2009 年 8 月 31 日作成

All electron Band structure CAlculation Package

— ABCAP —

HAMADA Noriaki

Tokyo University of Science

Crystal and Symmetry — TSPACE

Reciprocal space

LAPW basis function

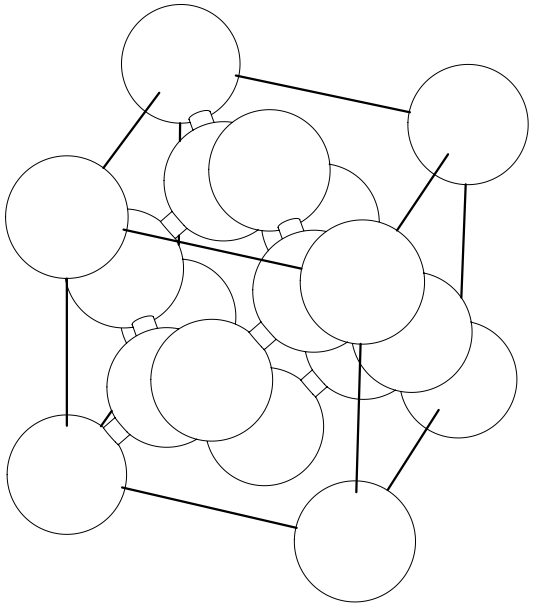
Totally symmetric basis function

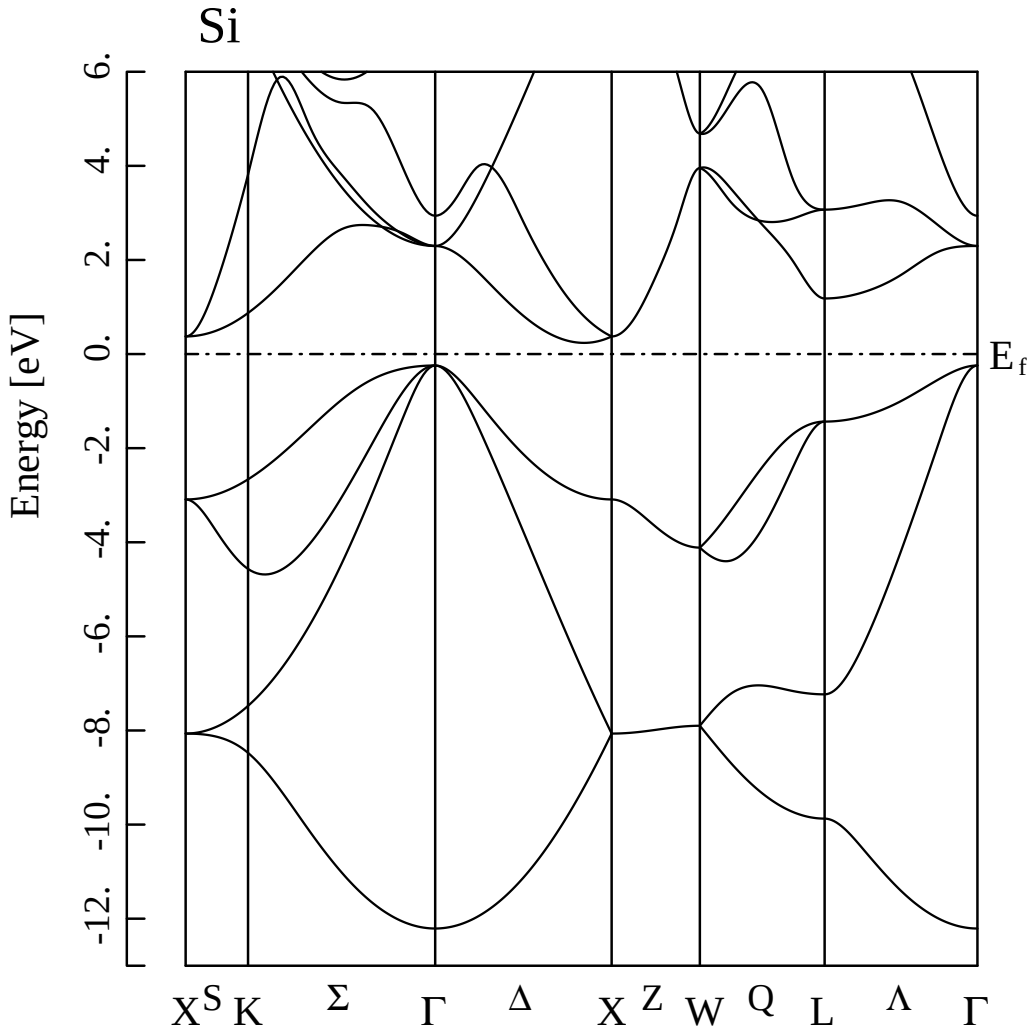
Silicon (Si)

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

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

Crystal structure

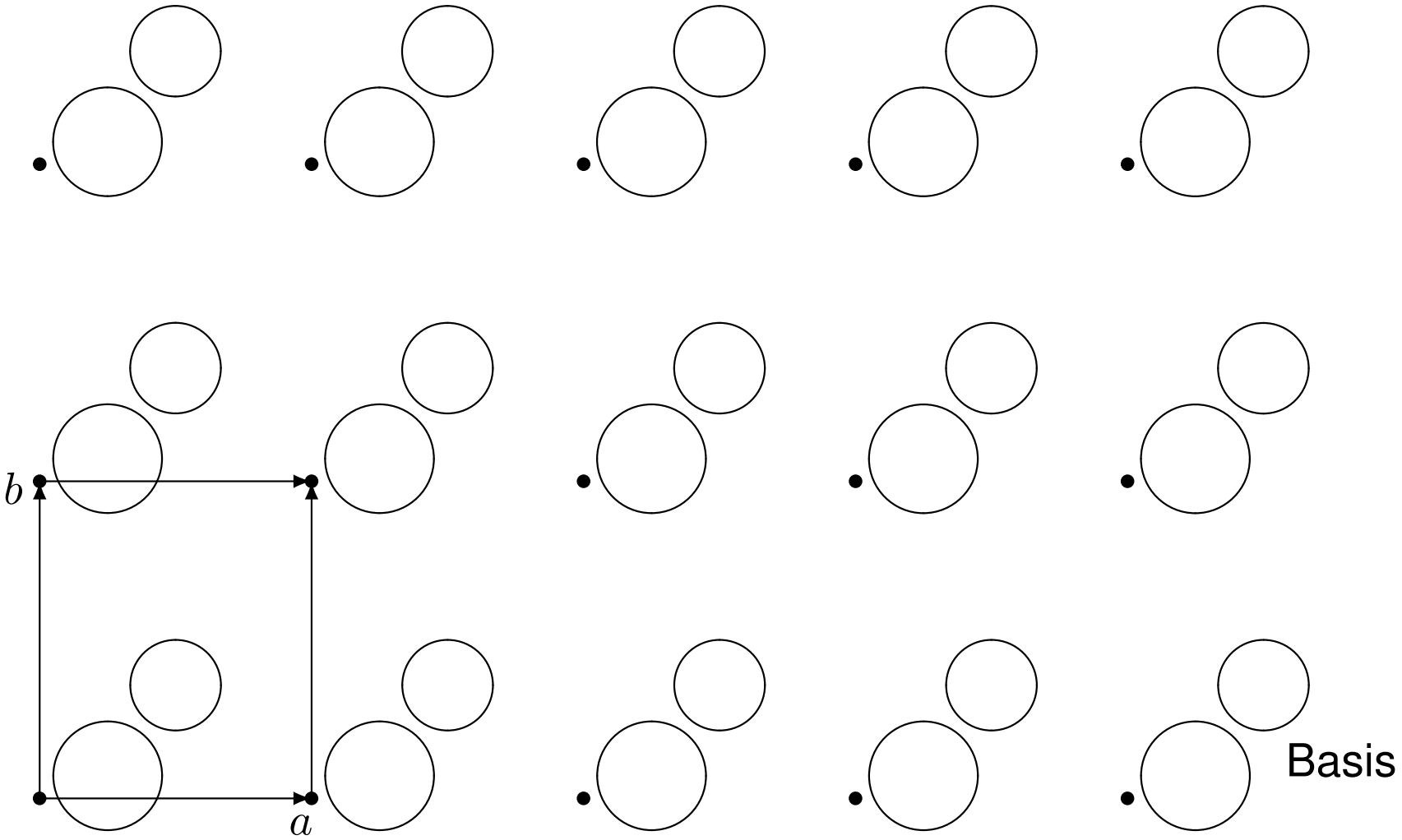




```
Input for Si (diamond)  ---ab_prp.data---
lattice parameter -2----*----3----*----4----*----5----*----6----*---
5.4296 5.4296 5.4296  90.0 90.0 90.0 !a,b,c[A], alpha,beta,gamma
space group       -2----*----3----*----4----*----5----*----6----*---
 3   2   3   0                !idim, il(R,H,P(1),F,I,C,A,B),ngen,inv
    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
-----------------------------------
```

Crystal $=$ Lattice $\otimes$ Basis



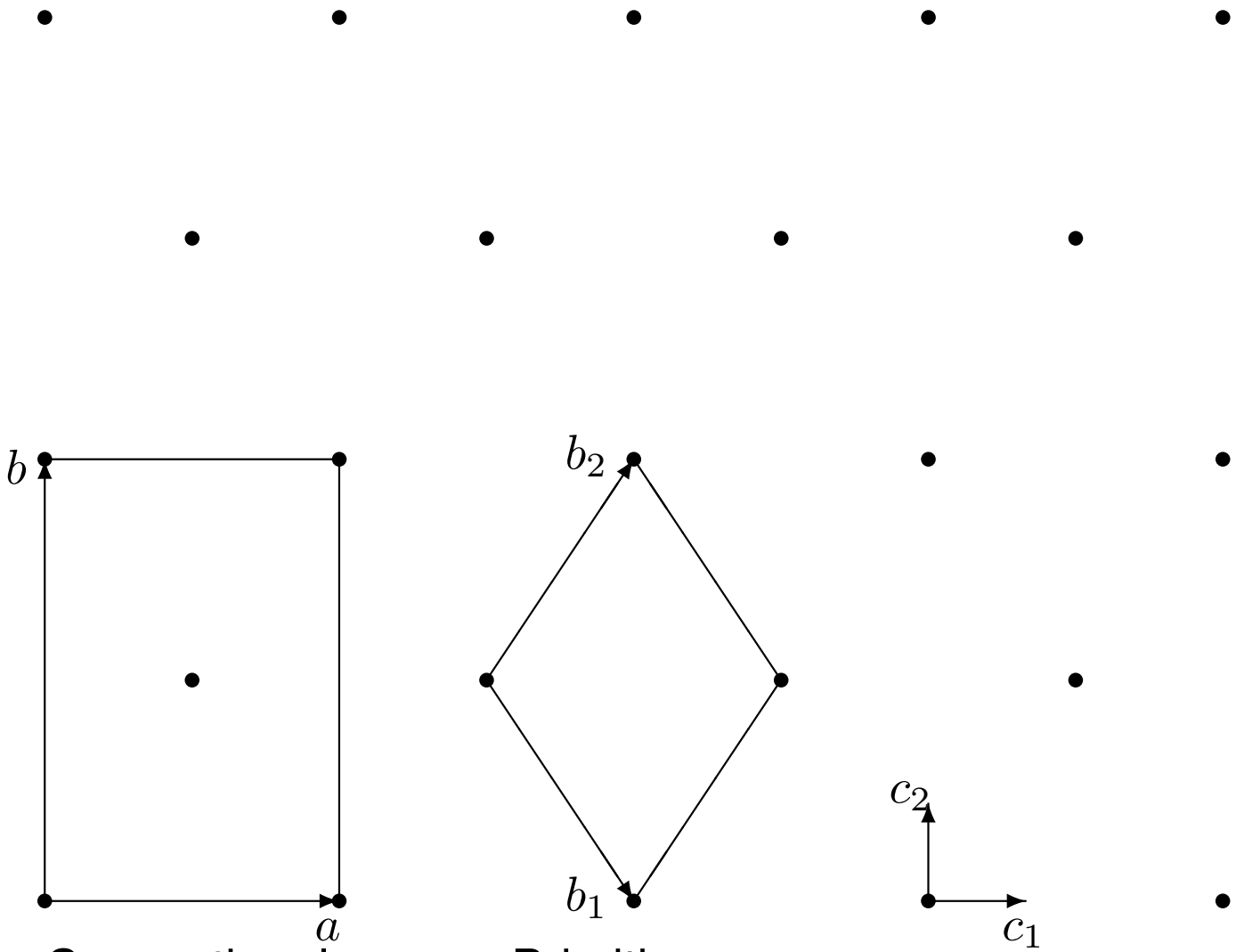
Lattice (14 Bravais lattices)

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

Hexagonal system : P6, Trigonal system : P3, R3

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	Internationl	
-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:

$$\boldsymbol{T} = p_1\boldsymbol{a} + p_2\boldsymbol{b} + p_3\boldsymbol{c}$$
$$p_1,\ p_2,\ p_3 \quad : \quad \text{integers and fractions} \tag{1}$$

Positions on a cell:

$$\boldsymbol{x} = x_1\boldsymbol{a} + x_2\boldsymbol{b} + x_3\boldsymbol{c}$$
$$x_1,\ x_2,\ x_3 \quad : \quad \text{real numbers} \tag{2}$$

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）:

$$T_{ab}^{P} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{3}$$

C-centered lattice（C）:

$$T_{ab}^{C} = \begin{pmatrix} 1/2 & 1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{4}$$

A-centered lattice（A）:

$$T_{ab}^{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 1/2 \\ 0 & -1/2 & 1/2 \end{pmatrix} \tag{5}$$

B-centered lattice（B）：

$$T^B_{ab} = \begin{pmatrix} 1/2 & 0 & -1/2 \\ 0 & 1 & 0 \\ 1/2 & 0 & 1/2 \end{pmatrix} \tag{6}$$

Body-centered lattice（I）：

$$T^I_{ab} = \begin{pmatrix} -1/2 & 1/2 & 1/2 \\ 1/2 & -1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{pmatrix} \tag{7}$$

Face-centered lattice（F）：

$$T^F_{ab} = \begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \\ 1/2 & 1/2 & 0 \end{pmatrix} \tag{8}$$

Rhombohedral lattice（R）：

$$T^R_{ab} = \begin{pmatrix} 2/3 & -1/3 & -1/3 \\ 1/3 & 1/3 & -2/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix} \tag{9}$$

Translational symmetry

Lattice translation vector

$$\boldsymbol{T} = p_1\boldsymbol{a} + p_2\boldsymbol{b} + p_3\boldsymbol{c} \quad (p_1,\ p_2,\ p_3 \ : \ \text{integers and fractions}) \tag{10}$$

$$= n_1\boldsymbol{b}_1 + n_2\boldsymbol{b}_2 + n_3\boldsymbol{b}_3 \quad (n_1,\ n_2,\ n_3 \ : \ \text{integer}) \tag{11}$$

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: $-\boldsymbol{T}$

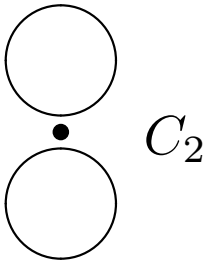
$\{T\}$: Abelian group **($T_2T_1 = T_1T_2$)**

(1) Irreducible representation: 1 dimentional

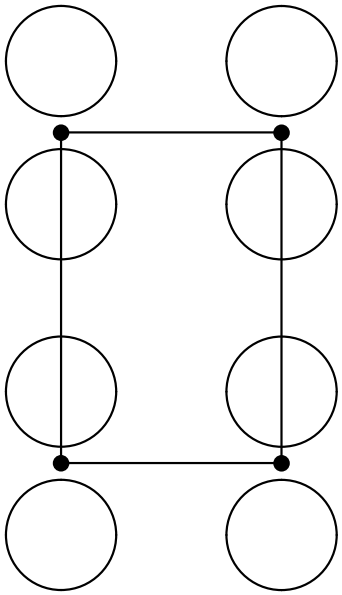
(2) Bloch's theorem

Rotational symmetry

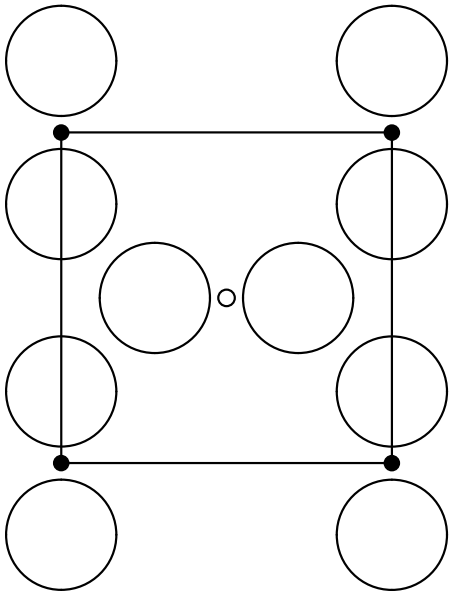
Example of rotation :



C_2



C_2



C_4
or
$\{C_4|(1/2,1/2,0)\}$

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

Space group

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

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

  $\boldsymbol{t}$: nonprimitive translation vector

230 space groups

- **symmorphic** : 73
- **nonsymmorphic** : 157

  $\boldsymbol{t}$: nonprimitive translation

(*) rotation axis

Rotations TSPACE code number

```
(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)
```

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

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	

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

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	

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 2 3 4	
	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 (lattice) space

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

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

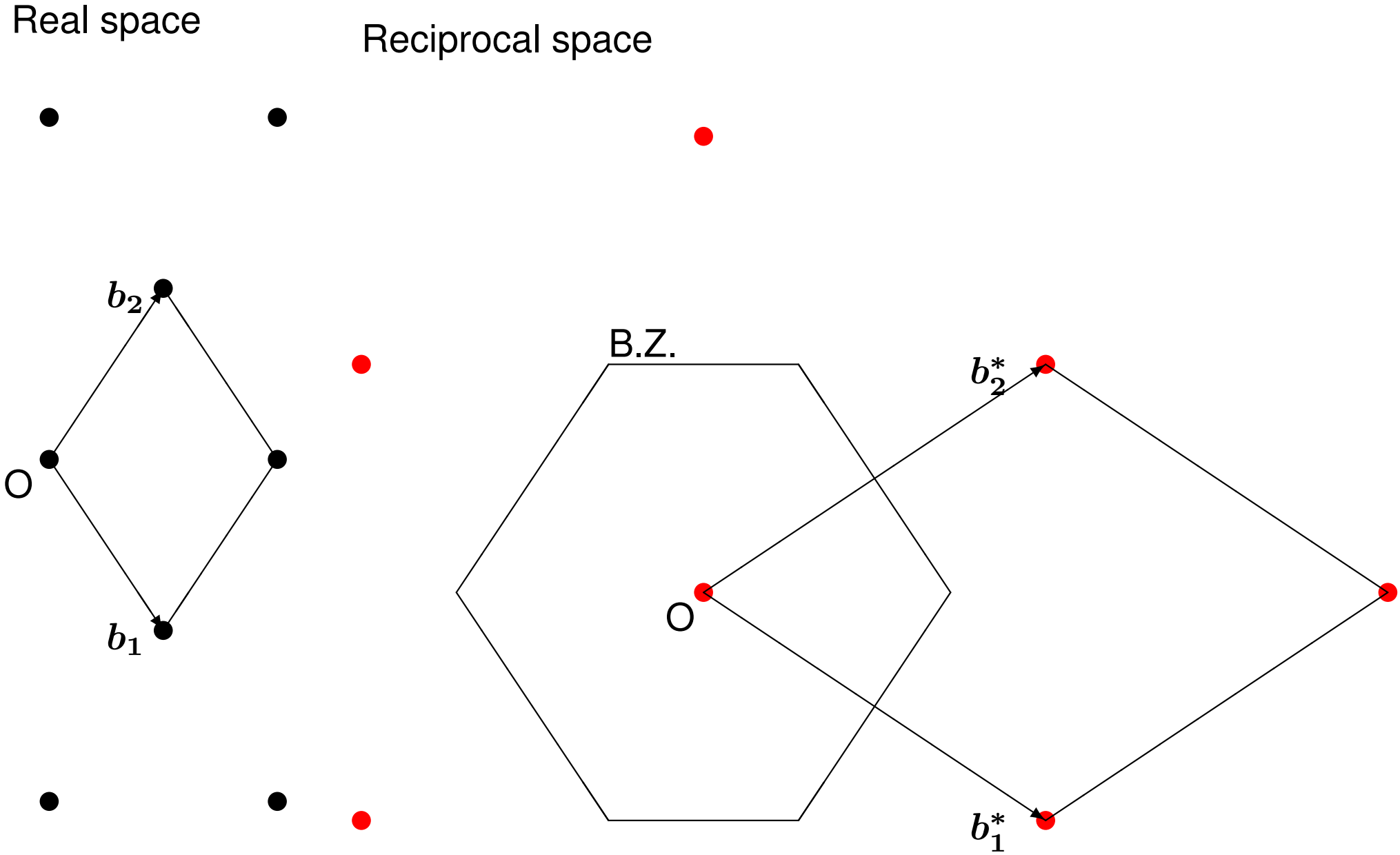
Reciprocal lattice vector

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

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

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

Face-centered rectangular lattice (2D)



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

(1) Wave vector

$e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ (plane wave)

(2) Crystal wave vector

Bloch's theorem $^{\forall}T$:

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

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

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

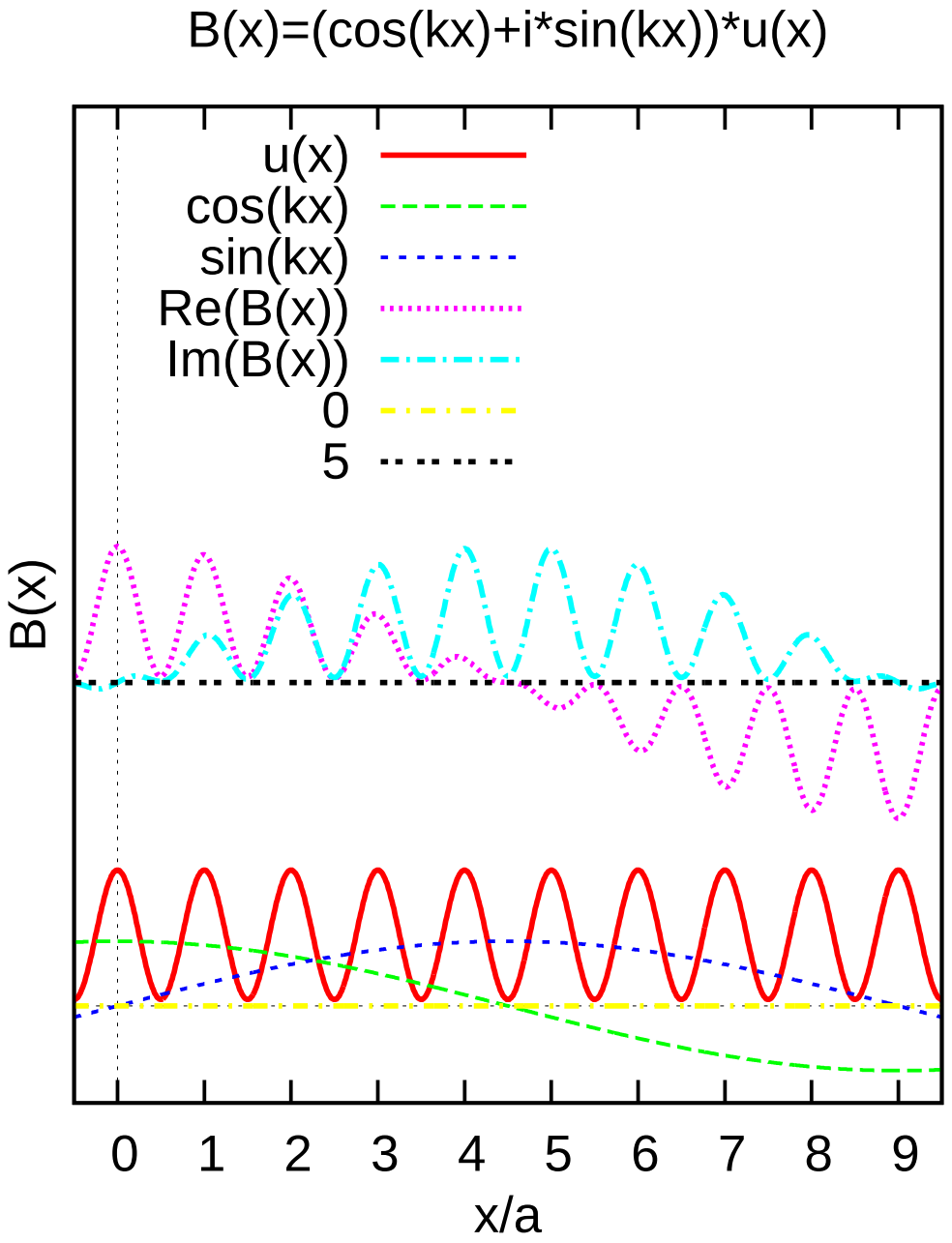
$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\ u(\boldsymbol{r})\ ; \qquad u(\boldsymbol{r}) = \sum_{\boldsymbol{G}} c_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}}$$

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} c_{\boldsymbol{G}} e^{i(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}}$$

Bloch function

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

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



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

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

Reciprocal lattice vector

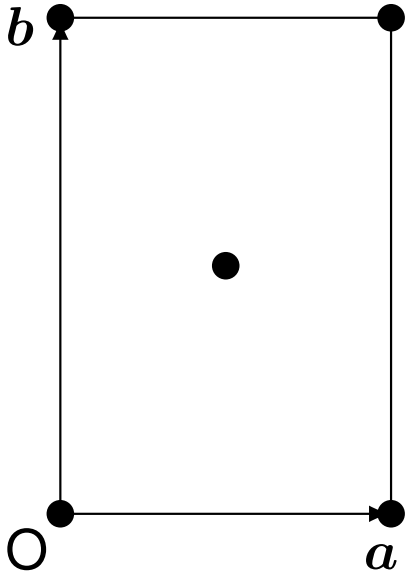
$$\boldsymbol{G} = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$$

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

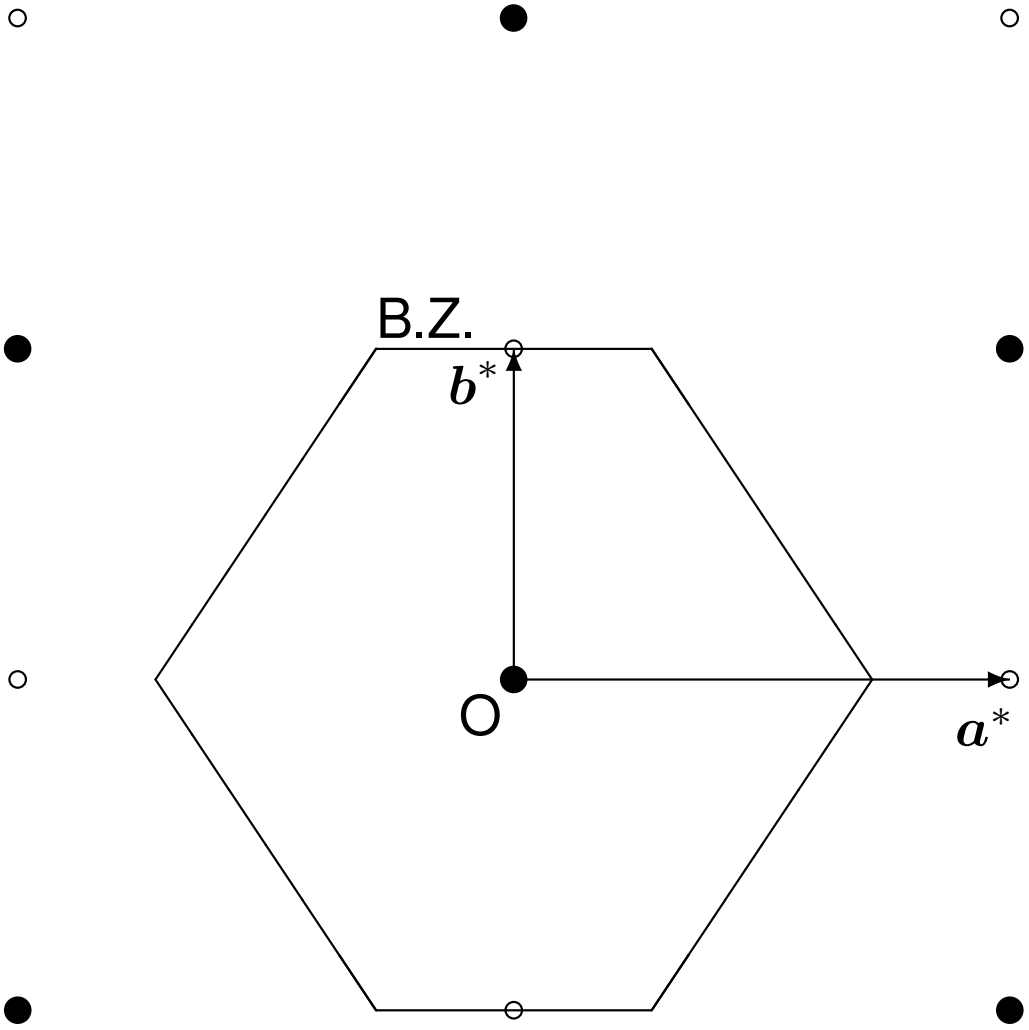
Face-centered rectangular lattice (2D)

Real space



Conventional unit cell

Reciprocal space (k-space)



One-electron state

One-electron Hamiltonian:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + v_{\text{eff}}(\boldsymbol{r})$$

$^{\forall}T$:

$$[H, T] = 0$$

$\Rightarrow$

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

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

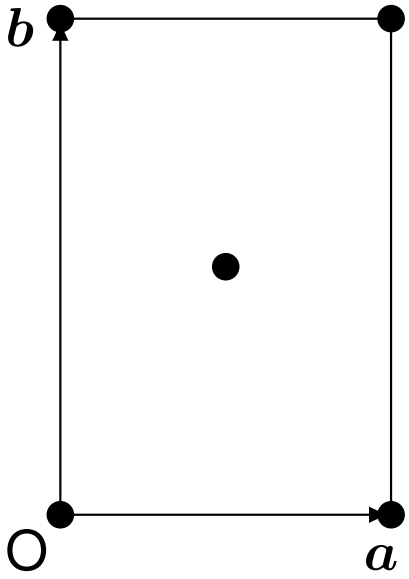
$\boldsymbol{k}$ space mesh : $\left(\frac{a^*}{n_x}, \frac{b^*}{n_y}, \frac{c^*}{n_z}\right)$

ABCAP
n_x, n_y, n_z

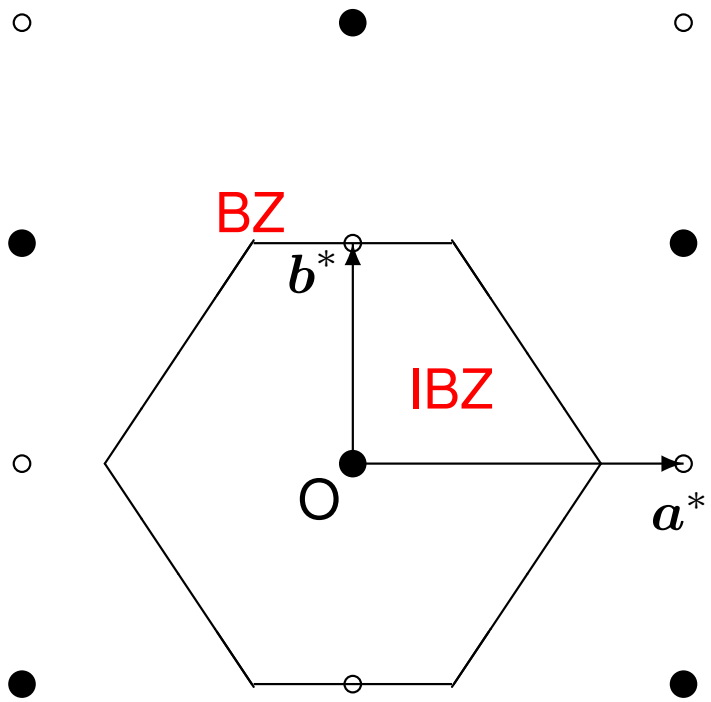
Irreducible brillouin zone (IBZ)

Face-centered rectangular lattice (2D)

Real space



Reciprocal space (k-space)



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

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

```
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)
  0.197601262613305 2E+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
ie=10(10)  e= 0.474056 Hr  :  Si* 2  0.000   0.000   0.294   0.000
ie=11(10)  e= 0.474056 Hr  :  Si* 2  0.000   0.000   0.294   0.000
```

```
ie=12( 7)  e= 0.597702 Hr  :  Si* 2  0.000  0.081  0.088  0.021
ie=13( 7)  e= 0.597702 Hr  :  Si* 2  0.000  0.081  0.088  0.021
ie=14( 7)  e= 0.597702 Hr  :  Si* 2  0.000  0.081  0.088  0.021
```

Iteration process of Kohn-Sham equations

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

Linearized Augmented Plane Wave Method

Muffin-Tin sphere (MT sphere)

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

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

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

LAPW : Basis function

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

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

(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

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

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

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

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

Schrödinger equation (matrix form)

$$\sum_{G'} H_{\boldsymbol{k}}^{\boldsymbol{G},\boldsymbol{G'}} c_{\boldsymbol{k}n}^{\boldsymbol{G'}} = E_{\boldsymbol{k}n} \sum_{G'} S_{\boldsymbol{k}}^{\boldsymbol{G},\boldsymbol{G'}} c_{\boldsymbol{k}n}^{\boldsymbol{G'}}$$

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

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

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:

$$G_p(\boldsymbol{r}) = \left\langle \boldsymbol{r} \middle| G_p \right\rangle = \sum_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}} c_{\boldsymbol{G}p} \tag{12}$$

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

$$\begin{aligned} F_{\nu s}(\rho; \boldsymbol{r}) &= \left\langle \boldsymbol{r} \middle| F_{\nu s}(\rho) \right\rangle \\ &= \sum_{\alpha} \Theta_{\nu\alpha}(\boldsymbol{r}) \delta(\rho - r_{\nu\alpha}) \sum_m Y_{lm}(\boldsymbol{r}_{\nu\alpha}) d_{\alpha m \nu s} \end{aligned} \tag{13}$$

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

Totally symmetric plane-wave basis (SPW)

Orthogonality:

$$\int_\Omega \mathrm{d}^3 r G_p^*(\boldsymbol{r}) G_{p'}(\boldsymbol{r}) = \Omega \sum_{\boldsymbol{G}} c^*_{\boldsymbol{G}p} c_{\boldsymbol{G}p'}$$
$$= \frac{\Omega}{N_p} \delta_{pp'} \tag{14}$$

Overlap integrals in the interstitial:

$$O_{pp'}^{\mathrm{SPW}} = \int_\Omega \mathrm{d}^3 r G_p^*(\boldsymbol{r}) G_{p'}(\boldsymbol{r}) [1 - \Theta(\boldsymbol{r})] \tag{15}$$