

All electron Band structure CAIculation 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

$$n^{\text{in}}(\mathbf{r})$$

↓

$$v_{\text{eff}}(\mathbf{r}) = v_{\text{H}}(\mathbf{r}) + v_{\text{xc}}(\mathbf{r}) + v(\mathbf{r})$$

↓

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + v_{\text{eff}}(\mathbf{r}) \right] \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r})$$

↓

$$n^{\text{out}}(\mathbf{r}) = \sum_{i=1}^N |\psi_i(\mathbf{r})|^2$$

↓

$$(1 - \delta) \cdot n^{\text{in}}(\mathbf{r}) + \delta \cdot n^{\text{out}}(\mathbf{r}) \Rightarrow n^{\text{in}}(\mathbf{r})$$

2 FLAPW method

Full-Potential
Linearized Augmented Plane Wave Method

Muffin-Tin spheres

Takeda-Kübler scheme (linearization)

Totally symmetric basis functions

Crystal Structure

Lattice :

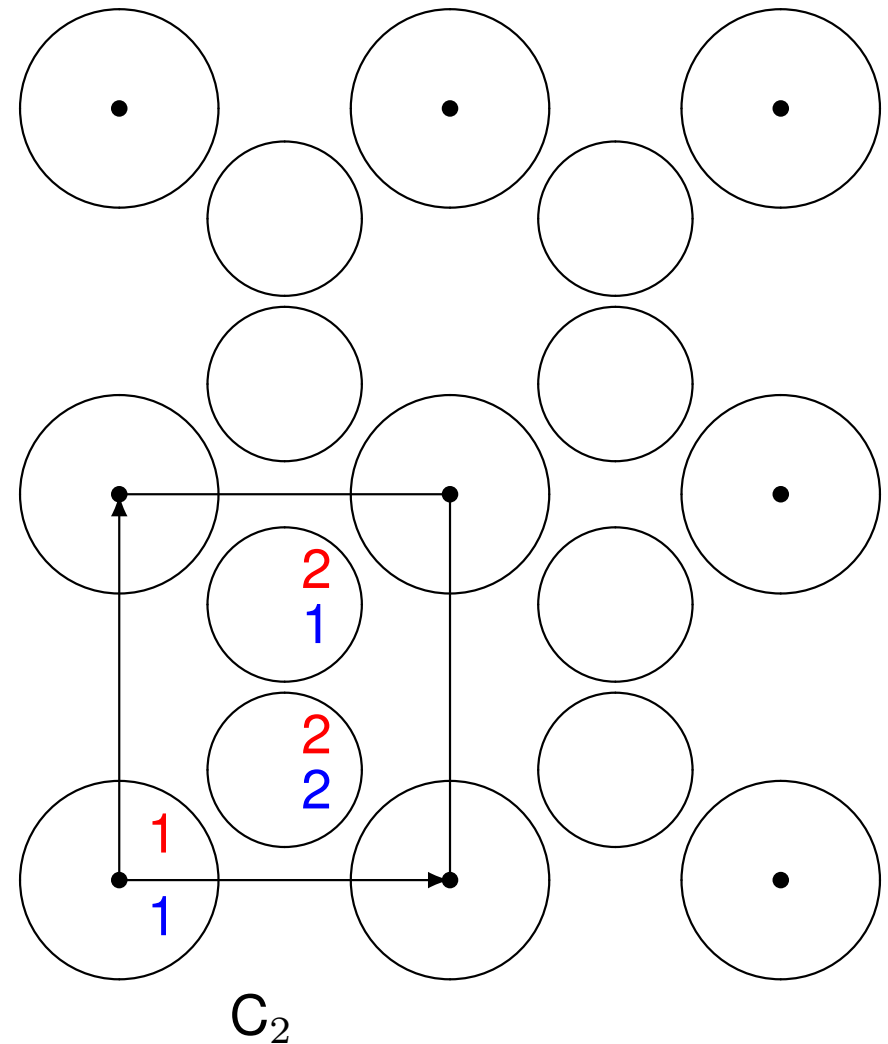
- a, b, c
- α, β, γ

Primitive cell :

- ν : kind of atom
- α : atom no.

Two regions in APW method

- Muffin-Tin (MT) Sphere
- Interstitial



Linearized Augmented Plane Wave Method

Muffin-Tin sphere (MT sphere)

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

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

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

LAPW : Basis function

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

\mathbf{k} : inside the Brillouin zone

\mathbf{G} : Reciprocal lattice vector

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

$\chi_{\nu\alpha}^{\mathbf{K}}(\mathbf{r})$: 'atomic' wavefunction

Fe₃O₄ magnetite

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

(1) Interstitial

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

ABCAP

ekmax1 cut-off energy

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

$$\chi_{\nu\alpha}^{\mathbf{K}}(\mathbf{r}) = 4\pi e^{i\mathbf{K}\cdot\mathbf{R}_{\nu\alpha}} \sum_{lm} i^l Y_{lm}^*(\hat{\mathbf{K}}) Y_{lm}(\hat{\mathbf{r}}_{\nu\alpha}) \Phi_{\nu l}^{\mathbf{K}}(r_{\nu\alpha})$$

$$\Phi_{\nu l}^{\mathbf{K}}(r) = \sum_{\beta=1}^2 \phi_{\nu l\beta}(r) a_{\nu l\beta}^{\mathbf{K}}$$

ABCAP

lmax1 maximum value of l

Schrödinger equation

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

Eigenfunction expanded by LAPW basis

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

Schrödinger equation (matrix form)

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

$$H_{\mathbf{k}}^{\mathbf{G},\mathbf{G}'} = \langle \chi_{\mathbf{k}+\mathbf{G}} | H | \chi_{\mathbf{k}+\mathbf{G}'} \rangle$$

$$S_{\mathbf{k}}^{\mathbf{G},\mathbf{G}'} = \langle \chi_{\mathbf{k}+\mathbf{G}} | \chi_{\mathbf{k}+\mathbf{G}'} \rangle$$

Full potential

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

(SPW) Totally symmetric basis function in the interstitial:

$$G_p(\mathbf{r}) = \langle \mathbf{r} | G_p \rangle = \sum_G e^{i\mathbf{G} \cdot \mathbf{r}} c_{Gp} \quad (1)$$

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

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

ABCAP	
<i>egmax0</i>	cut-off energy
<i>lmax0</i>	maximum value of <i>l</i>

Totally symmetric plane-wave basis (SPW)

Orthogonality:

$$\begin{aligned}\int_{\Omega} d^3r G_p^*(\mathbf{r}) G_{p'}(\mathbf{r}) &= \Omega \sum_{\mathbf{G}} c_{\mathbf{G}p}^* c_{\mathbf{G}p'} \\ &= \frac{\Omega}{N_p} \delta_{pp'}\end{aligned}\quad (3)$$

Overlap integrals in the interstitial: (OSPW matrix)

$$O_{pp'}^{\text{SPW}} = \int_{\Omega} d^3r G_p^*(\mathbf{r}) G_{p'}(\mathbf{r}) [1 - \Theta(\mathbf{r})] \quad (4)$$

3 Example : Si

Two important input files

`ab_prp.data`
Crystal structure

`ab_atom.data`
Electron configuration of atom

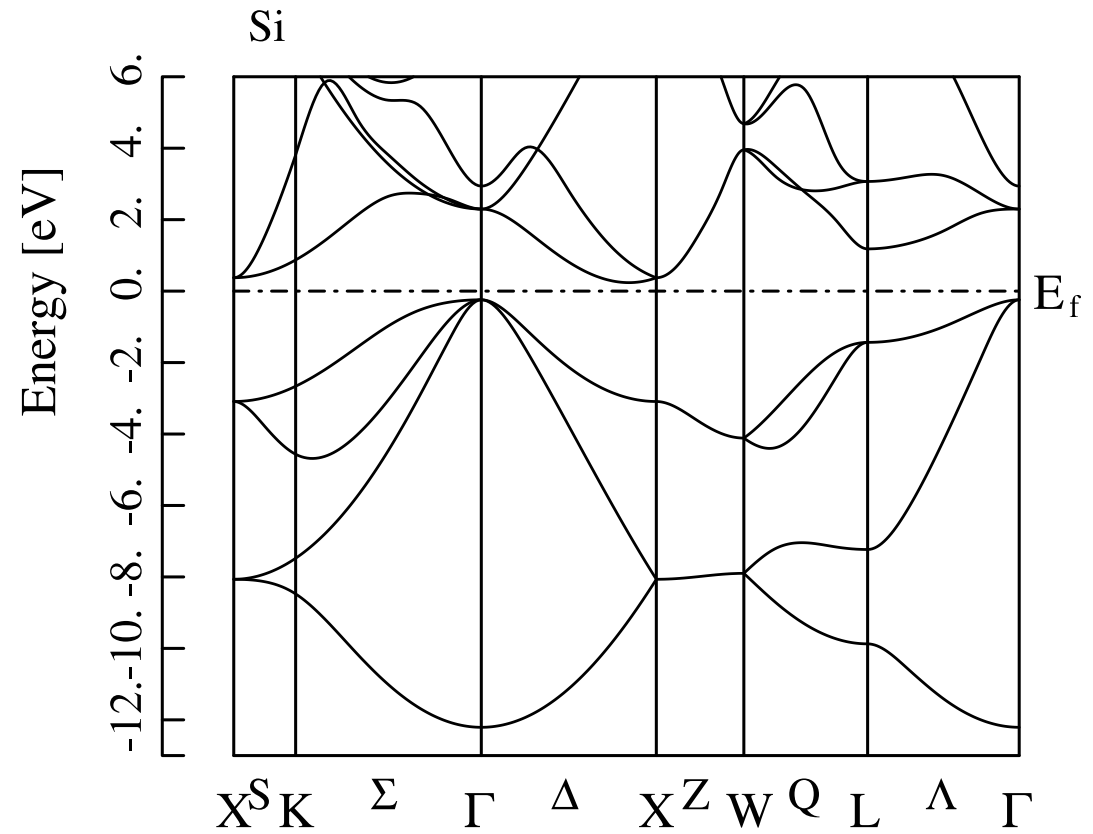
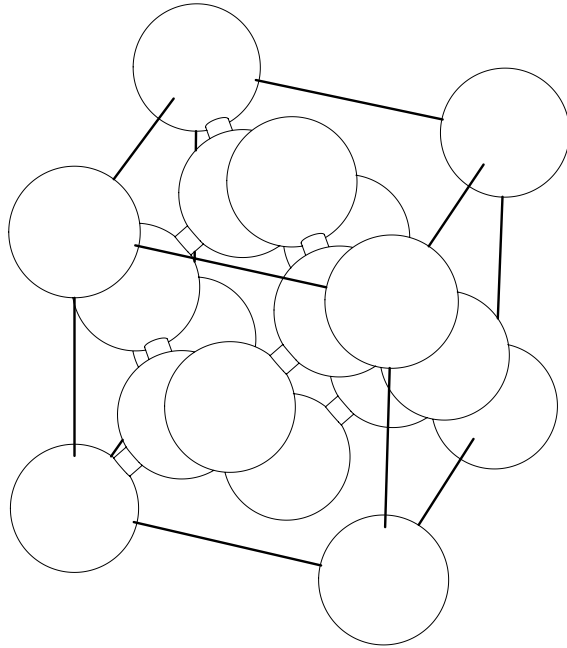
Parameters on the calculational scheme

Silicon (Si)

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

$\hbar\mathbf{k}$: crystal momentum (\mathbf{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

4 Crystal structure

”TSPACE”

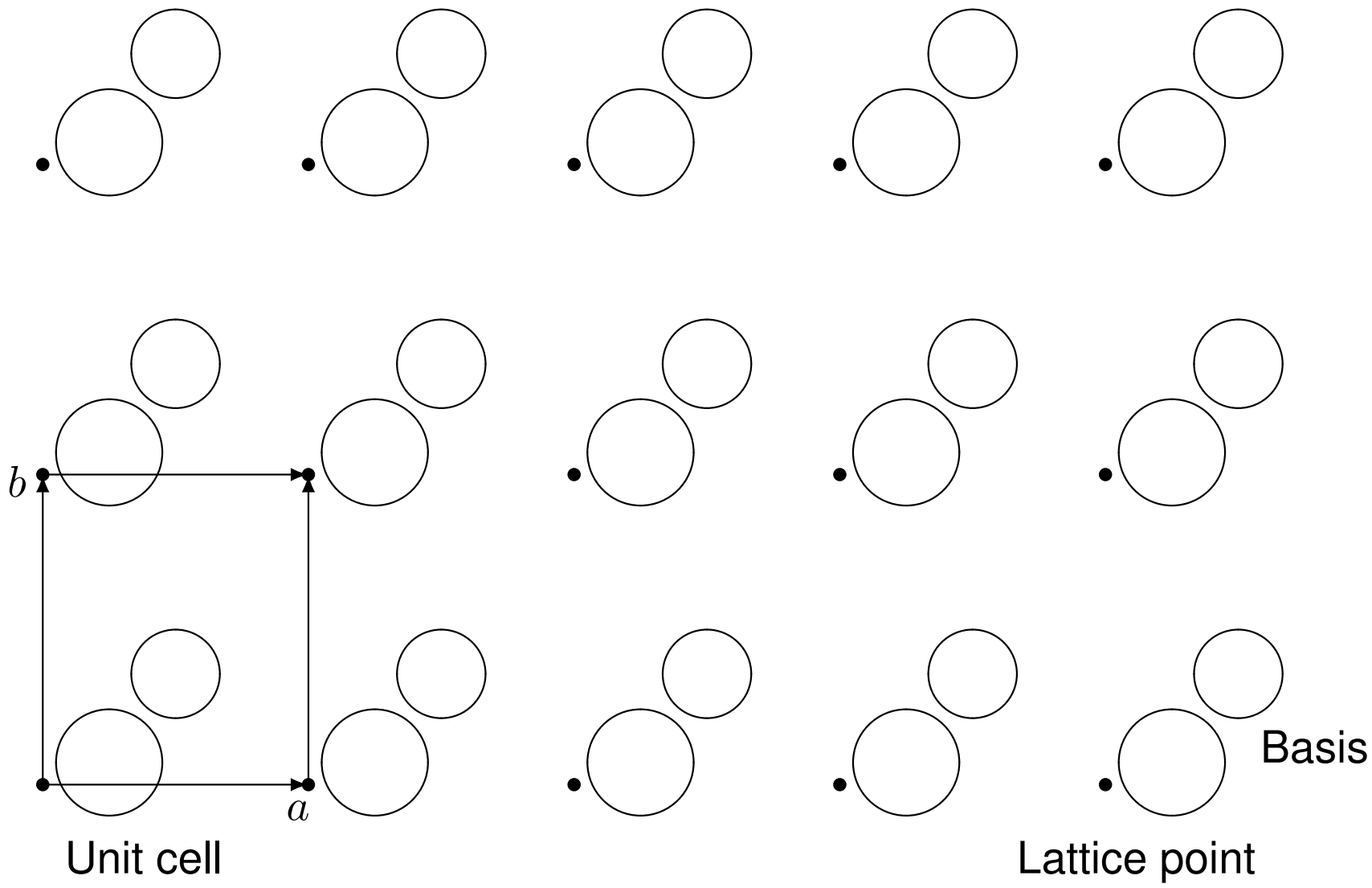
Translational symmetry
Bravais lattice

Rotational symmetry

Crystal point group
with non-primitive translation

”International Tables for Crystallography”

Crystal = Lattice \otimes Basis



Lattice (14 Bravais lattices)

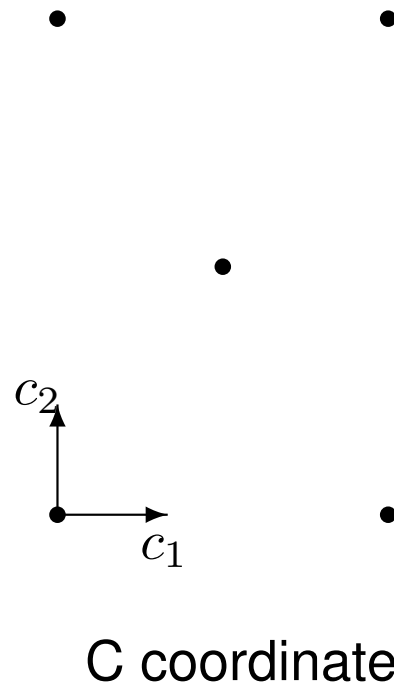
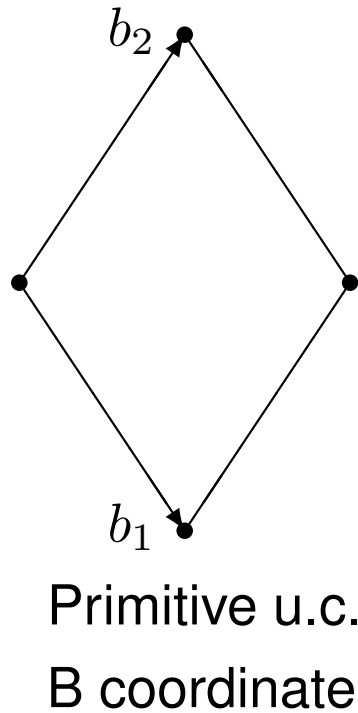
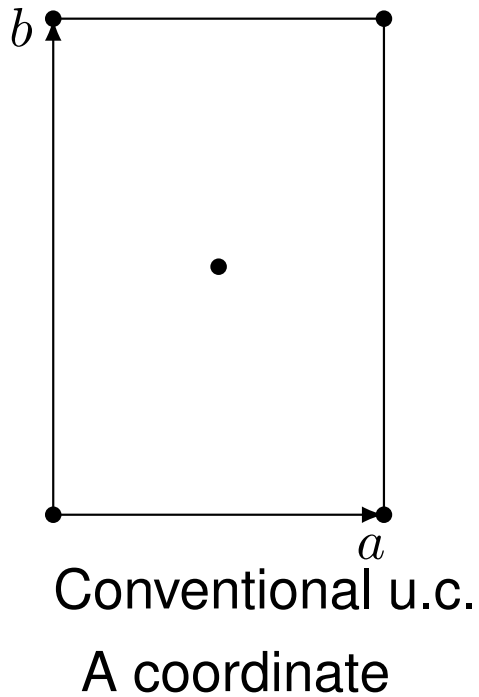
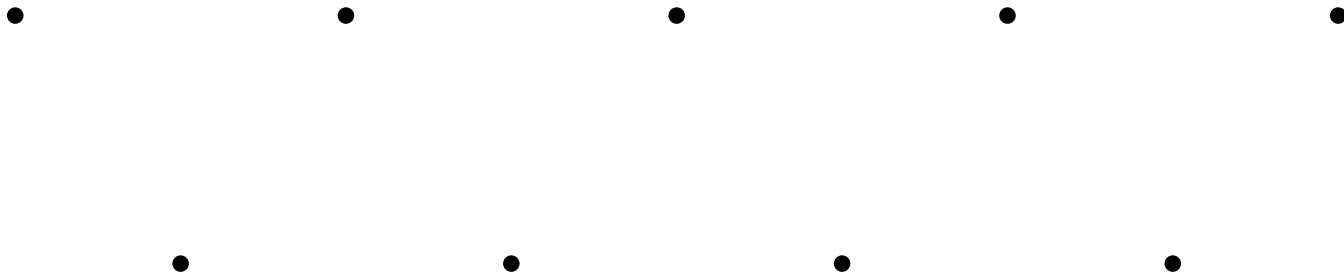
Crystal System	Lattice Parameter	Bravais lattice
Triclinic		P
Monoclinic	$\beta = \gamma = 90^\circ$	P C
Orthorhombic	$\alpha = \beta = \gamma = 90^\circ$	P C I F
Tetragonal	$a = b$	P I
Cubic	$a = b = c$	P I F
Hexagonal, Trigonal	$a = b, \gamma = 120^\circ$	P R

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 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	$(0, 1/2, 1/2), (1/2, 0, 1/2), (1/2, 1/2, 0)$ $(1/2, 1/2, 1/2)$ $(1/2, 1/2, 0)$ $(0, 1/2, 1/2)$ $(1/2, 0, 1/2)$
2	F	
3	I	
4	C	
	A	
	B	

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

Lattice translation vector:

$$\mathbf{T} = p_1 \mathbf{a} + p_2 \mathbf{b} + p_3 \mathbf{c}$$

p_1, p_2, p_3 : integers and fractions (5)

Positions in a cell:

$$\mathbf{x} = x_1 \mathbf{a} + x_2 \mathbf{b} + x_3 \mathbf{c}$$

x_1, x_2, x_3 : real numbers (6)

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

Primitive coordinate system $\{b_1, b_2, b_3\}$: **B coordinate system**

$$(b_1, b_2, b_3) = (a, b, c)T_{ab}$$

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

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

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

Lattice translation operator : T

Lattice translation group $\{T\}$

(i) Closure: $T_2 T_1 \in \{T\}$

(ii) Associativity: $(T_3 T_2) T_1 = T_3 (T_2 T_1)$

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

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

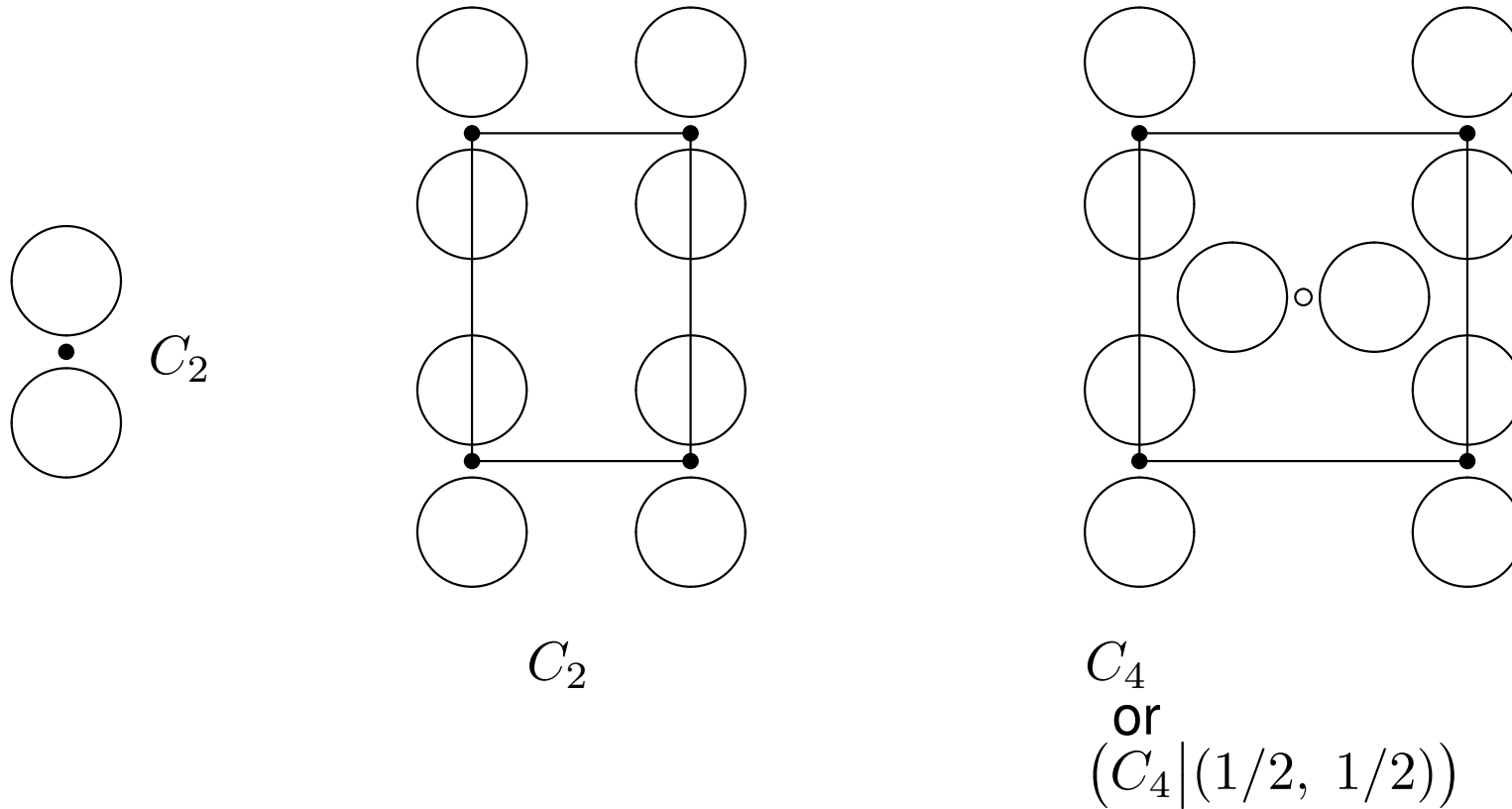
$\{T\}$: Abelian group ($T_2 T_1 = T_1 T_2$)

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

(2) Bloch's theorem (k : label of irrep.)

Rotational symmetry

Example of rotation :



Point group $\{E, C_2\}$,

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

$\{E, C_2, C_4\}$

symmorphic

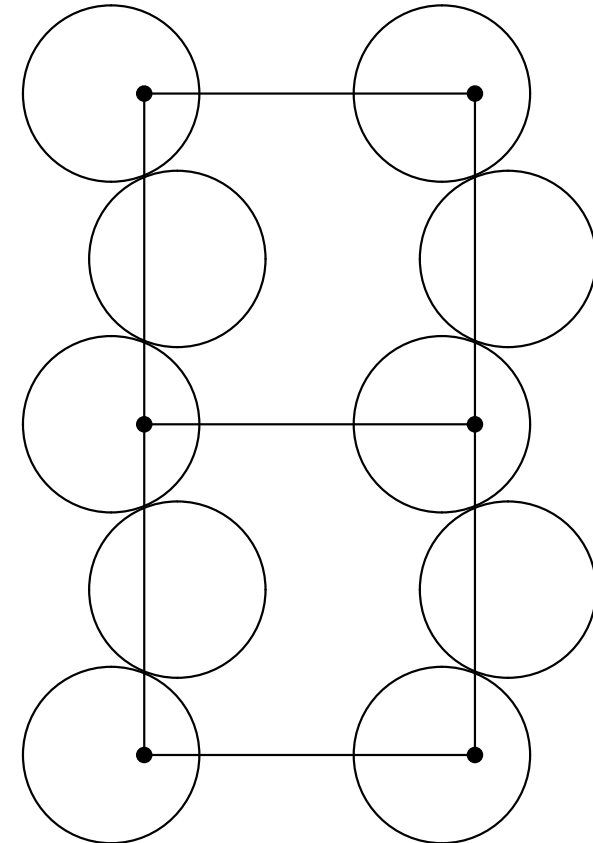
Space group

Group element (Seitz notation): $(R|\mathbf{T} + t_R)$

- R : E, C_2, C_3, C_4, C_6, I
- \mathbf{T} : lattice translation vector
- t_R : nonprimitive translation vector

230 space groups

- $t_R = 0$
symmorphic : 73
- $t_R \neq 0$ (screw, glide)
nonsymmorphic : 157



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

"TSPACE"

TSPACE convention

Rotations

"TSPACE" symmetry operation code (Hexagonal and Trigonal)

(i1=-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)

(i1=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

$$\{b_1^*, b_2^*, b_3^*\}$$

Reciprocal (lattice) space

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

$$\mathbf{b}_1^* \cdot \mathbf{b}_1 = 2\pi, \quad \mathbf{b}_1^* \cdot \mathbf{b}_2 = 0, \quad \mathbf{b}_1^* \cdot \mathbf{b}_3 = 0,$$

$$\mathbf{b}_2^* \cdot \mathbf{b}_1 = 0, \quad \mathbf{b}_2^* \cdot \mathbf{b}_2 = 2\pi, \quad \mathbf{b}_2^* \cdot \mathbf{b}_3 = 0,$$

$$\mathbf{b}_3^* \cdot \mathbf{b}_1 = 0, \quad \mathbf{b}_3^* \cdot \mathbf{b}_2 = 0, \quad \mathbf{b}_3^* \cdot \mathbf{b}_3 = 2\pi$$

Reciprocal lattice vector

$$\mathbf{G} = m_1 \mathbf{b}_1^* + m_2 \mathbf{b}_2^* + m_3 \mathbf{b}_3^*$$

$$m_1, m_2, m_3 = \text{integer}$$

\mathbf{G} and \mathbf{T}

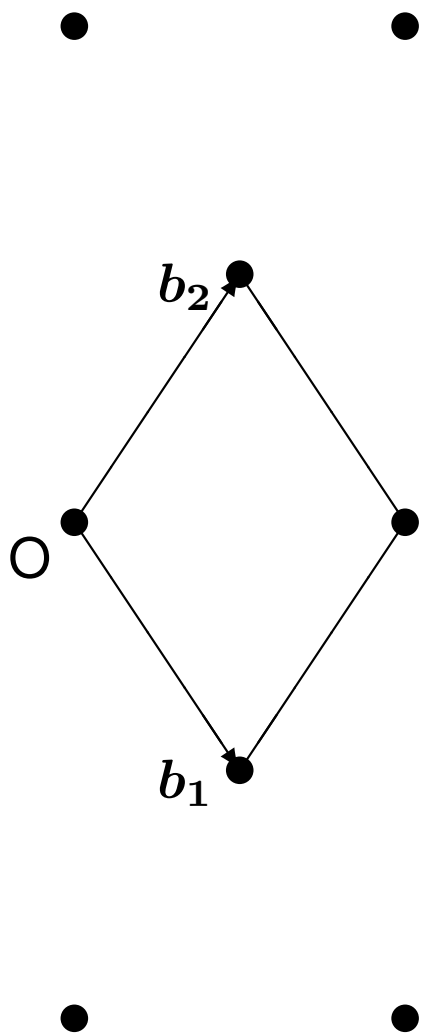
$$\mathbf{G} \cdot \mathbf{T} = 2\pi n \quad (n : \text{integer})$$

or

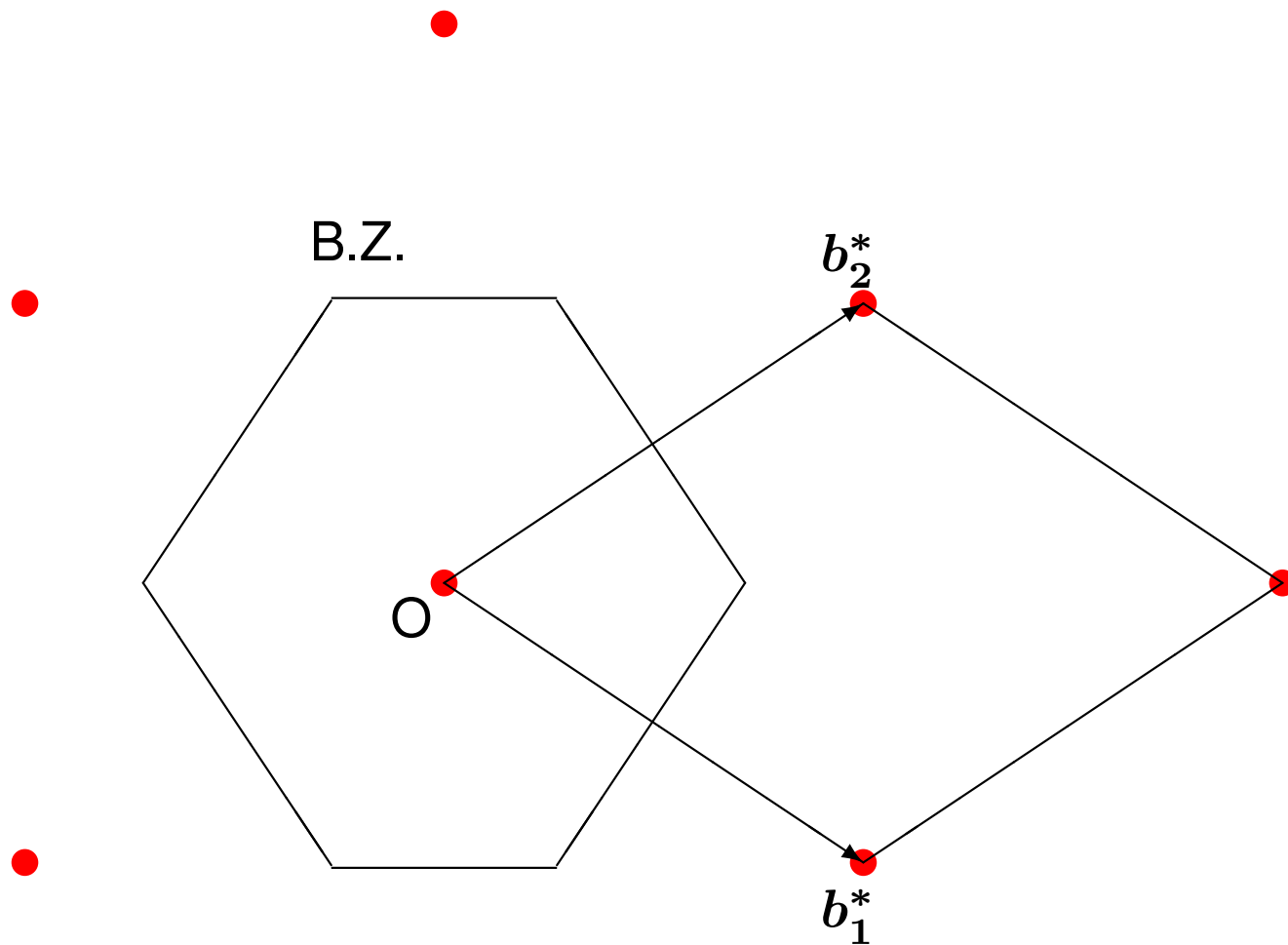
$$e^{i\mathbf{G} \cdot \mathbf{T}} = 1$$

Face-centered rectangular lattice (2D)

Real space



Reciprocal space



”

Conventional reciprocal-space coordinate

The A coordinate system in reciprocal space

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

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

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

Reciprocal lattice vector

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

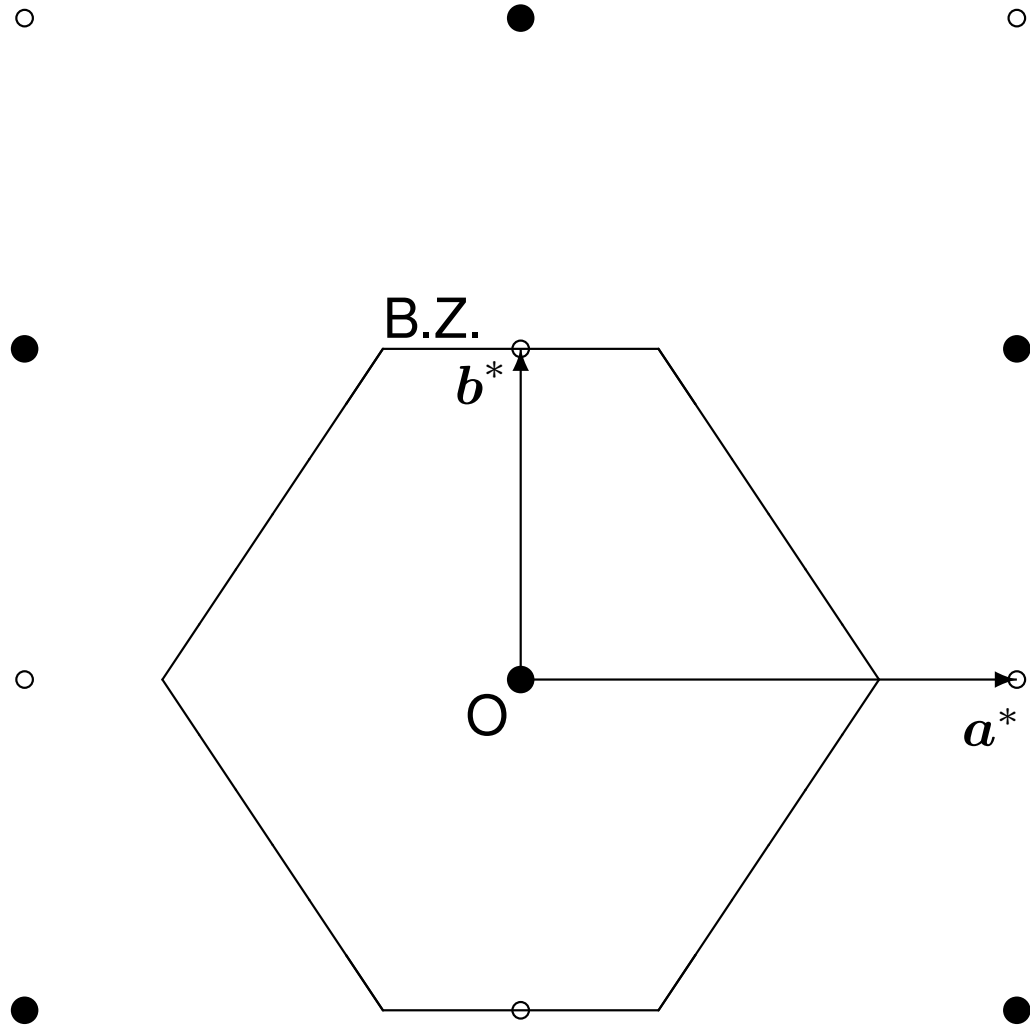
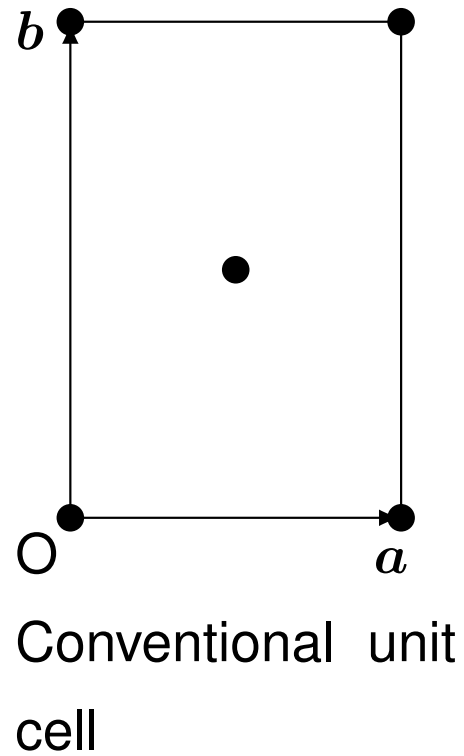
lattice type	allowed (h,k,l)
Rhombohedral ($il = -1$)	$-h + k + l = \text{multiple of } 3$
Hexagonal ($il = 0$)	all integer
Primitive ($il = 1$)	all integer
Face-centered ($il = 2$)	all odd or all even
Body-centered ($il = 3$)	$h + k + l = \text{even}$
C-centered ($il = 1$)	$h + k = \text{even}$

Extinction Rule

Face-centered rectangular lattice (2D)

Reciprocal space (k -space)

Real space



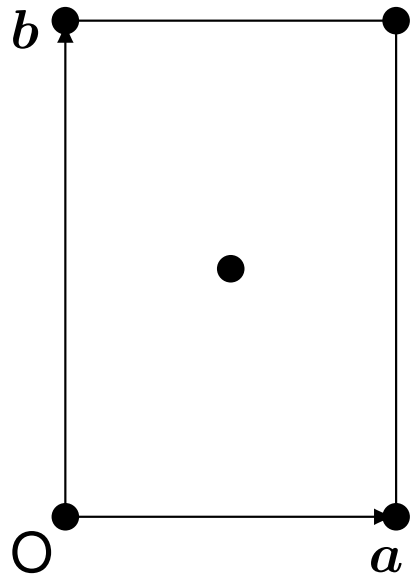
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Rotational symmetry in the k space

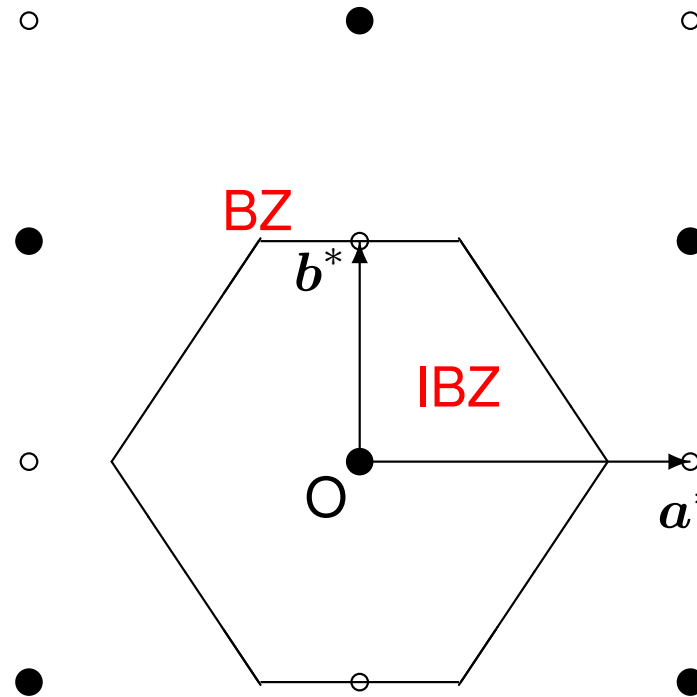
Irreducible brillouin zone (IBZ)

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 : $h \Rightarrow \text{IBZ} = \frac{\text{BZ}}{h}$

” ”

Bloch function

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

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

Simultaneous eigenfunction for all T :

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

\mathbf{k} is a 'good quantum number'.

Group theoretical interpretation:

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

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

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

Bloch function

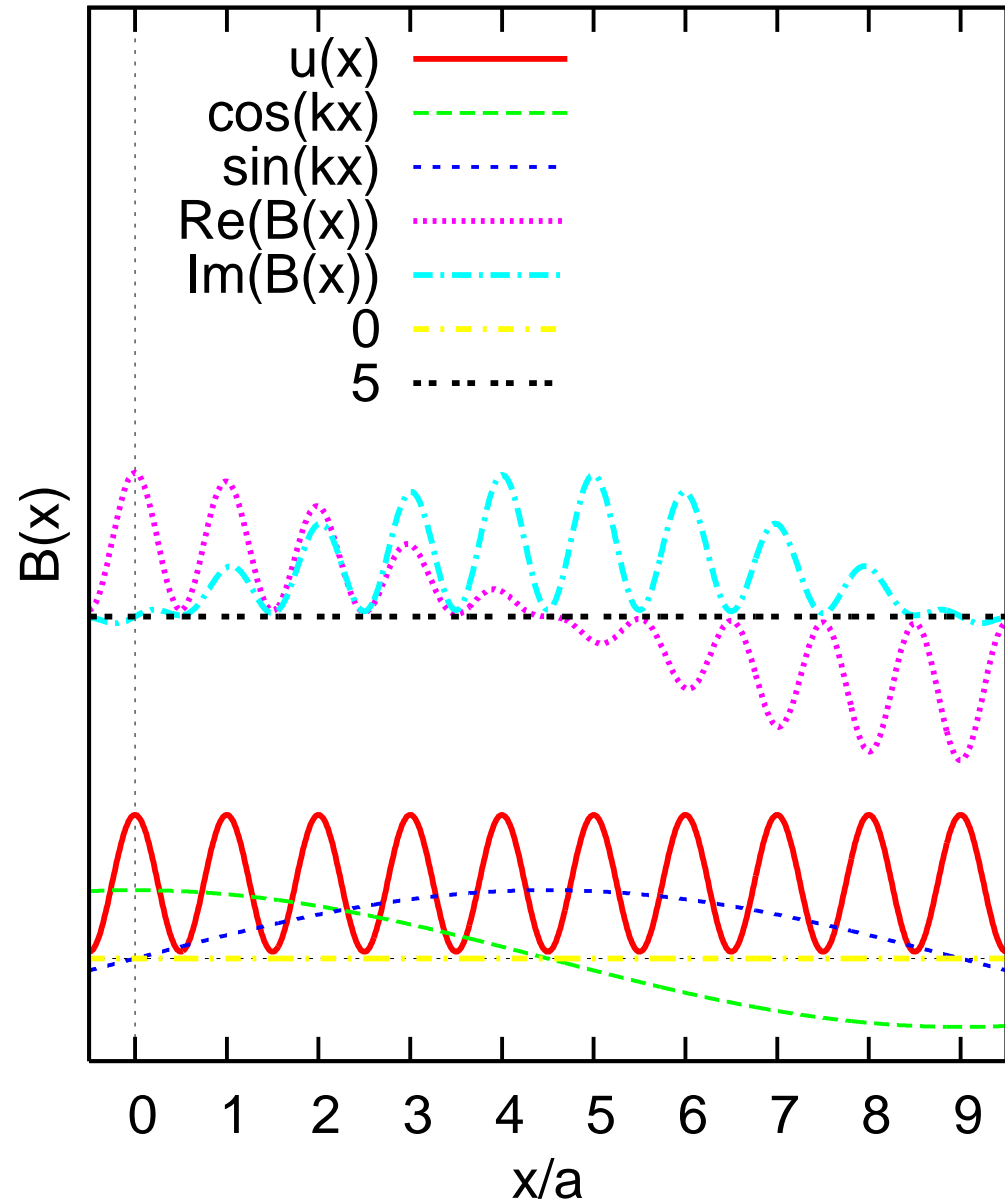
$$B(x) = e^{ikx} u(x)$$

$$= [\cos(kx) + i \sin(kx)] u(x)$$

$$u(x) = u(x - T) \quad (\forall T)$$

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

$$B(x) = (\cos(kx) + i \sin(kx)) u(x)$$



” ”

Energy eigenstate

One-electron state

One-electron Hamiltonian:

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

$$[H, T] = 0 \quad (\forall T)$$

↓

$$H\psi_{\mathbf{k}n} = \epsilon_{\mathbf{k}n}\psi_{\mathbf{k}n}$$

$$T\psi_{\mathbf{k}n} = e^{-i\mathbf{k}\cdot\mathbf{T}}\psi_{\mathbf{k}n} \quad (\forall T)$$

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

\mathbf{k} space mesh : $\frac{a^*}{n_x}, \frac{b^*}{n_y}, \frac{c^*}{n_z}$

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
- wyckoff.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
0.000000000E+00  0.400000000E+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 $\psi_{\mathbf{k}}(\mathbf{r})$

Irreducible representation of \mathbf{k} group

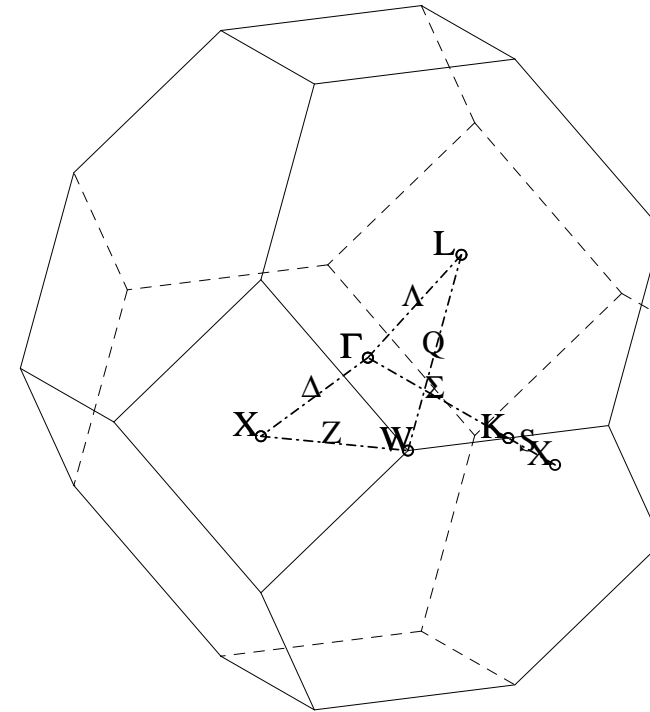
$$\exp(-i\mathbf{k} \cdot (\mathbf{u}_\alpha + \mathbf{T})) D_{\mathbf{k}}^{(\lambda)}(\alpha)$$

α : \mathbf{k} -invariant rotation

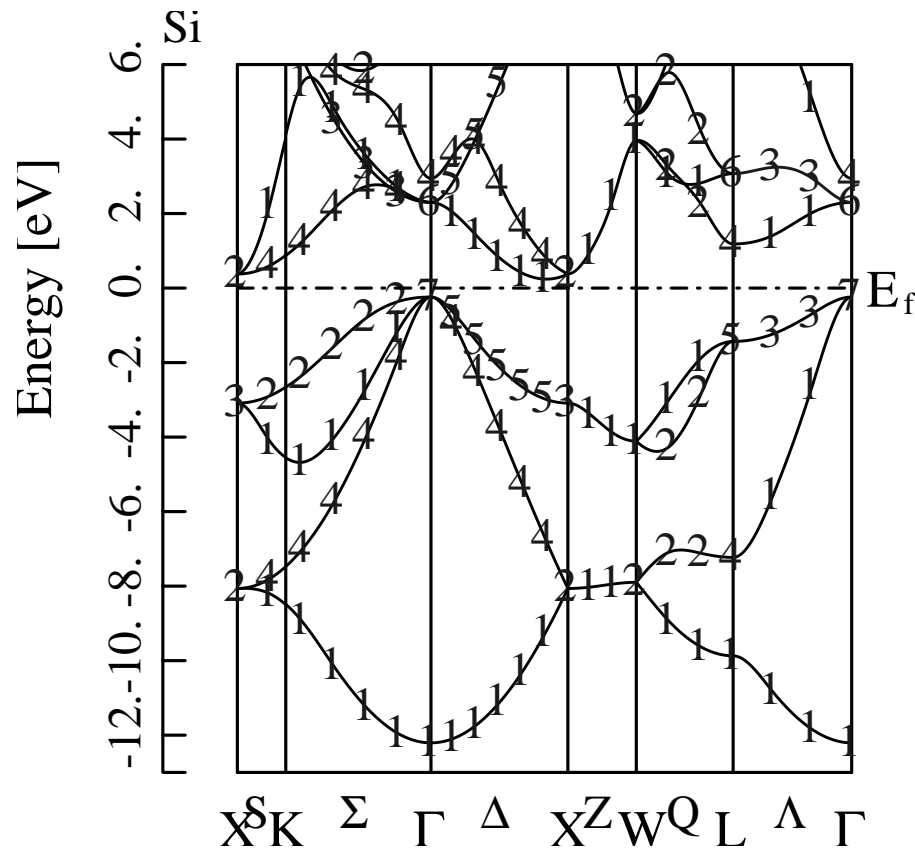
Nonsymmorphic space group ($Fd\bar{3}m$)

$D_{\mathbf{k}}^{(\lambda)}(\alpha)$:

- 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 <i>u_d</i>)	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)				

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

(T): TSPACE code,

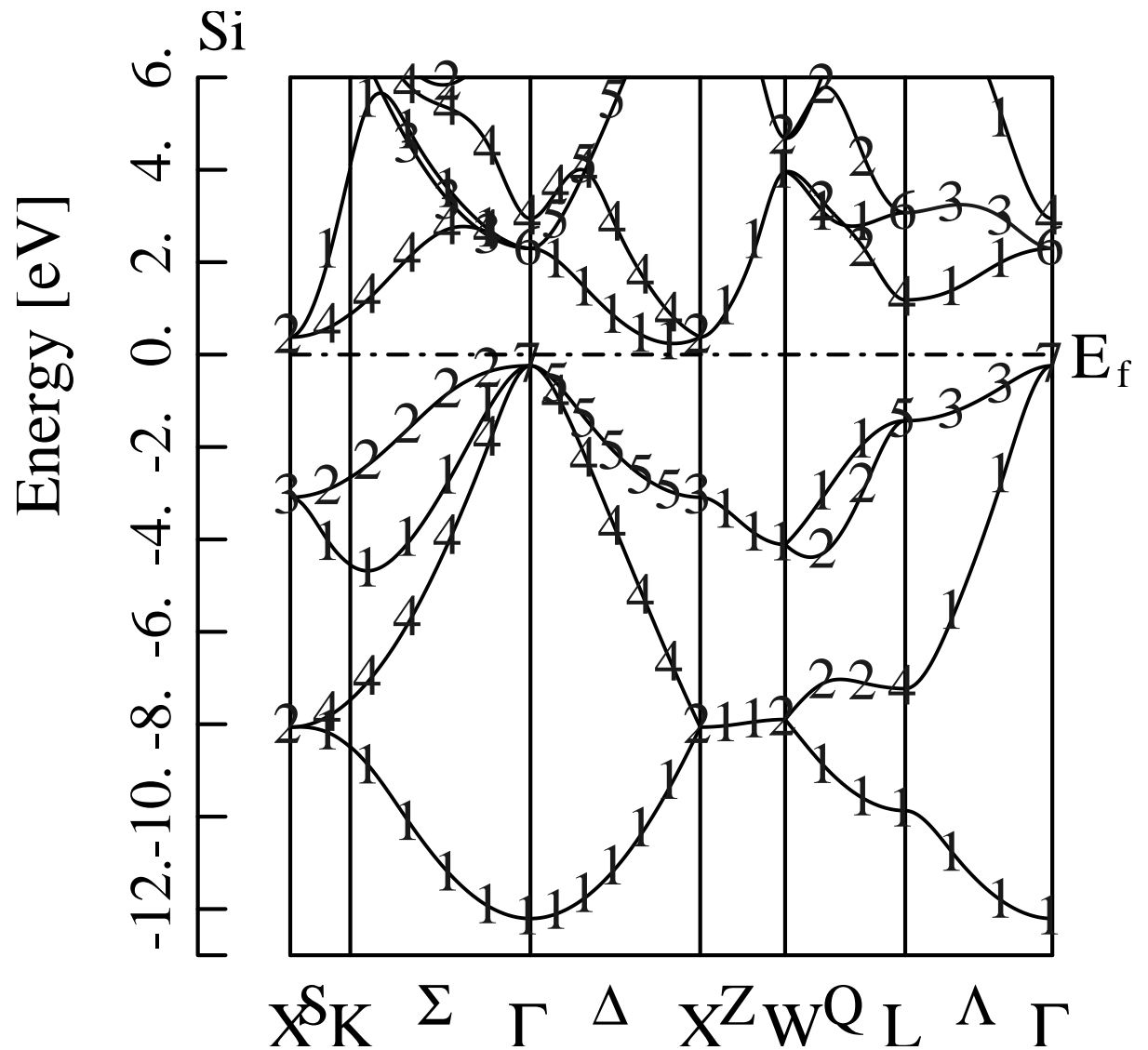
(B): BSW notation at the X point in diamond (nonsymmorphic)

Optical transition — Si —

Dipole allowed:

At the Γ point,

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



Optical transition — AIP —

Dipole allowed:

At the Γ point,

- $1 \leftrightarrow 4$

