618327-2560

PHYSICS OF ELECTRONIC MATERIALS AND DEVICES

Dr. Orrathai Watcharakitchakorn

Lecture 2

Quantum numbers

- As Pauli exclusion principle stating that no two electrons in an interacting system can have the same set of quantum numbers **n, *l*, m, s**. ควอนตัม Number

- Only two electrons can have the same three quantum numbers **n, *l*, m**, and those two must have opposite spin. These can be summarized as

ชั้น 1 อยู่ 2
ชั้น 2 อยู่ 8
ชั้น 3 อยู่ 18

การจัดเรียงตัว e : Ex! ^{14}S : 2 8 $\underline{\underline{4}}$

หมู่ที่ 4 เวเลนซ์อิเล็กตรอน คาบ 3

ชั้นใหญ่ ← $\mathbf{n} = 1, 2, 3, \ldots$

ชั้นย่อยของ n ← $\boldsymbol{l} = 0, 1, 2, \ldots, (\mathbf{n}-1)$

ชั้นย่อยของ n ← $\mathbf{m} = -\boldsymbol{l}, \ldots, -1, 0, 1, \ldots, +\boldsymbol{l}$

Spin ขึ้น-ลง ← $\mathbf{s} = \pm 1/2$

เป็นตามกฎเพาลี ควอนตัมจ.ไม่ซ้ำกันอาจมีทิศทางตรงข้ามได้

- The quantum states shown in the table are used to indicate the electronic configurations for atoms in the lowest energy state.

Quantum numbers

l　　สามารถใส่แต่ละชั้นได้ (ท)

n	*l*	m	s	Allowable states in subshell	Allowable states in complete shell
1	0	0	±1/2	2	2
	0	0	±1/2	2	s
		-1	±1/2		
2	1	0	±1/2	6	p 8
		1	±1/2		
	0	0	±1/2	2	
		-1	±1/2		
	1	0	±1/2	6	
		1	±1/2		
3		-2	±1/2		18
		-1	±1/2		
	2	0	±1/2	10	
		1	±1/2		
		2	±1/2		

Quantum numbers

Shell(**n**)	K 1	L 2		M 3			N 4			
Subshell (*l*)	0	0	1	0	1	2	0	1	2	3
	s	s	p	s	p	d	s	p	d	f
# of electrons	2	2	6	2	6	10	2	6	10	14
	2	8		18			32			

Quantum numbers

- There is a simple shorthand notation for electronic structures that is the naming of ***l*** values expressed as

$$\boldsymbol{l} = 0, 1, 2, 3, 4$$

$$s, p, d, f, g$$

n: 1, 2, 3

- These **s, p, d, f** stand for *sharp*, *principal*, *diffuse*, *and fundamental*.
- The rest will be written in alphabetical order beyond **f**.

Ex!. Si^{14} n:1 n:2 n:3

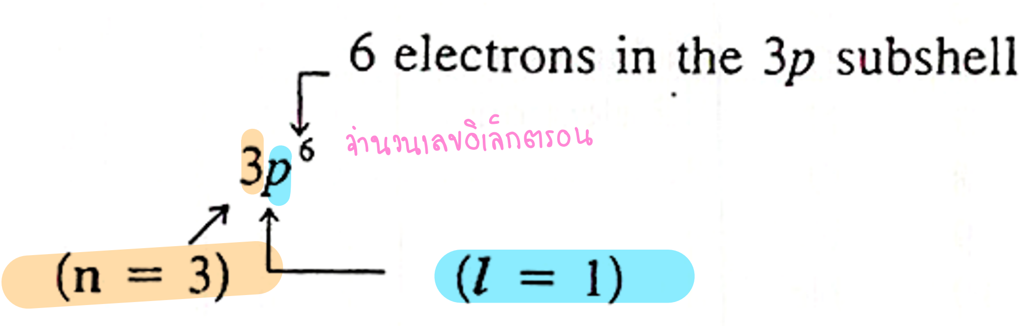
แบ่งเป็น 2

แบ่งเป็น 6

Si^{14} : 2 8 4

$1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^2$

Quantum numbers



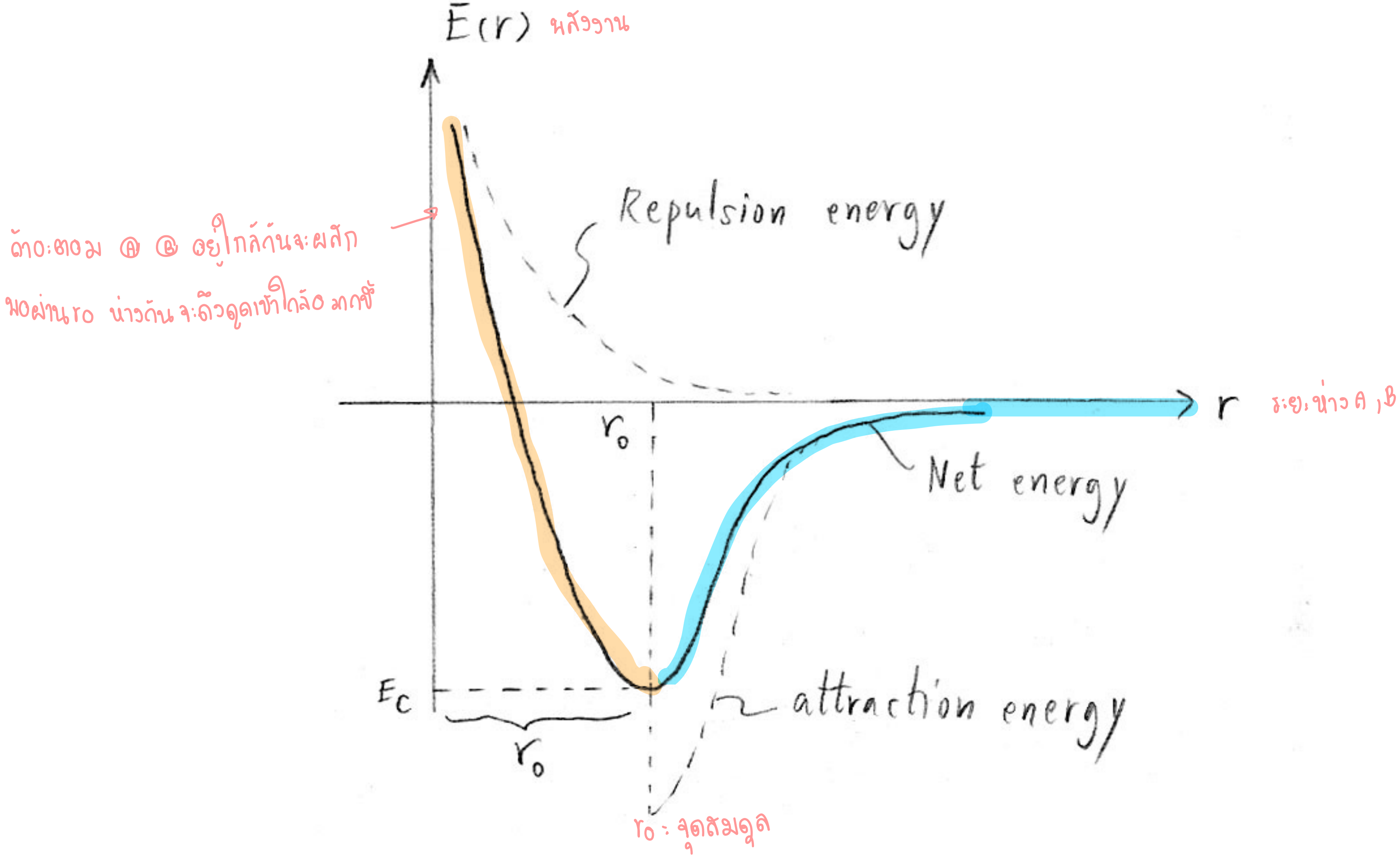
- For example, Si (atomic number = 14):

$$1s^2 2s^2 2p^6 3s^2 3p^2$$

Atomic number (Z)	Element	$n = 1$, $l = 0$	$n = 2$, $l = 0$	$n = 2$, $l = 1$	$n = 3$, $l = 0$	$n = 3$, $l = 1$	$n = 3$, $l = 2$	$n = 4$, $l = 0$	$n = 4$, $l = 1$	Shorthand notation
		$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	
		Number of electrons								
1	H	1								$1s^1$
2	He	2								$1s^2$
3	Li		1							$1s^2\ 2s^1$
4	Be		2							$1s^2\ 2s^2$
5	B		2	1						$1s^2\ 2s^2\ 2p^1$
6	C	helium core, 2 electrons	2	2						$1s^2\ 2s^2\ 2p^2$
7	N		2	3						$1s^2\ 2s^2\ 2p^3$
8	O		2	4						$1s^2\ 2s^2\ 2p^4$
9	F		2	5						$1s^2\ 2s^2\ 2p^5$
10	Ne		2	6						$1s^2\ 2s^2\ 2p^6$
11	Na				1					[Ne] $3s^1$
12	Mg				2					$3s^2$
13	Al				2	1				$3s^2\ 3p^1$
14	Si	neon core, 10 electrons			2	2				$3s^2\ 3p^2$
15	P				2	3				$3s^2\ 3p^3$
16	S				2	4				$3s^2\ 3p^4$
17	Cl				2	5				$3s^2\ 3p^5$
18	Ar				2	6				$3s^2\ 3p^6$
19	K							1		[Ar] $4s^1$
20	Ca							2		$4s^2$
21	Sc						1	2		$3d^1\ 4s^2$
22	Ti						2	2		$3d^2\ 4s^2$
23	V						3	2		$3d^3\ 4s^2$
24	Cr						5	1		$3d^5\ 4s^1$
25	Mn						5	2		$3d^5\ 4s^2$
26	Fe						6	2		$3d^6\ 4s^2$
27	Co	argon core, 18 electrons					7	2		$3d^7\ 4s^2$
28	Ni						8	2		$3d^8\ 4s^2$
29	Cu						10	1		$3d^{10}\ 4s^1$
30	Zn						10	2		$3d^{10}\ 4s^2$
31	Ga						10	2	1	$3d^{10}\ 4s^2\ 4p^1$
32	Ge						10	2	2	$3d^{10}\ 4s^2\ 4p^2$
33	As						10	2	3	$3d^{10}\ 4s^2\ 4p^3$
34	Se						10	2	4	$3d^{10}\ 4s^2\ 4p^4$
35	Br						10	2	5	$3d^{10}\ 4s^2\ 4p^5$
36	Kr						10	2	6	$3d^{10}\ 4s^2\ 4p^6$

Bonds

แรงยึดเหนี่ยวระหว่างอะตอม <พันธะ>



Bonds

พลังงานดูด

$$E(r) = -\frac{a}{r^m} + \frac{b}{r^n}$$

พลังงานผลัก

where r = interatomic distance
a = attraction constant
b = repulsion constant
m,n = constant of characteristic of each type of bond or structure

- Therefore, $-\frac{a}{r^m}$ and $\frac{b}{r^n}$ are attraction and repulsion energy, respectively.

Bonds

อธิบายกราฟด้านบน

We may conclude that

- $E \rightarrow 0$ at $r \rightarrow \infty$: Zero energy as the energy in the absence of interaction.

- At $r > r_o$, atoms attract each other from $r \rightarrow \infty$ to $r \rightarrow r_o$.

- At $r < r_o$, atoms repel each other up to the point r_o.

- At r_o, equilibrium position occurs. It is where the attraction energy and repulsion energy balance each other.

Types of bonds

- Bonds may be classified into **4** types as ชนิดพันธะแบ่ง 2 ประเภทใหญ่ๆ

1. ionic bond: non-directional

primary bond

2. metallic bond: non-directional

3. covalent bond: directional

4. van der Waals bond: very weak → secandary bond

Ionic bond คล้าย Metallic Bond

- This happens from electrostatic attraction between ions with different charges such as NaCl or LiF. The cohesive energy, Ec, the energy needed to take the crystal apart, may be written as

ประจุ e = 1.6×10^{-19} คูลอมบ์

$$E_c = -\frac{Mq^2}{4\pi\varepsilon_0 r} + \frac{b}{r^n}$$

ค่าคงที่

where M = Madelung constant

$-\dfrac{q^2}{4\pi\varepsilon_0 r}$ = Coulomb electrostatic attraction energy between 2 ions.

Metallic bond

อยู่ในโลหะเป็นส่วนใหญ่

ใช้พลังเยอะในการทำให้แตกแยก

- Metallic bond is similar to the ionic bond as electrostatic forces play big part on it, but this electrostatic forces are everywhere and come from all directions.

- In metals, the negative charges are highly mobile, electrons act like a glue to hold the lattice together.

- The cohesive forces in metals are very strong and hard to break.

Covalent bond

พันธะที่แชร์ e วงนอกสุดด้วยกัน

(ต้องครบ 8 ตัวถึงเสถียร)

- This bond happens from the sharing of electrons between two atoms.
- The simplest example of covalent bond is shown by hydrogen atom.
- Hydrogen atom needs another electron to fill its 1*s* shell.
- It would find that extra electron from another hydrogen atom as they both finally share their electrons.

Covalent bond

- In covalent bond, all electrons pair up and orbit around a pair of atoms, so more of them can wander away to conduct electricity.

- In case of carbon, it acts like an insulator, but this bond in silicon or germanium is weaker.

- Some of electrons in the latter case might be shaken off and able to conduct electricity, so we call them "semiconductors".

Covalent bond

จะเกิดนสววานก์ต่อเมื่อเกิดการกระตุ้นให้นำไฟฟ้า

└→ อุณหภูมิ, สนามไฟฟ้า, สนามแม่เหล็ก, การเจือปน

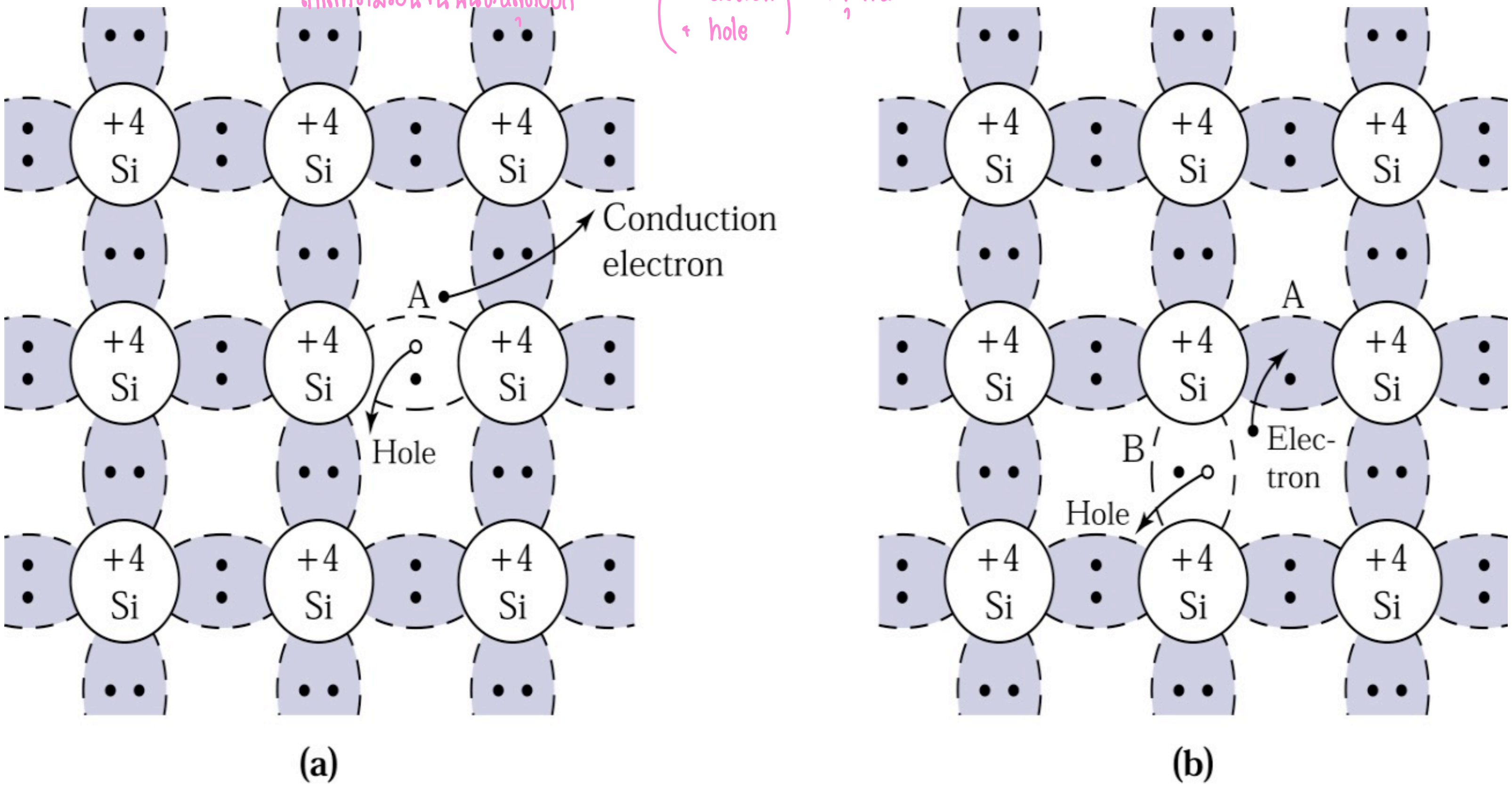
ถ้าใส่ความร้อนจนพันธะหลุดออก

↗ ทำให้ธาตุไม่บริสุทธิ์

↳ เกิดคุณสมบัติเปลี่ยนไป

(- eletron
+ hole) = ประจุพาหะ

↗ ถ้าประจุพาหะเคลื่อนที่จะเกิดกระแสไฟฟ้า



- (*a*) A broken bond at Position A, resulting in a conduction electron and a hole.
- (*b*) A broken bond at position B.

The van der Waals bond มันจะอ่อนสุด

- This is like a *secondary* bond since its force is very weak.
- This bond can be seen in atoms that their outer shell is fully filled.
- Consider atom A has a dipole moment then it will induce an opposite dipole moment on atom B.
- This attraction force is called "van der Waals bond".

Example 1

- The potential energy E per Na^+ Cl^- pair within the NaCl crystal depends on the inter-ionic separation r as

1.6×10^{-19} คูลอมบ์

$\varepsilon_0 : 8.85 \times 10^{-12}\ Fm^{-1}$

$$E(r) = -\frac{e^2 M}{4\pi\varepsilon_o r} + \frac{B}{r^n}$$

where n = 8, M = 1.7476, B = 6.972×10^{-96} $J.m^8$.

- (a) Find the equilibrium separation (r_o) of the ions in the crystal. หา r_0 0.28
- การบ้าน → (b) Find the ionic bonding energy, defined as $-E(r_o)$.

1) $E(r) = \frac{-e^2 M}{4\pi\varepsilon_0 r} + \frac{B}{r^n}$

$$\frac{dE(r)}{dr} = \frac{d}{dr}\left[\frac{-e^2 M}{4\pi\varepsilon_0 r} + \frac{B}{r^n}\right]$$

$$0 = -\frac{d}{dr}\frac{e^2 M}{4\pi\varepsilon_0 r} + \frac{d}{dr}\frac{B}{r^n}$$

$$0 = \frac{-e^2 M}{4\pi\varepsilon_0}\frac{d}{dr}\frac{1}{r} + B\frac{d}{dr}\frac{1}{r^n}$$

$$0 = \frac{-e^2 M}{4\pi\varepsilon_0}\frac{d}{dr} r^{-1} + B\frac{d}{dr} r^{-n}$$

$$0 = \frac{-e^2 M}{4\pi\varepsilon_0}(-1) r^{-1-1} + B(-n) r^{-n-1}$$

$$0 = \frac{e^2 M}{4\pi\varepsilon_0} r^{-2} - Bn r^{-n-1}$$

$$0 = \frac{e^2 M}{4\pi\varepsilon_0 r^2} - Bn r^{-(n+1)}$$

$$0 = \frac{e^2 M}{4\pi\varepsilon_0 r^2} - \frac{Bn}{r^{n+1}}$$

แทน $r = r_0$

$$\frac{Bn}{r_0^{n+1}} = \frac{e^2 M}{4\pi\varepsilon_0 r_0^2}$$

$$\frac{r_0^2}{r_0^n \cdot r_0} = \frac{e^2 M}{4\pi\varepsilon_0 B n}$$

$$\frac{r_0}{r_0^n} = \frac{e^2 M}{4\pi\varepsilon_0 B n}$$

$$r_0^{1-n} = \frac{e^2 M}{4\pi\varepsilon_0 B n}$$

ยกกำลัง $\frac{1}{1-n}$

$$\left(r_0^{1-n}\right)^{\frac{1}{1-n}} = \left(\frac{e^2 M}{4\pi\varepsilon_0 B n}\right)^{\frac{1}{1-n}}$$

$$r_0^{\cancel{\frac{1-n}{1-n}}} = \left(\frac{e^2 M}{4\pi\varepsilon_0 B n}\right)^{\frac{1}{1-n}}$$

$$\frac{-1}{1-n} = \frac{\cancel{-}1}{\cancel{-}(n-1)} = \frac{1}{n-1}$$

กลับเศษเป็นส่วน

$$r_0 = \left(\frac{4\pi\varepsilon_0 B n}{e^2 M}\right)^{\frac{1}{n-1}} \quad \#$$