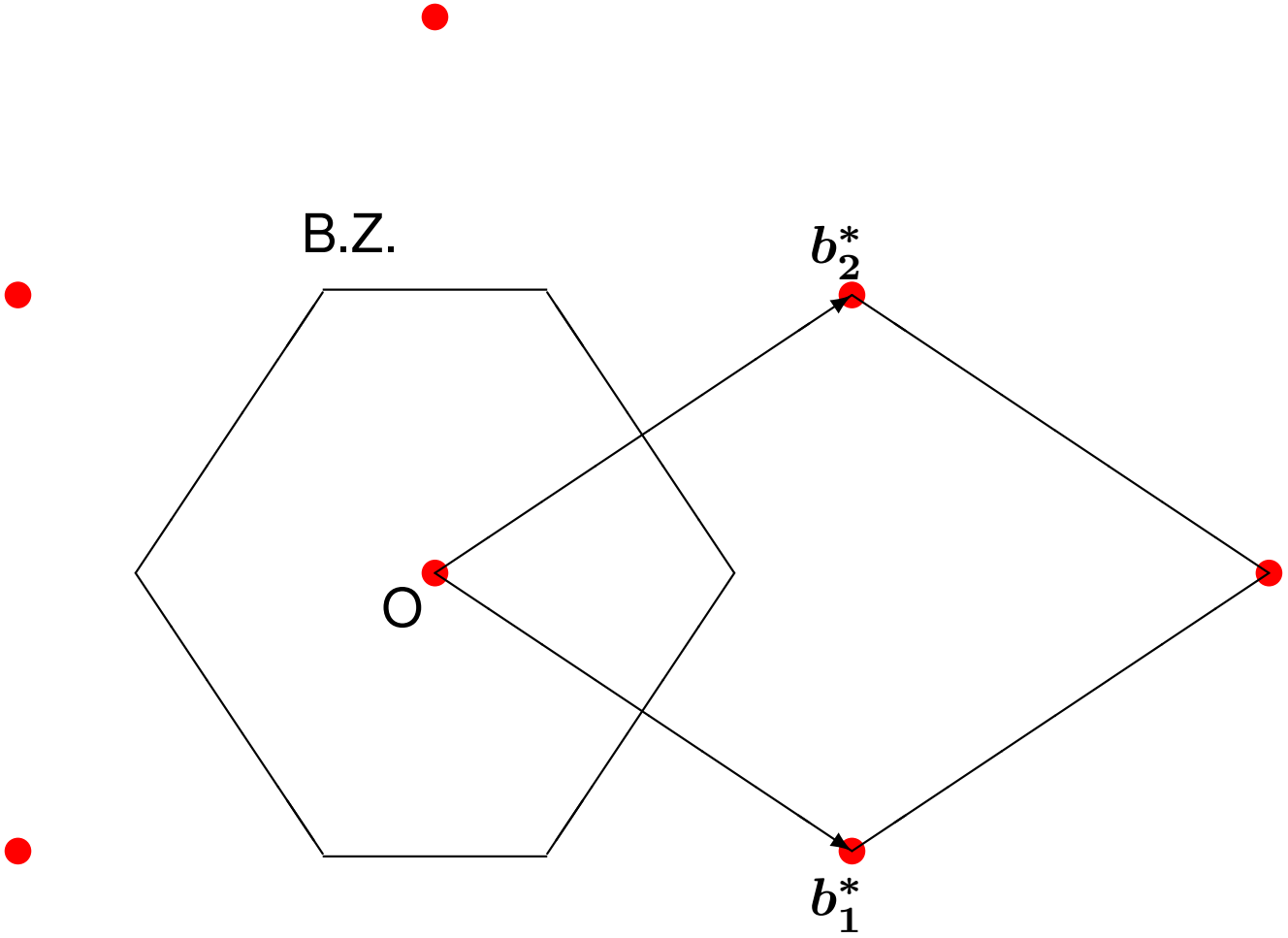
$$\begin{aligned}
&\boldsymbol{G} \cdot \boldsymbol{T} = 2\pi n \quad (n:\ \text{integer}) \\
&\quad \text{or} \\
&e^{i\boldsymbol{G}\cdot\boldsymbol{T}} = 1
\end{aligned}$$

Face-centered rectangular lattice (2D)

Real space



Reciprocal space



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Conventional reciprocal-space coordinate

The A coordinate system in reciprocal space

$$\{\boldsymbol{a}^*,\ \boldsymbol{b}^*,\ \boldsymbol{c}^*\}$$

Conventional reciprocal-lattice unit vector : $\{\boldsymbol{a}^*,\ \boldsymbol{b}^*,\ \boldsymbol{c}^*\}$

$$\begin{aligned}
&\boldsymbol{a}^* \cdot \boldsymbol{a} = 2\pi, \quad &&\boldsymbol{a}^* \cdot \boldsymbol{b} = 0, \quad &&\boldsymbol{a}^* \cdot \boldsymbol{c} = 0, \\
&\boldsymbol{b}^* \cdot \boldsymbol{a} = 0, \quad &&\boldsymbol{b}^* \cdot \boldsymbol{b} = 2\pi, \quad &&\boldsymbol{b}^* \cdot \boldsymbol{c} = 0, \\
&\boldsymbol{c}^* \cdot \boldsymbol{a} = 0, \quad &&\boldsymbol{c}^* \cdot \boldsymbol{b} = 0, \quad &&\boldsymbol{c}^* \cdot \boldsymbol{c} = 2\pi
\end{aligned}$$

Reciprocal lattice vector

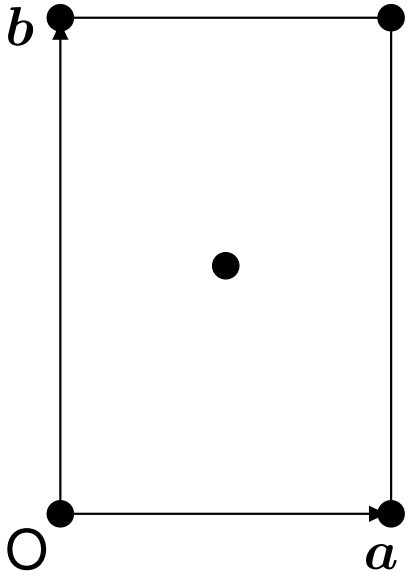
$$\boldsymbol{G} = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$$

lattice type	allowed (h,k,l)
Rhombohedral ($il = -1$)	$-h + k + l =$multiple of 3
Hexagonal ($il = 0$)	all integer
Primitive ($il = 1$)	all integer
Face-centered ($il = 2$)	all odd or all even
Body-centered ($il = 3$)	$h + k + l =$even
C-centered($il = 1$)	$h + k =$even

Extinction Rule

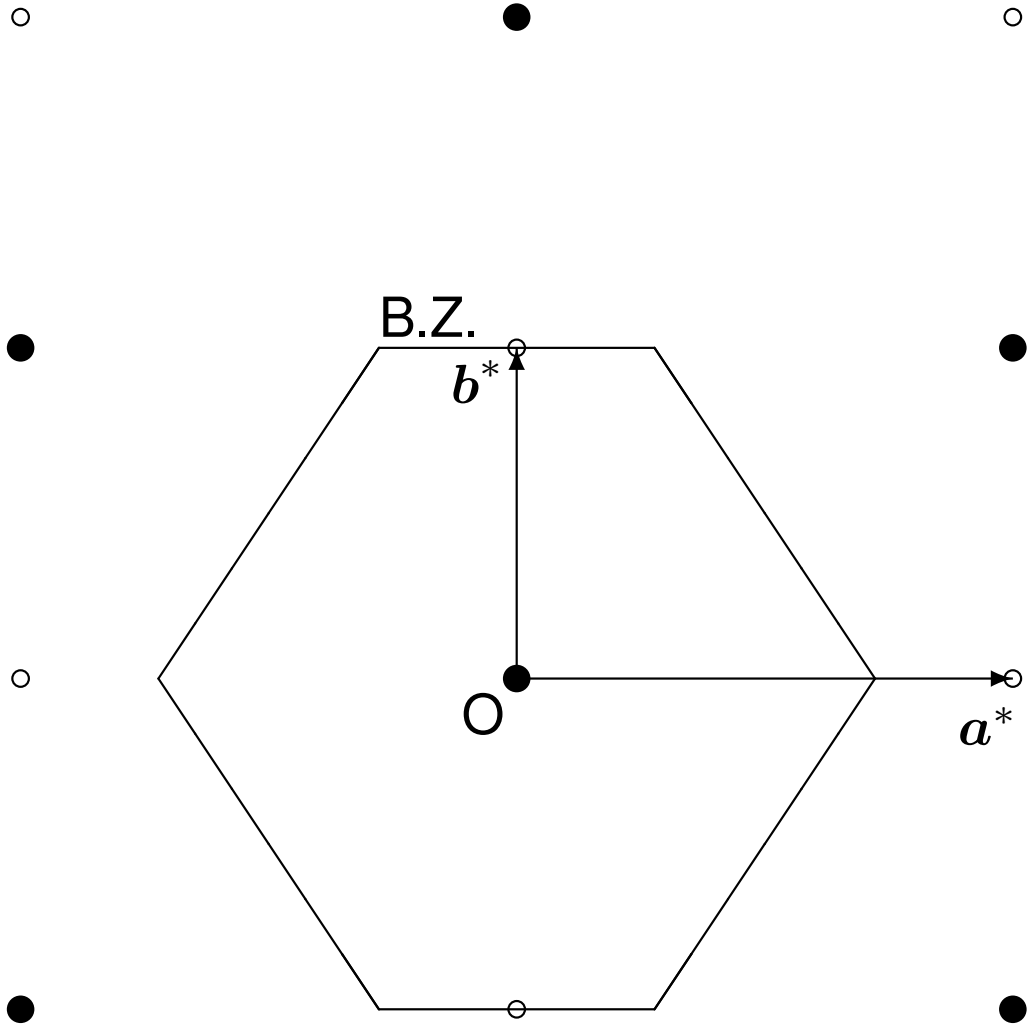
Face-centered rectangular lattice (2D)

Real space



Conventional unit cell

Reciprocal space (k-space)



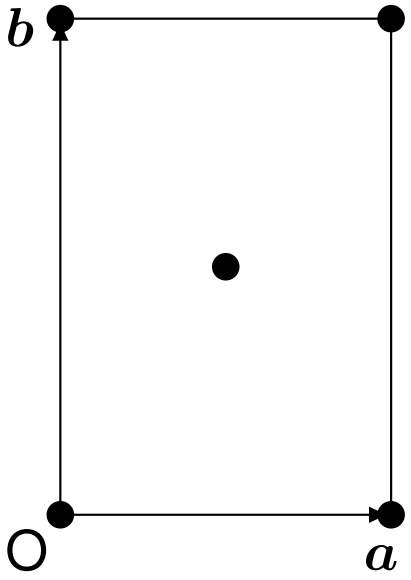
” ”

Rotational symmetry in the k space

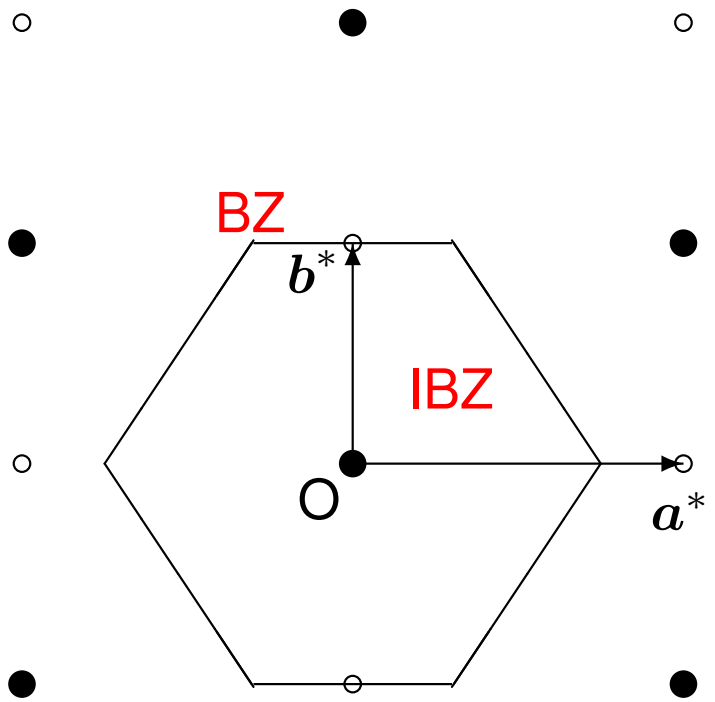
Irreducible brillouin zone (IBZ)

Face-centered rectangular lattice (2D)

Real space



Reciprocal space ($\boldsymbol{k}$-space)



Crystal point group : $\{E, C_2, \sigma_x, \sigma_y\}$ $(h = 4)$

Order of the crystal point group : h $\Rightarrow$ $\mathrm{IBZ} = \dfrac{\mathrm{BZ}}{h}$

” ”

Bloch function

$\boldsymbol{k}$ vector : $\boldsymbol{k} = k_1\boldsymbol{b}_1^* + k_2\boldsymbol{b}_2^* + k_3\boldsymbol{b}_3^*$

Bloch function $\psi_{\boldsymbol{k}}(\boldsymbol{r})$

Simultaneous eigenfunction for all T:

$$T\psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{T}}\psi_{\boldsymbol{k}}(\boldsymbol{r}) \qquad ({}^{\forall}T)$$

$\boldsymbol{k}$ is a 'good quantum number'.

Group theoretical interpretation:

- $e^{-i\boldsymbol{k}\cdot\boldsymbol{T}}$: Irreducible representation (Irrep)
- $\psi_{\boldsymbol{k}}(\boldsymbol{r})$: basis of irrep
- $\boldsymbol{k}$: label of irrep ($\boldsymbol{k} + \boldsymbol{G} \doteq \boldsymbol{k}$: crystal wave vector)

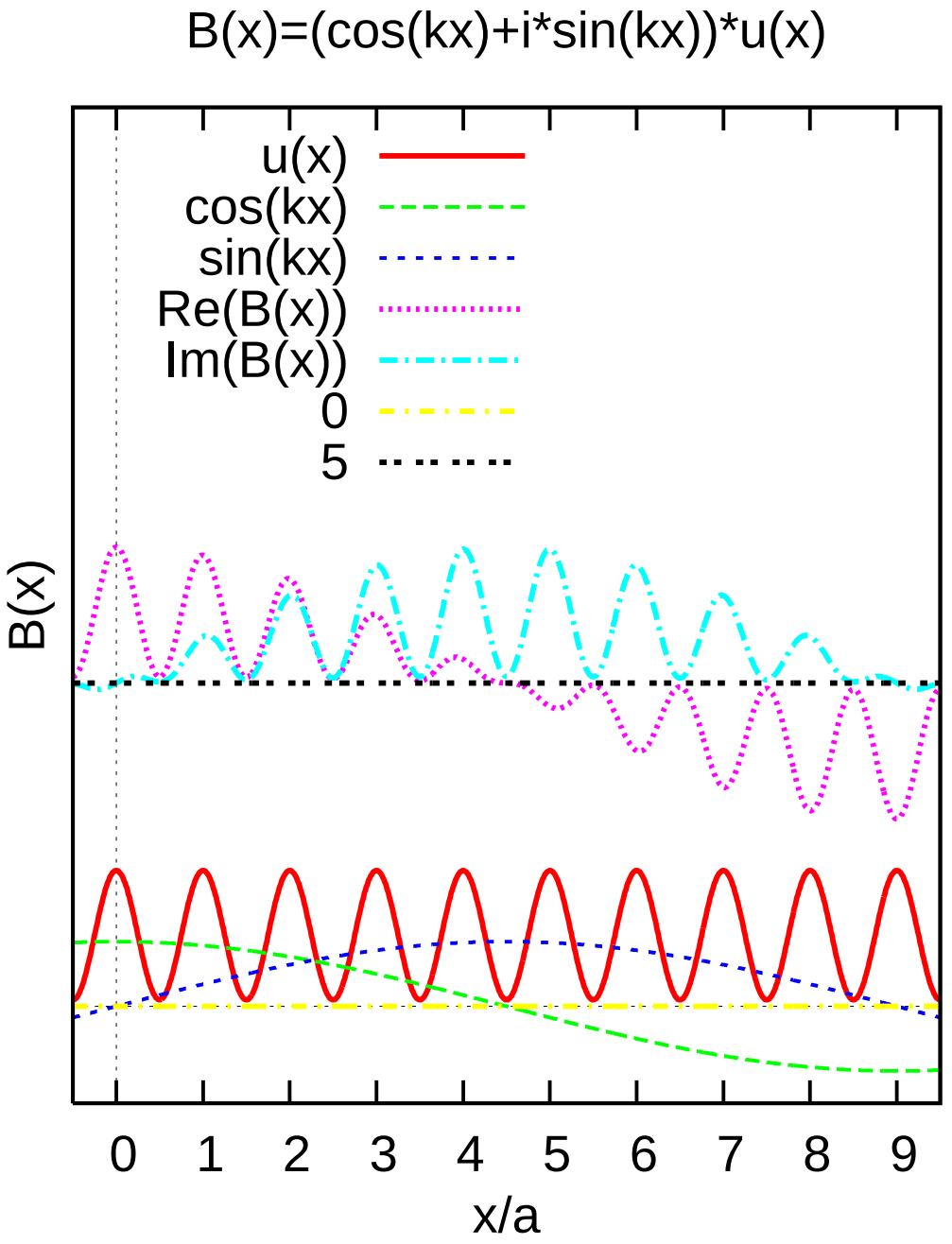
Bloch's theorem: ($u(\boldsymbol{r})$: periodic function)

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\ u(\boldsymbol{r})\ ; \qquad u(\boldsymbol{r}-\boldsymbol{T}) = u(\boldsymbol{r})$$

Bloch function

$$B(x) = e^{ikx}u(x)$$
$$= [\cos(kx) + i\sin(kx)]u(x)$$
$$u(x) = u(x - T) \qquad (^{\forall}T)$$

$$|B(x)|^2 = |u(x)|^2$$



” ”

Energy eigenstate

One-electron state

One-electron Hamiltonian:

$$
\begin{aligned}
H &= -\frac{\hbar^2}{2m}\nabla^2 + v_{\mathrm{eff}}(\boldsymbol{r}) \\
[H, T] &= 0 \qquad\qquad ({}^{\forall}T) \\
&\Downarrow \\
H\psi_{\boldsymbol{k}n} &= \epsilon_{\boldsymbol{k}n}\psi_{\boldsymbol{k}n} \\
T\psi_{\boldsymbol{k}n} &= e^{-i\boldsymbol{k}\cdot\boldsymbol{T}}\psi_{\boldsymbol{k}n} \qquad ({}^{\forall}T)
\end{aligned}
$$

- $\boldsymbol{k}$: label of irrep of translation group (= crystal wave vector)
- n : band index (ascending order)

$\boldsymbol{k}$ space mesh : $\dfrac{a^*}{n_x}, \quad \dfrac{b^*}{n_y}, \quad \dfrac{c^*}{n_z}$

ABCAP
n_x, n_y, n_z

5 Example : Si

Important files

ab_prp.data, ab_prp.log

---

ab_input.data

ab_in.log, a_kp0.dta

f_ef.dta, fl_bnd.log

```
Input for Si (diamond)  ---ab_prp.data---
lattice parameter -2----*----3----*----4----*----5----*----6----*---
5.4296 5.4296 5.4296  90.0 90.0 90.0 !a,b,c[A], alpha,beta,gamma
space group       -2----*----3----*----4----*----5----*----6----*---
 3   2   3   0                !idim, il(R,H,P(1),F,I,C,A,B),ngen,inv
    5   0 1  0 1  0 1                              !igen,jgen(2,3)
   19   1 4  1 4  1 4                              !igen,jgen(2,3)
   25   1 4  1 4  1 4                              !igen,jgen(2,3)
kinds of atoms    -2----*----3----*----4----*----5----*----6----*---
 1                                                 !# of kinds
 1   0.0        0.0        0.0       Si           !jpos,position,name
magnetic state    -2----*----3----*----4----*----5----*----6----*---
 0                                                 !jmag(0,1,2)
k-points (# of division)  ---3----*----4----*----5----*----6----*---
  8  8  8                             !nx,ny,nz
!---*----1----*----2----*----3----*----4----*----5----*----6----*---
```

Information (Diamond structure)

- generator.data : 227, $Fd\bar{3}m$, O_h^7
- wycoff.data : Wyckoff position = 8a
- ab_prp.log : Order of crystal point group $=$ 48
- ab_input.data : Input data for almost all programs
- ab_in.txt : Interatomic distance, Bond angle
- a_kp0.dta : $n_x = n_y = n_z = 8 \;\; \Rightarrow \;\;$ 2048 k-points in BZ, 85 k-points in IBZ

ab_in.txt

Bond length:

```
 atom0=    1
atom1=   2  wa=  0.250  0.250  0.250   r= 4.442908[B] ( 2.351086[A])
atom1=   2  wa= -0.250 -0.250  0.250   r= 4.442908[B] ( 2.351086[A])
atom1=   2  wa=  0.250 -0.250 -0.250   r= 4.442908[B] ( 2.351086[A])
atom1=   2  wa= -0.250  0.250 -0.250   r= 4.442908[B] ( 2.351086[A])
```

Bond angle:

```
 atom0=    1
   2   2  109.47
   2   2  109.47    2   2  109.47
   2   2  109.47    2   2  109.47    2   2  109.47
```

f_ef.dta

Fermi-level information:

```
abcap-ef[Hr]:   Fermi-level, dos, vale, band-E (/spin)
  0.1976012626133052E+00           1   22
    4    4   22     # of fully-occ. bands, # of occ. bands
  0.00000000E+00  0.40000000E+01  0.92388815E-02 spin=1
```

fl_bnd.log

core level:

```
  ===== eigenenergy of core state (ryd.) =====
          100         -129.881656
          200           -9.388127
          210           -6.215834
```

fl_bnd.log

eigenenergy and (s,p,d,f)-component:

```
sub.fl_pw0001: k=    0    0    0  512       no. of plane waves =  181
                                      s       p       d       f
ie= 1( 1)  e=-0.251070 Hr  :  Si* 2  0.435   0.000   0.000   0.001
ie= 2( 7)  e= 0.188678 Hr  :  Si* 2  0.000   0.442   0.062   0.001
ie= 3( 7)  e= 0.188678 Hr  :  Si* 2  0.000   0.442   0.062   0.001
ie= 4( 7)  e= 0.188678 Hr  :  Si* 2  0.000   0.442   0.062   0.001
ie= 5( 6)  e= 0.282010 Hr  :  Si* 2  0.000   0.310   0.068   0.003
ie= 6( 6)  e= 0.282010 Hr  :  Si* 2  0.000   0.310   0.068   0.003
ie= 7( 6)  e= 0.282010 Hr  :  Si* 2  0.000   0.310   0.068   0.003
ie= 8( 4)  e= 0.305603 Hr  :  Si* 2  0.726   0.000   0.000   0.007
ie= 9( 1)  e= 0.471272 Hr  :  Si* 2  0.208   0.000   0.000   0.015
```

Symmetry of Bloch function $\psi_{\boldsymbol{k}}(\boldsymbol{r})$

Irreducible representation of $\boldsymbol{k}$ group

$$\exp\big(-i\boldsymbol{k}\cdot(\boldsymbol{u_\alpha}+\boldsymbol{T})\big)\; D^{(\lambda)}_{\boldsymbol{k}}(\alpha)$$

α : $\boldsymbol{k}$-invariant rotation

Nonsymmorphic space group (F$d\bar{3}m$)

$D^{(\lambda)}_{\boldsymbol{k}}(\alpha)$:

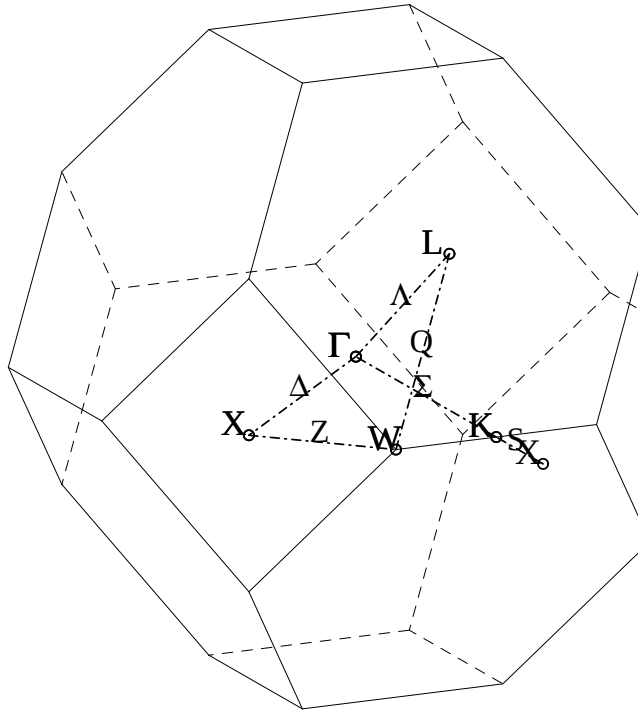
- Inside the Brillouin zone,

  Usual point group representation

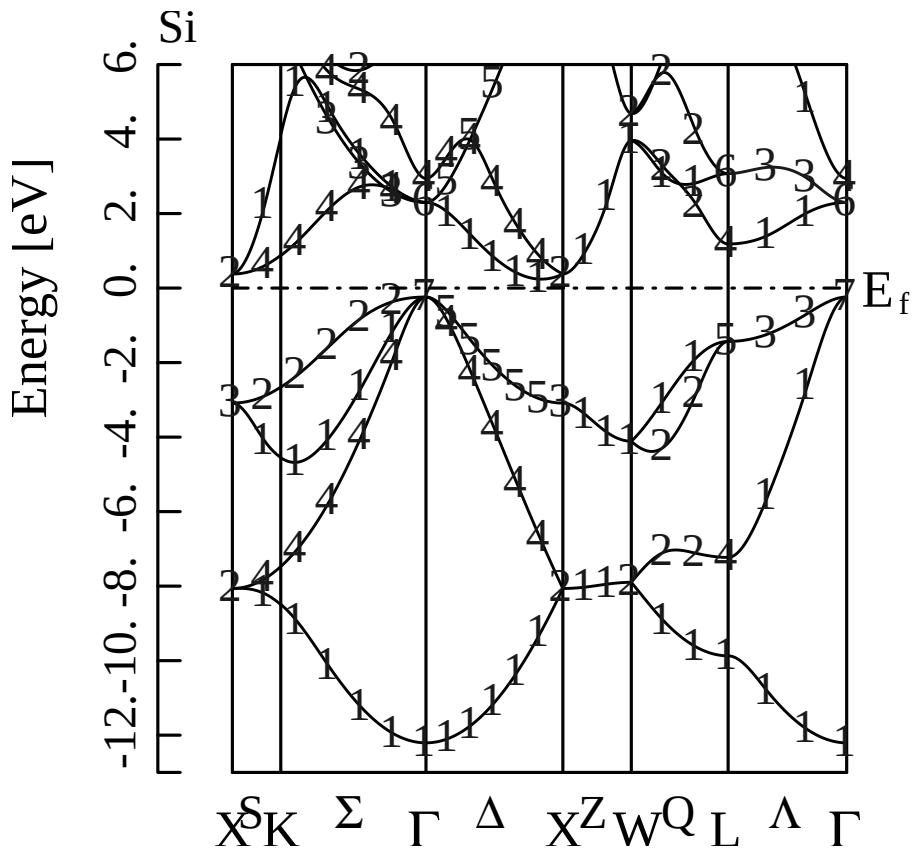
  example) Γ: O$_h$
- On the Brillouin zone surface,

  Projective representation

  example) X: D$_{4h}$



Symmetry of eigenenergy states



Irreducible representations at the Γ point

TSPACE	BSW	basis f.
1	Γ_1	r^2
4	Γ'_2	xyz
6	Γ_{15}	x, y, z
7	Γ'_{25}	xy, yz, zx

Irreducible representations at the X point

(All are 2-D rep.)

TSPACE	BSW
2	X_1
3	X_3

BSW:

L. P. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. 50 , 58 (1936).

For the Γ point, character table of O_h is available.

	O_h		E	$3C_2$	$8C_3$	$6C'_2$	$6C_4$	I	$3\sigma_h$	$8IC_3$	$6\sigma_d$	$6IC_4$
1	Γ_1	A_{1g}	1	1	1	1	1	1	1	1	1	1
3	Γ_2	A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
2	Γ'_1	A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
4	Γ'_2	A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
9	Γ_{12}	E_g	2	2	-1	0	0	2	2	-1	0	0
10	Γ'_{12}	E_u	2	2	-1	0	0	-2	-2	1	0	0
5	Γ'_{15}	T_{1g}	3	-1	0	-1	1	3	-1	0	-1	1
7	Γ'_{25}	T_{2g}	3	-1	0	1	-1	3	-1	0	1	-1
6	Γ_{15}	T_{1u}	3	-1	0	-1	1	-3	1	0	1	-1
8	Γ_{25}	T_{2u}	3	-1	0	1	-1	-3	1	0	-1	1
(T)	(B)	(M)										

(T): TSPACE code, (B): BSW notation at the Γ point, (M): Mulliken notation

For the X point in diamond (nonsymmorphic), character table

(Projective representation)

		(E|0)	(C_2|0)	2(C_2''|$\boldsymbol{u}_d$)	2(σ_d|0)
2	X_1	2	2	0	2
1	X_2	2	2	0	-2
3	X_3	2	-2	-2	0
4	X_4	2	-2	2	0
(T)	(B)				

$\boldsymbol{u}_d = (1/4, 1/4, 1/4)a$

(T): TSPACE code,

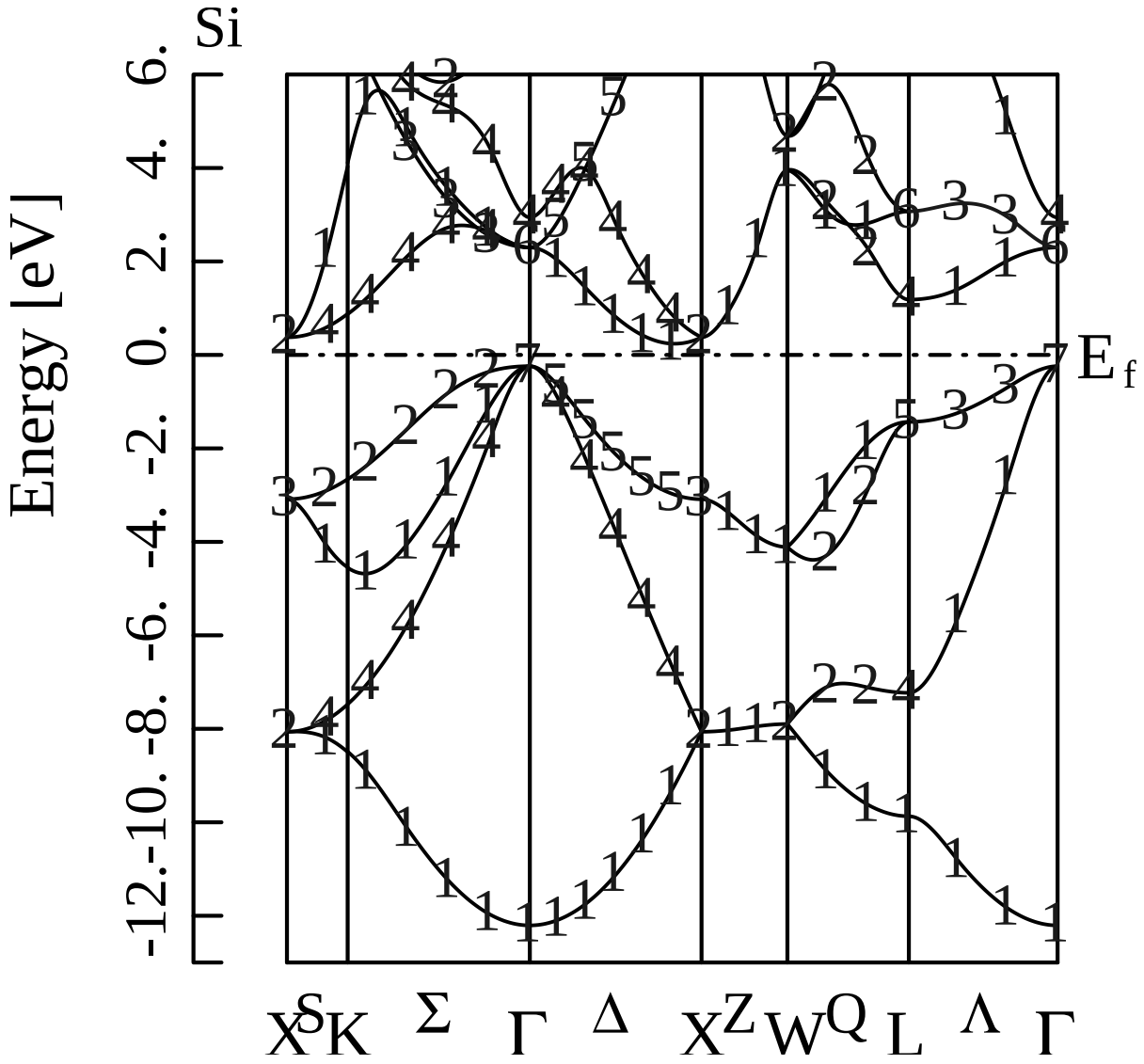
(B): BSW notation at the X point in diamond (nonsymmorphic)

Optical transition — Si —

Dipole allowed:

At the Γ point,

- $1 \leftrightarrow 6$
- $7 \leftrightarrow 4, 6$



Optical transition — AlP —

Dipole allowed:

At the Γ point,

- $1 \leftrightarrow 4$