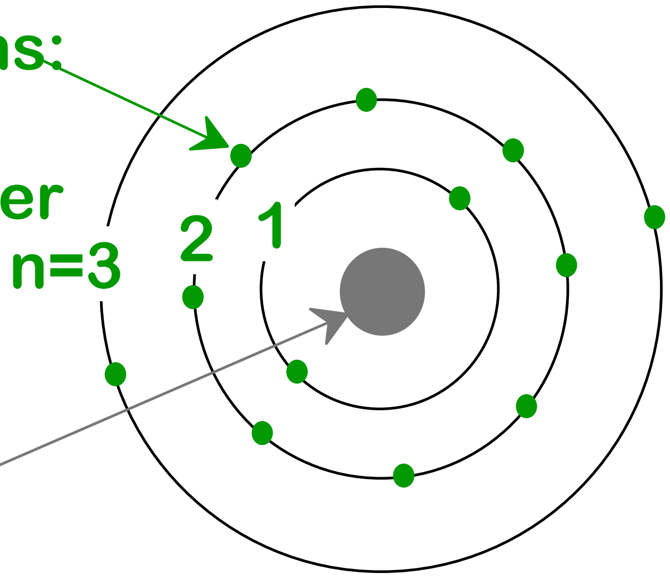
CHAPTER 2:
Atomic Structure and Interatomic Bonding

ISSUES TO ADDRESS...

- Atomic structure (2.1~2.4)
- What types of bonds are there?
- What properties are inferred from bonding?

Bohr Atom

orbital electrons:
n = principal
quantum number



Adapted from Fig. 2.1, *Callister 6e.*

Nucleus: Z = # protons

= 1 for hydrogen to 94 for plutonium

N = # neutrons

Atomic mass A ≈ Z + N

Atomic mass unit (amu)

$M_{proton} \approx M_{neutron} = 1.66 \times 10^{-24}$ g = 1 amu

Atomic Structure (Freshman Chem.)

- atom – electrons – 9.11×10^{-31} kg

  protons
  neutrons } 1.67×10^{-27} kg

- atomic number (Z) = # of protons in nucleus of atom
  = # of electrons of neutral species

- A [=] atomic mass unit = amu = 1/12 mass of ^{12}C

Atomic wt = wt of 6.023×10^{23} molecules or atoms

1 amu/atom = 1g/mol

C 12.011
H 1.008 etc.

Electronic Structure

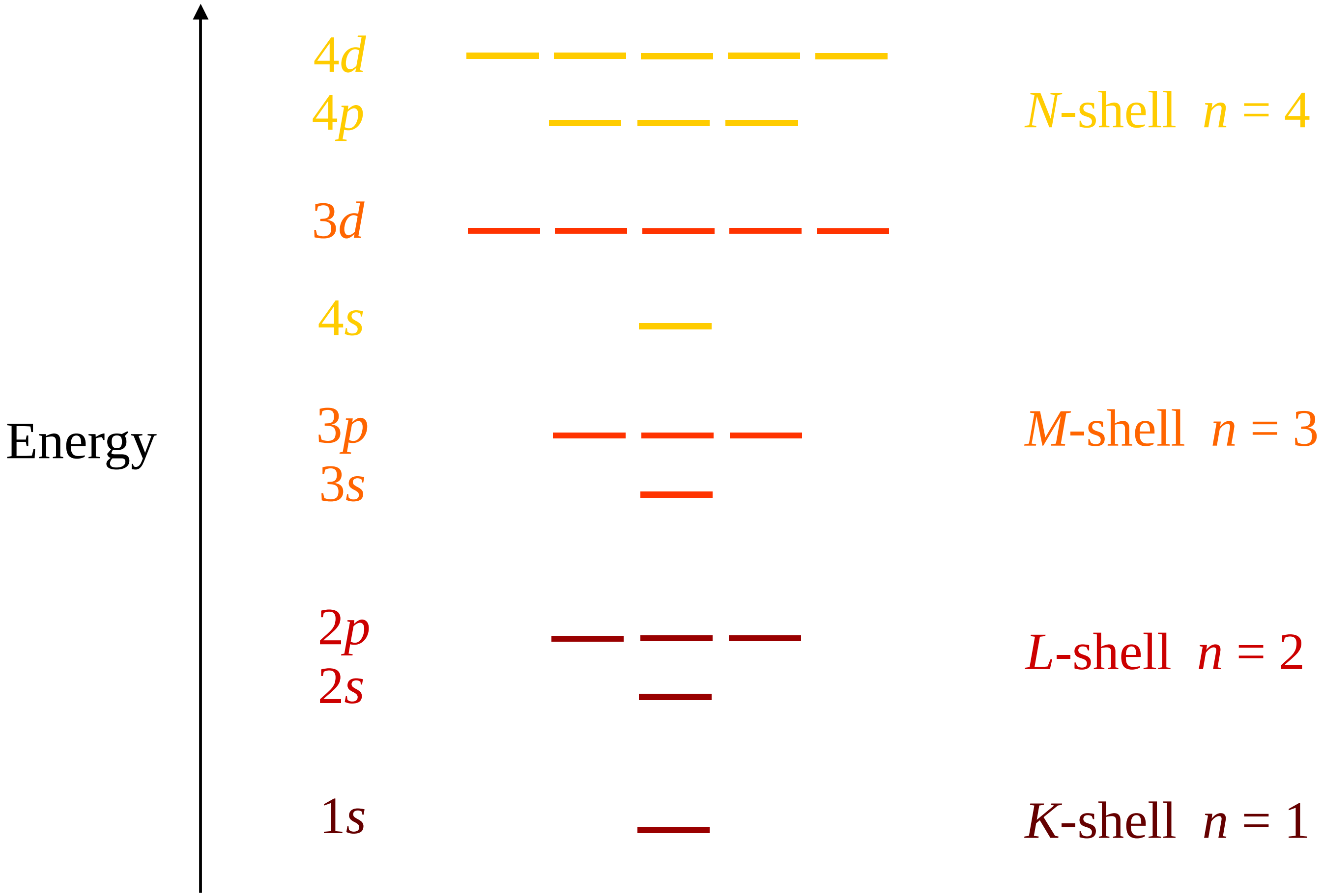
- Electrons have wavelike and particulate properties.
  - This means that electrons are in orbitals defined by a probability.
  - Each orbital at discrete energy level determined by quantum numbers.

Quantum #	Designation
n = principal (energy level-shell)	K, L, M, N, O (1, 2, 3, etc.)
l = subsidiary (orbitals)	s, p, d, f (0, 1, 2, 3,…, n-1)
m_l = magnetic	1, 3, 5, 7 (-l to +l)
m_s = spin	½, -½

Electron Energy States

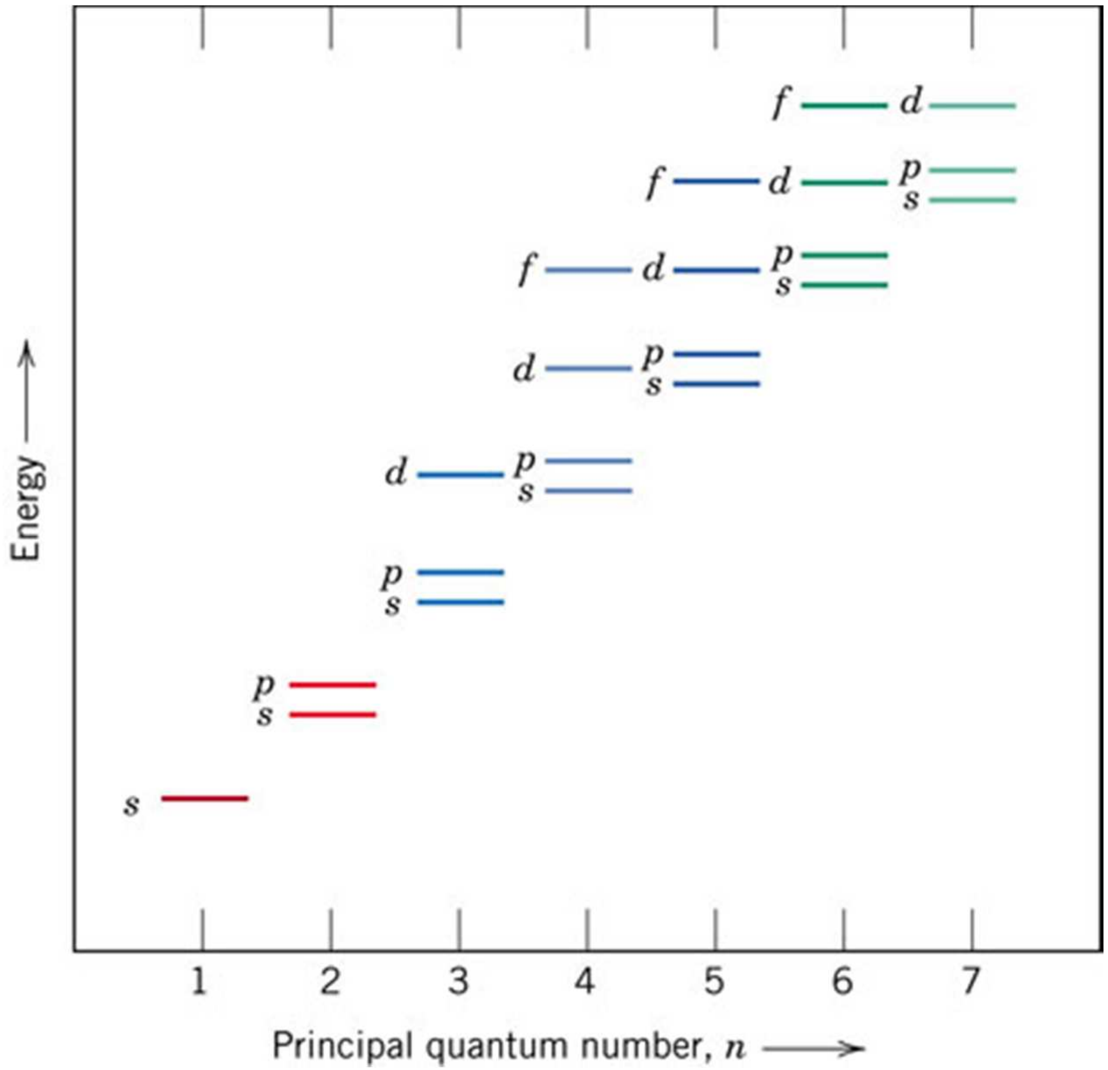
Electrons...

- have discrete energy states
- tend to occupy lowest available energy state.



Adapted from Fig. 2.4, *Callister 7e.*

Order of Filling Sublevels with Electrons



http://www.fordhamprep.org/gcurran/sho/sho/lessons/lesson36.htm

Element	*Symbol*	*Atomic Number*	*Electron Configuration*
Hydrogen	H	1	$1s^1$
Helium	He	2	$1s^2$
Lithium	Li	3	$1s^2 2s^1$
Beryllium	Be	4	$1s^2 2s^2$
Boron	B	5	$1s^2 2s^2 2p^1$
Carbon	C	6	$1s^2 2s^2 2p^2$
Nitrogen	N	7	$1s^2 2s^2 2p^3$
Oxygen	O	8	$1s^2 2s^2 2p^4$
Fluorine	F	9	$1s^2 2s^2 2p^5$
Neon	Ne	10	$1s^2 2s^2 2p^6$
Sodium	Na	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	Mg	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	Al	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
Silicon	Si	14	$1s^2 2s^2 2p^6 3s^2 3p^2$
Phosphorus	P	15	$1s^2 2s^2 2p^6 3s^2 3p^3$
Sulfur	S	16	$1s^2 2s^2 2p^6 3s^2 3p^4$
Chlorine	Cl	17	$1s^2 2s^2 2p^6 3s^2 3p^5$
Argon	Ar	18	$1s^2 2s^2 2p^6 3s^2 3p^6$
Potassium	K	19	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
Calcium	Ca	20	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
Scandium	Sc	21	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$
Titanium	Ti	22	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$
Vanadium	V	23	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$
Chromium	Cr	24	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$
Manganese	Mn	25	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^2$
Iron	Fe	26	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$
Cobalt	Co	27	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$
Nickel	Ni	28	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$
Copper	Cu	29	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$
Zinc	Zn	30	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$
Gallium	Ga	31	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$
Germanium	Ge	32	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$
Arsenic	As	33	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$
Selenium	Se	34	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^4$
Bromine	Br	35	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$
Krypton	Kr	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

[a] When some elements covalently bond, they form *sp* hybrid bonds. This is especially true for C, Si, and Ge.

t02_02_pg22

Stable Electron Configurations

Stable electron configurations...

- have complete s and p subshells
- tend to be unreactive.

Z	Element	Configuration
2	He	$1s^2$
10	Ne	$1s^2 2s^2 2p^6$
18	Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$
36	Kr	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

Adapted from Table 2.2, *Callister 6e.*

$\boxed{s^2\ p^6}$ Completely filled (8 electrons)

valence electrons

SURVEY OF ELEMENTS

- Most elements: Electron configuration not stable.

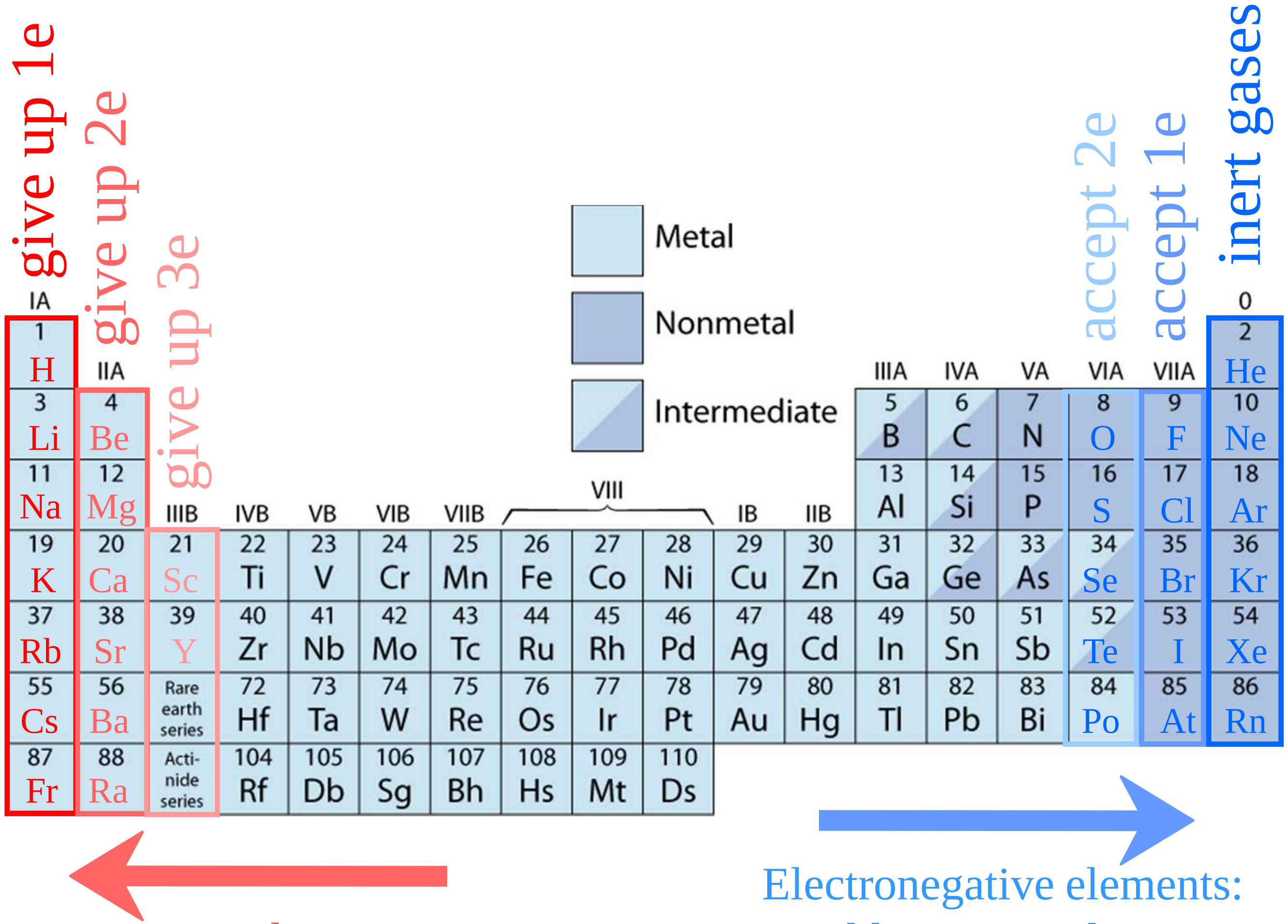
Element	Atomic #	Electron configuration	
Hydrogen	1	$1s^1$	
Helium	2	$1s^2$	(stable)
Lithium	3	$1s^2 2s^1$	
Beryllium	4	$1s^2 2s^2$	
Boron	5	$1s^2 2s^2 2p^1$	
Carbon	6	$1s^2 2s^2 2p^2$	
...		...	
Neon	10	$1s^2 2s^2 2p^6$	(stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$	
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$	
Aluminum	13	$1s^2 2s^2 2p^6 3s^2 3p^1$	
...		...	
Argon	18	$1s^2 2s^2 2p^6 3s^2 3p^6$	(stable)
...	...	...	
Krypton	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$	(stable)

Chloride	17	$1s^2 2s^2 2p^6 3s^2 3p^5$
Sulfur	16	$1s^2 2s^2 2p^6 3s^2 3p^4$

Adapted from Table 2.2, *Callister 7e.*

The Periodic Table

- Columns: Similar Valence Structure



Adapted from Fig. 2.6, *Callister 7e.*

Electropositive elements: Readily give up electrons to become + ions.

Electronegative elements: Readily acquire electrons to become - ions.

Electronegativity

- Ranges from 0.7 to 4.0,
- Large values: tendency to acquire electrons.

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe –
Cs 0.7	Ba 0.9	La–Lu 1.1–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn –
Fr 0.7	Ra 0.9	Ac–No 1.1–1.7															

Smaller electronegativity

Larger electronegativity

Adapted from Fig. 2.7, *Callister 7e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

2.5 Bonding Forces and Energies

- **Ionic**: Strong Coulomb interaction among negative atoms (have an extra electron each) and positive atoms (lost an electron).

  Example - Na^+Cl^-

- **Covalent**: Electrons are shared between the molecules, to saturate the valency.

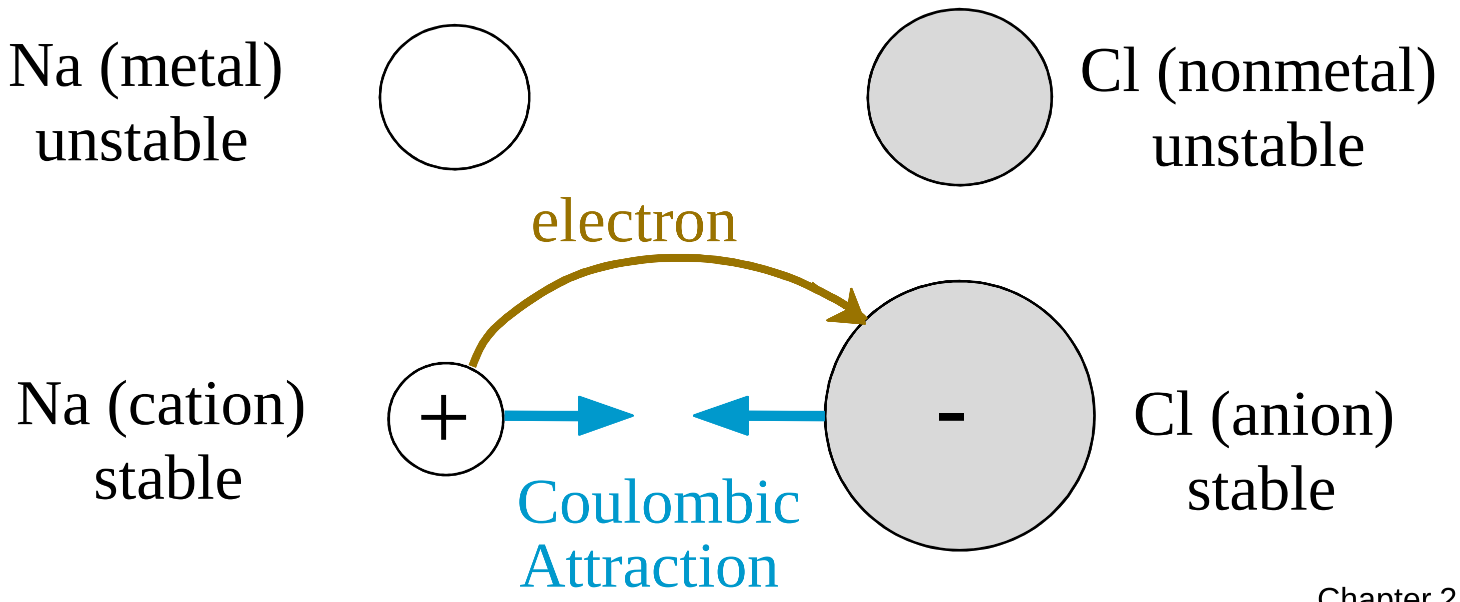
  Example - H_2

- **Metallic**: The atoms are ionized, loosing some electrons from the valence band. Those electrons form a electron sea, which binds the charged nuclei in place.

Ionic Bonding

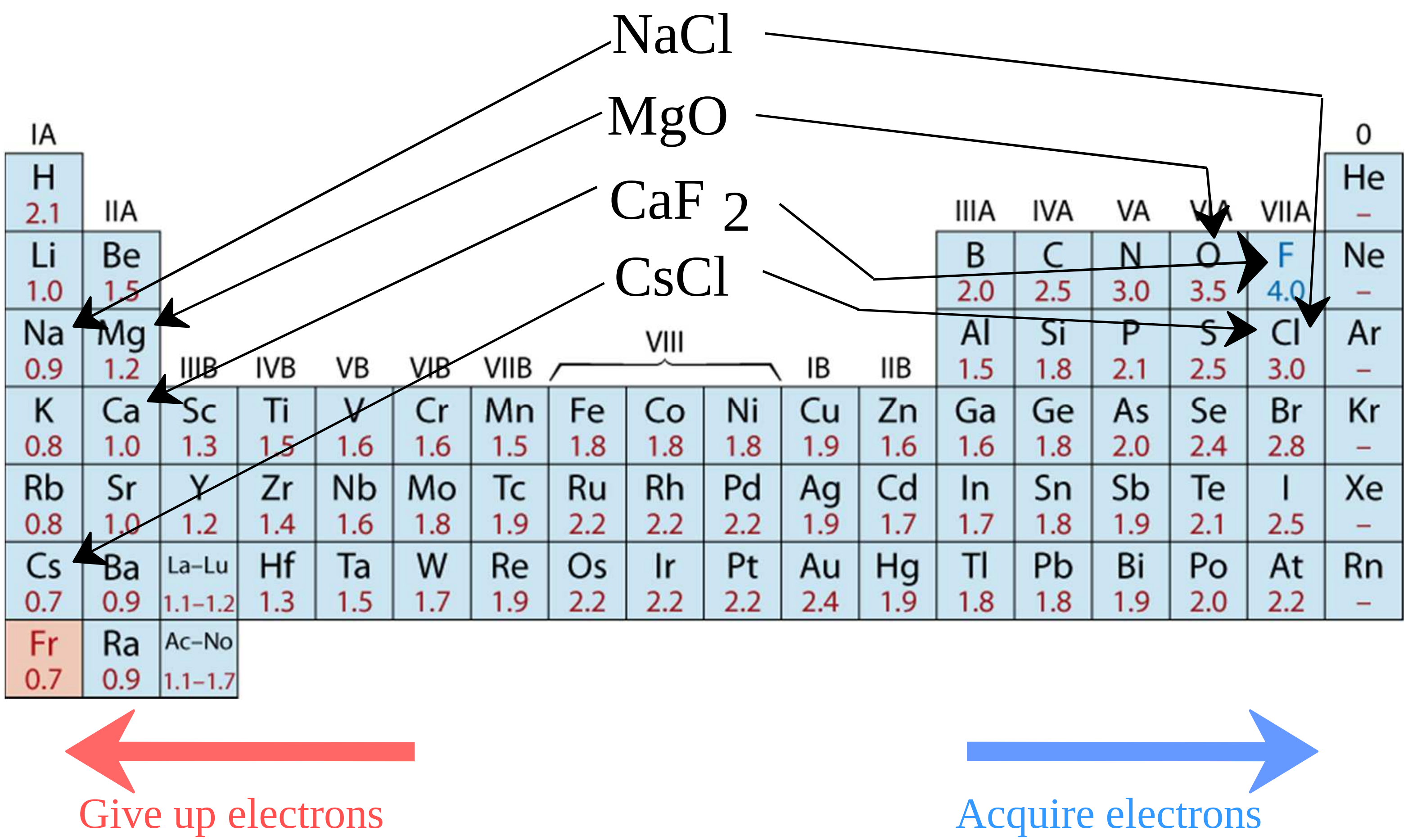
(Ionic bond – metal + nonmetal)

- Large difference in electronegativity required.
- Requires electron transfer.
- Occurs between + and - ions.
- Example: NaCl



Examples: Ionic Bonding

- Predominant bonding in Ceramics

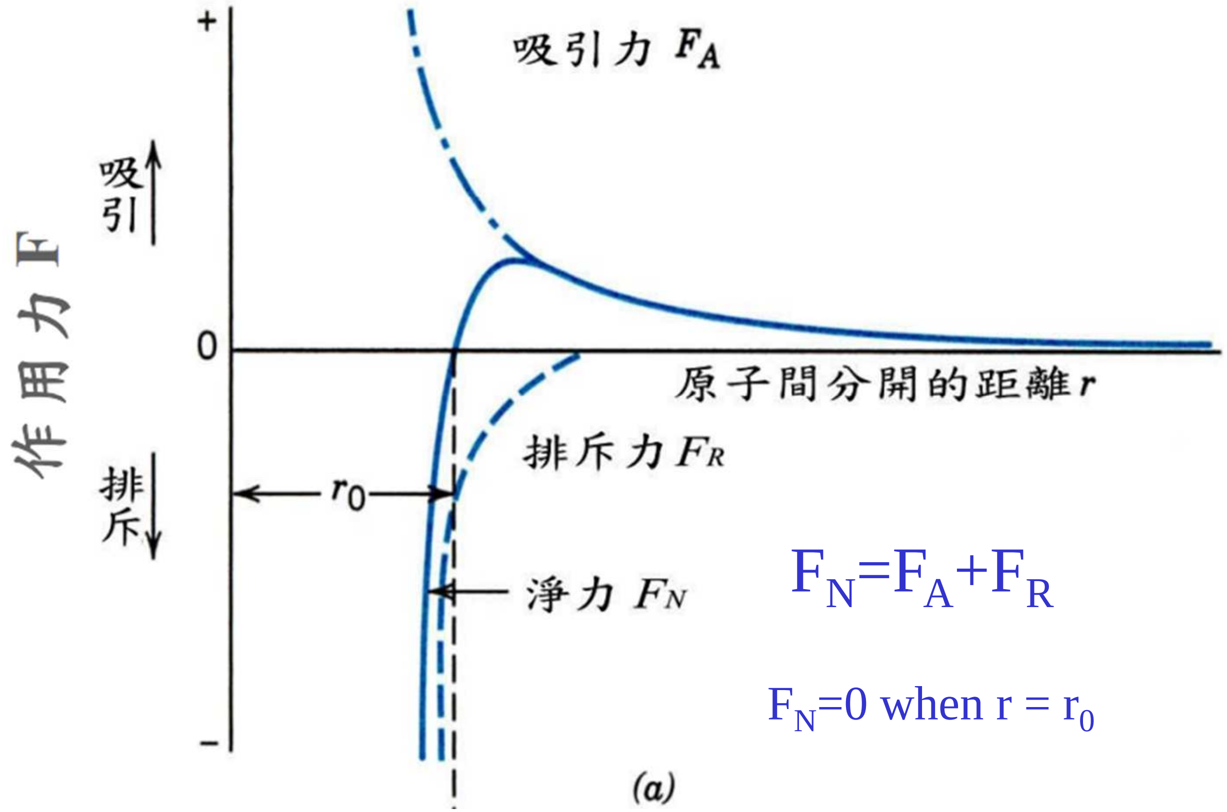


Adapted from Fig. 2.7, *Callister 7e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

Ionic Bonding

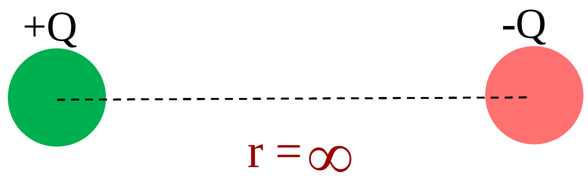
- Bonding Force

-- Attractive, Repulsive and Net force

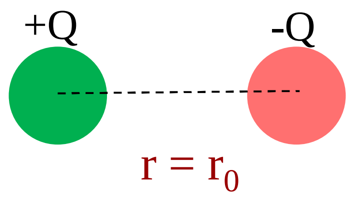


$F_N=F_A+F_R$

$F_N=0$ when $r = r_0$



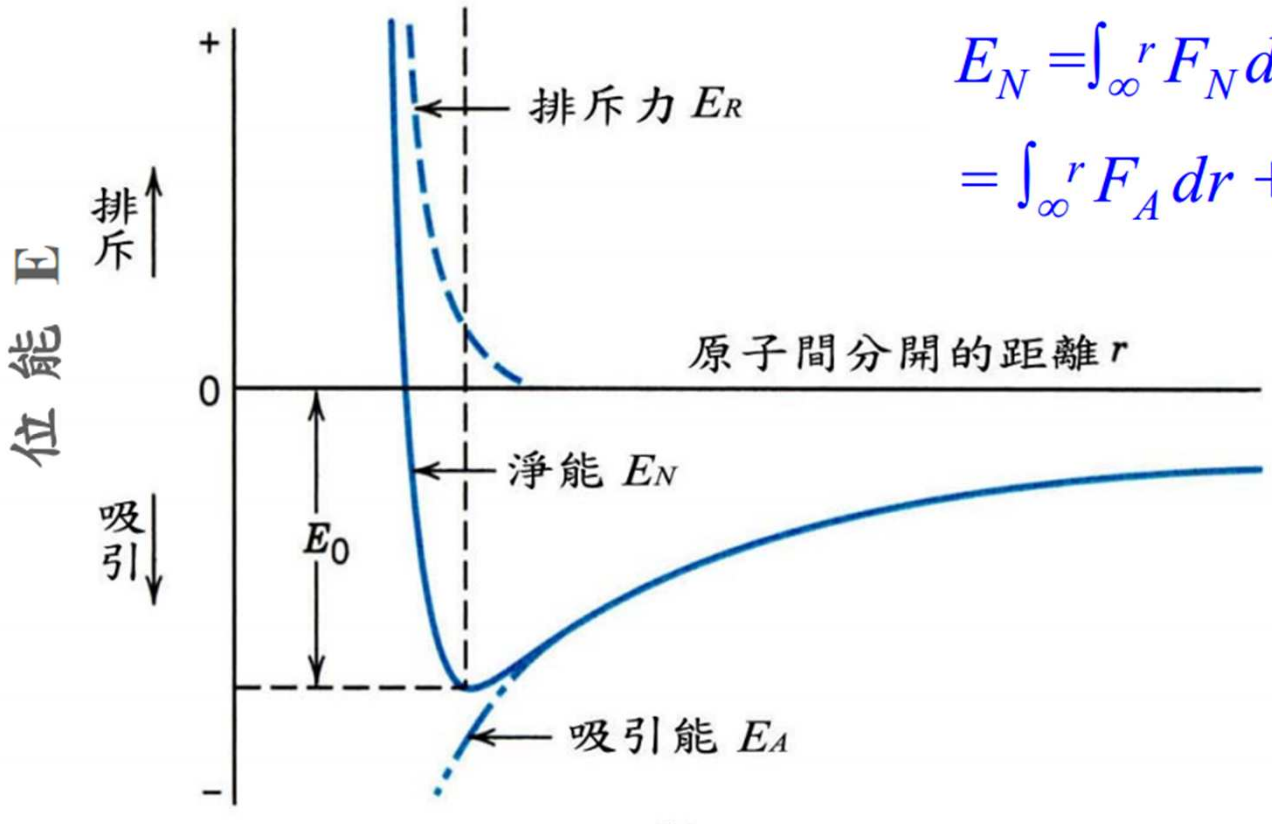
F_A & F_R 可忽略



http://blog.ncut.edu.tw/userfile/2819/CH02.pdf

Ionic Bonding

- Energy – minimum energy most stable
  - Energy balance of attractive and repulsive terms



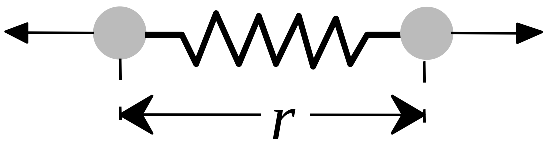
(b)

$$E_N = \int_\infty^r F_N dr$$
$$= \int_\infty^r F_A dr + \int_\infty^r F_R dr = E_A + E_R$$

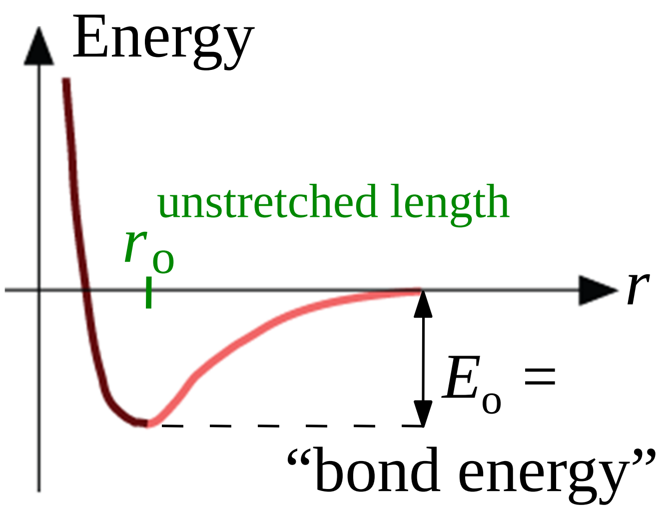
http://blog.ncut.edu.tw/userfile/2819/CH02.pdf

Properties From Bonding: T_m

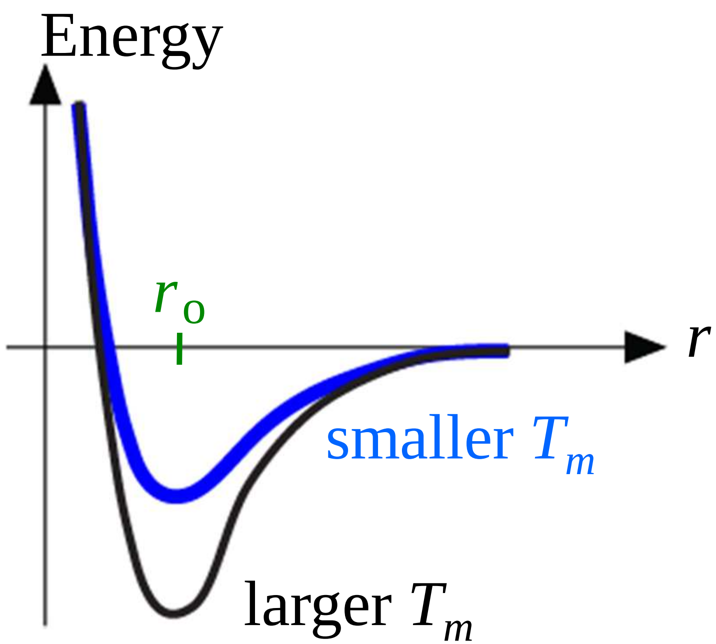
- Bond length, r



- Bond energy, E_o



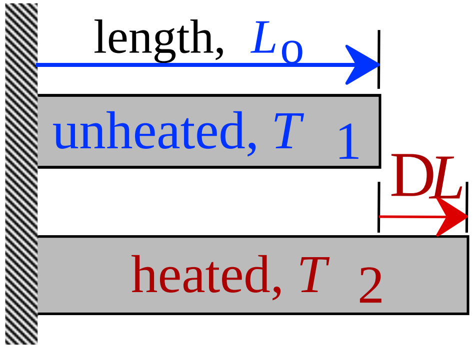
- Melting Temperature, T_m



T_m is larger if E_o is larger.

Properties From Bonding : α

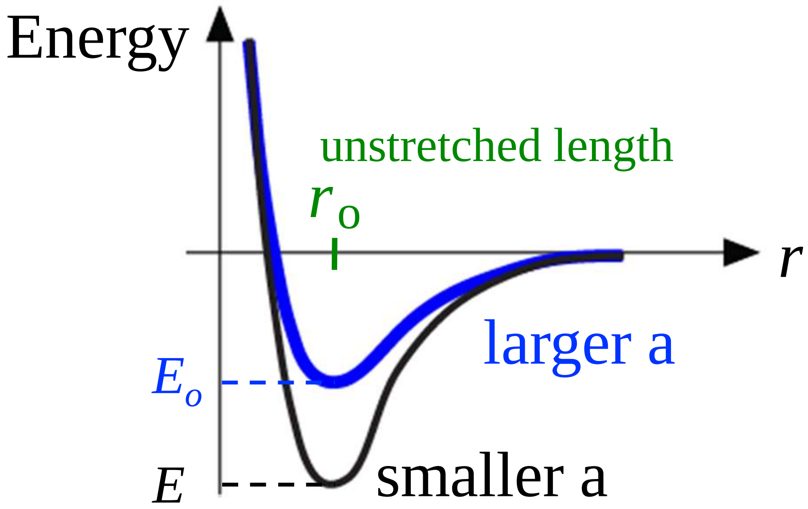
- Coefficient of thermal expansion, a



coeff. thermal expansion

$$\frac{DL}{L_o} = a\,(T_2 - T_1)$$

- a ~ symmetry at r_o



a is larger if E_o is smaller.

Covalent Bonding

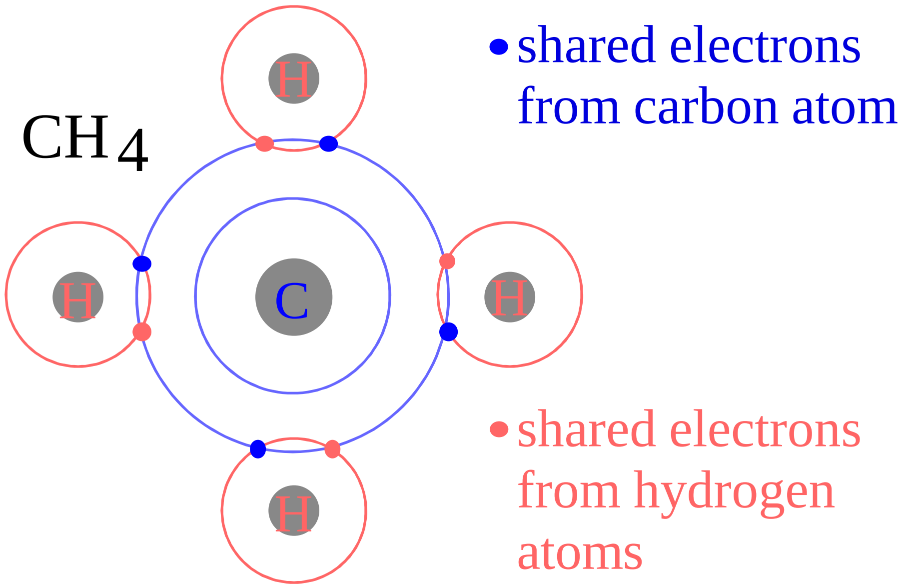
- Sharing of electrons between adjacent atoms.
- Two atoms that are covalently bonded will each contribute at least one electron to the bond
- The shared electrons may be considered to belong to both atoms

- Example: CH_4

C: has 4 valence e^-,
needs 4 more

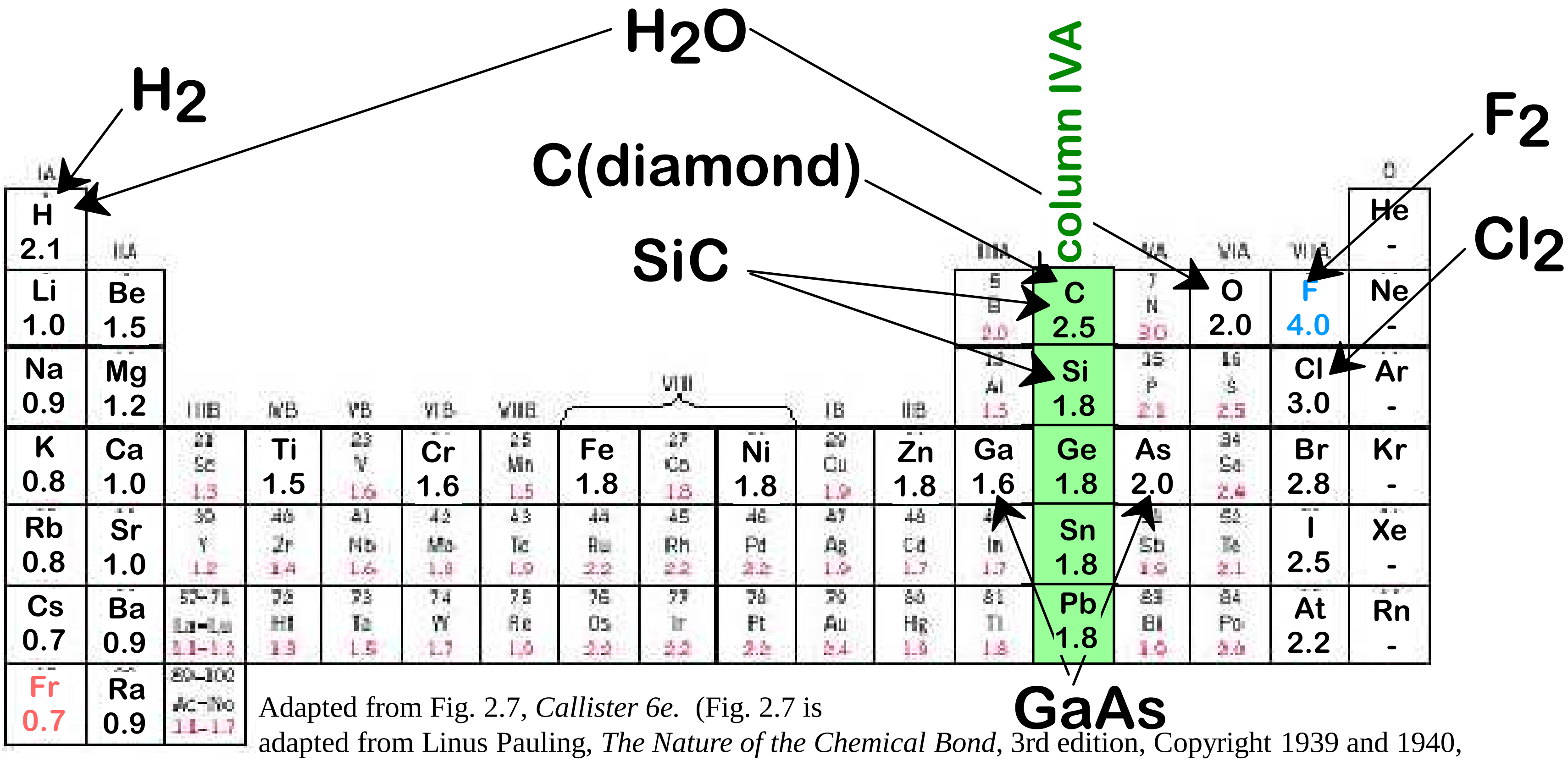
H: has 1 valence e^-,
needs 1 more

Electronegativities
are comparable.

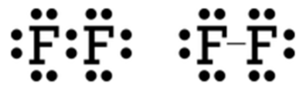


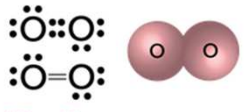
Adapted from Fig. 2.10, *Callister 7e.*

EXAMPLES: COVALENT BONDING



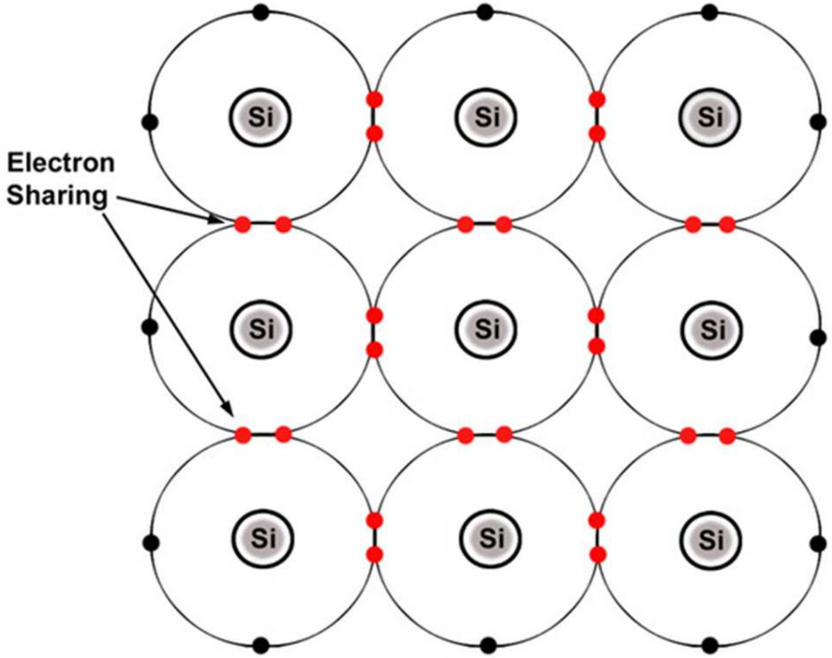
Adapted from Fig. 2.7, *Callister 6e*. (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

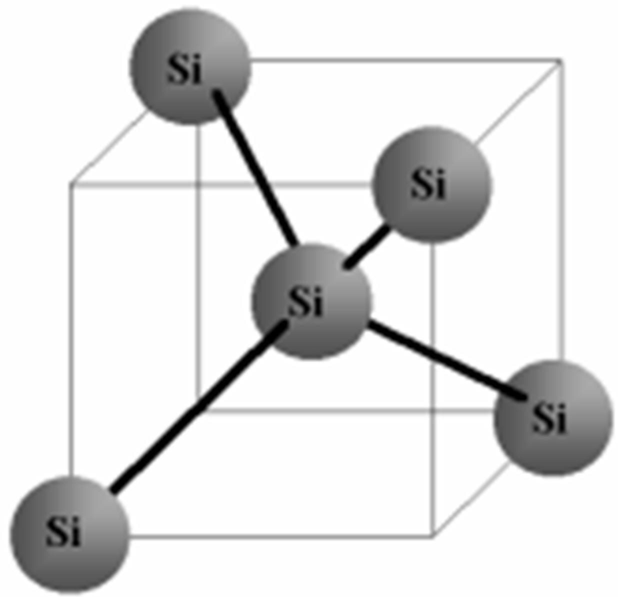




- Molecules with nonmetals (e.g., F_2, O_2)
- Molecules with nonmetals (e.g., H_2O, CH_4)
- Elemental solids (e.g., Ge, Si)
- Compound solids (about column IVA, e.g., GaAs)

Covalent Bonding ：Silicon



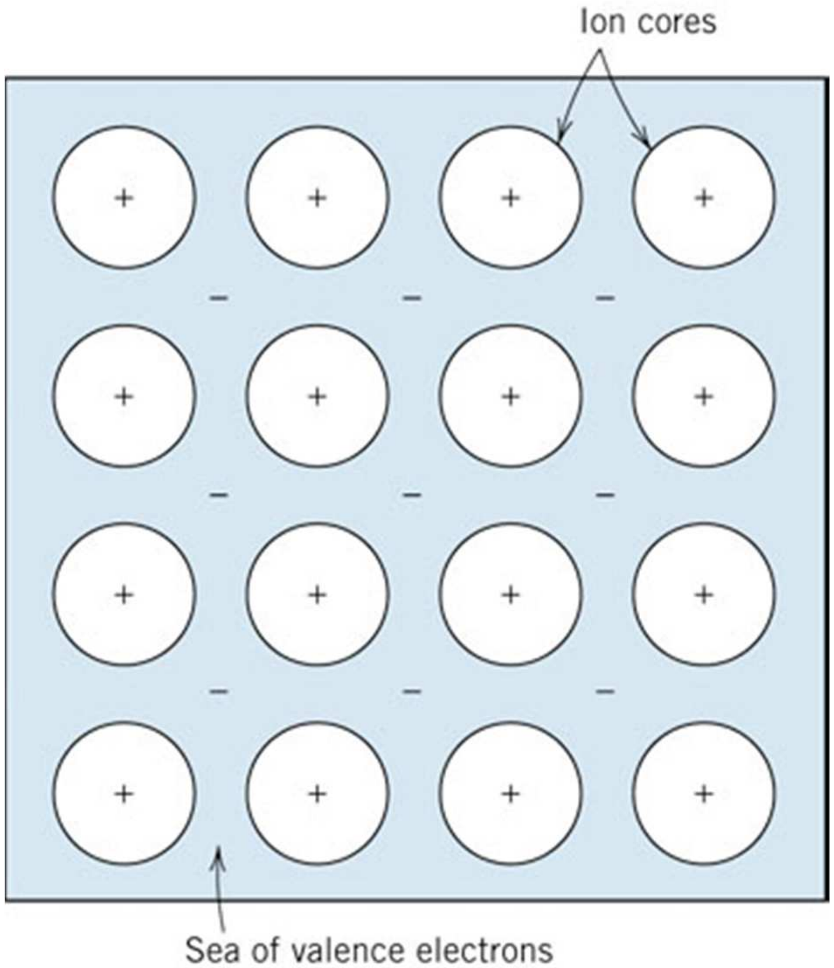


The covalent bond is directional !

http://solarwiki.ucdavis.edu/The_Science_of_Solar/Solar_Basics/A._Introductory_Physics_for_Solar_Application/I._Atoms_and_Materials/4._Covalent_Bonds

http://www.austincc.edu/HongXiao/overview/basic-semi/sld007.htm

Metallic Bonding



- These valence electrons are not bound to any particular atoms.
- More or less free to drift throughout the entire metal.
- Sea of electrons or an electron cloud.
- Remaining nonvalence electrons and atomic nuclei → ion cores.
- Nondirectional
- Group IA and IIA

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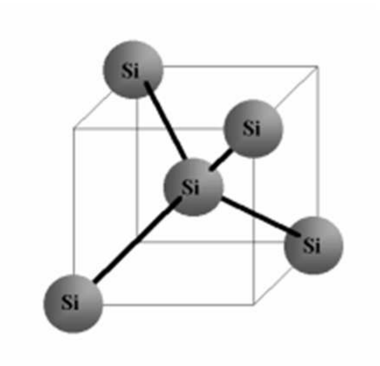
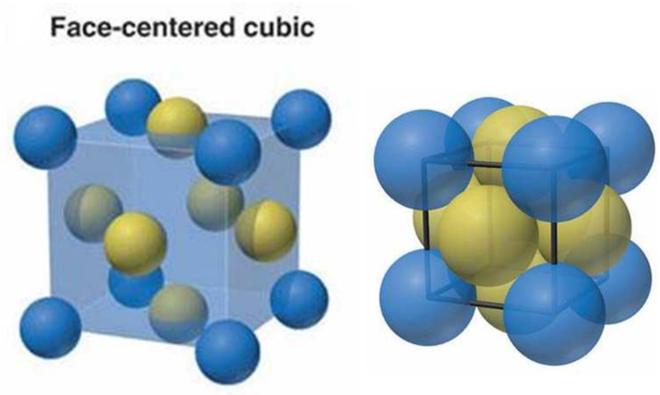
Concept Check 2.3

Q：Why covalently bonded materials are generally less dense than ionically or metallically bonded ones ?

Answer: Covalently bonded materials are less dense than metallic or ionically bonded ones because covalent bonds are directional in nature whereas metallic and ionic are not; when bonds are directional, the atoms cannot pack together in as dense a manner, yielding a lower mass density.



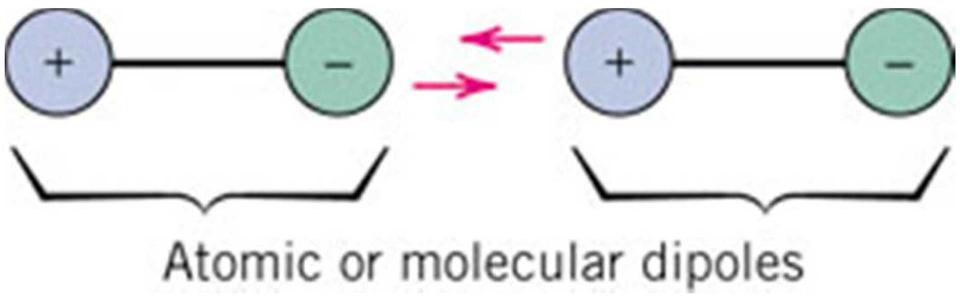


Au, Cu, Al…

http://www.learneasy.info/MDME/focus/materials/enmat/LECTURES/Lecture-04/webpages/crystals.html

Secondary Bonding

- Secondary = van der Waals
- Physical bonds (primary bounds →chemical)
- Weak (10 KJ/mol)
- No e- transferred or shared Interaction of atomic/molecular dipoles
- Inert gases
- Arise from atomic or molecular dipoles



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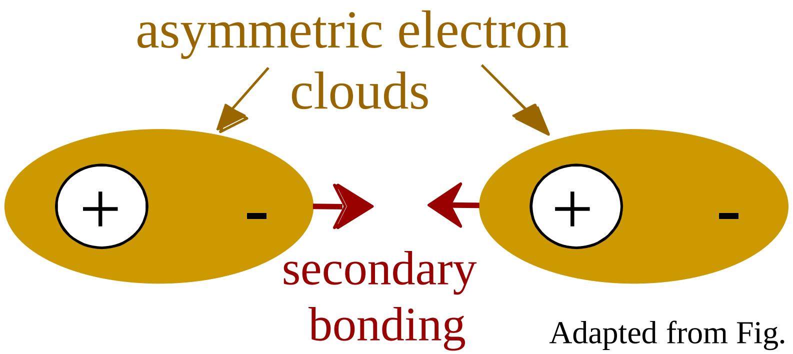
SECONDARY BONDING

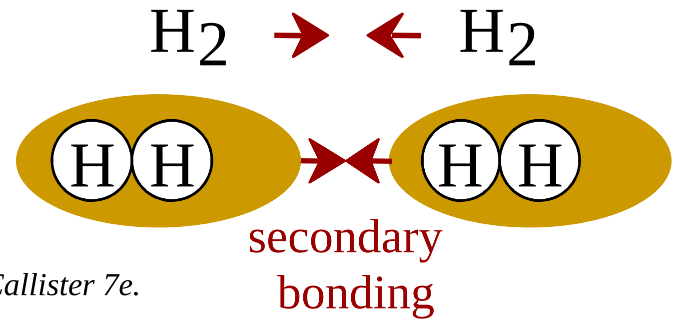
Arises from interaction between **dipoles**

- Fluctuating dipoles



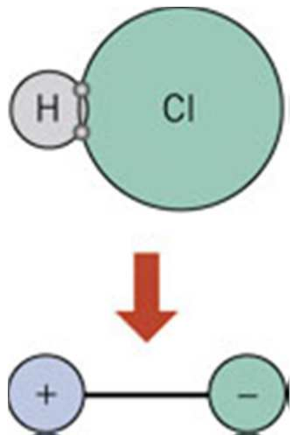
Adapted from Fig. 2.13, *Callister 7e.*

ex: liquid H_2



- Polar molecule-induced dipoles

-ex: liquid HCl



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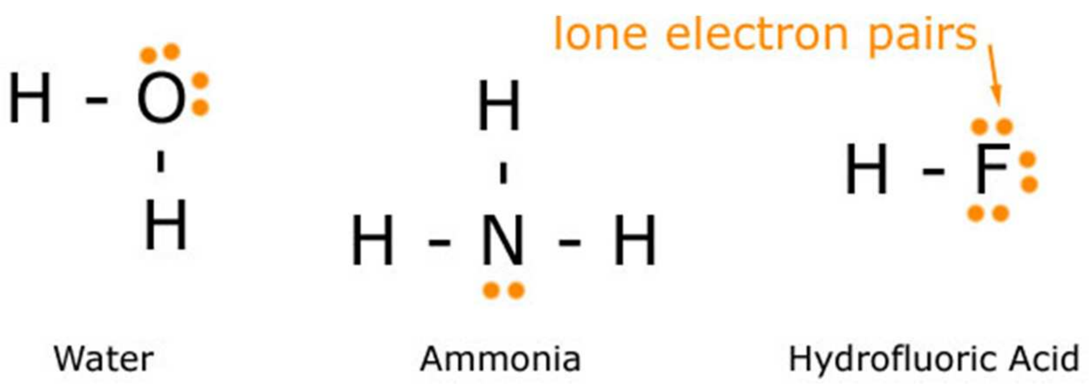
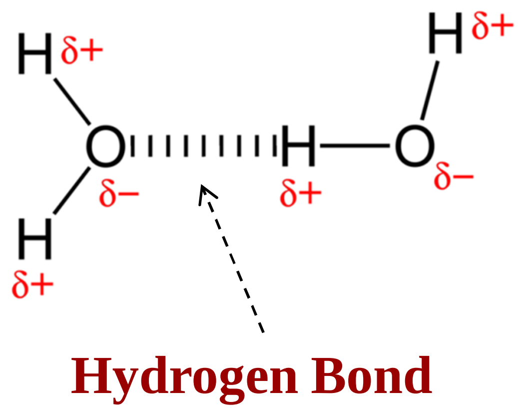
Secondary Bonding : **permanent dipoles**

"Hydrogen bond" – secondary bond formed between two **permanent dipoles** in adjacent molecules.

It only happens in molecules where hydrogen bonds with the following: Oxygen (O), Nitrogen (N) and Fluorine (F).
→ **high electronegativities**.





http://scienceaid.co.uk/chemistry/fundamental/inter.html

http://commons.wikimedia.org/wiki/File:Hydrogen-bonding-in-water-2D.png

Summary: Bonding

Type	Bond Energy	Comments
Ionic	Large!	Nondirectional (ceramics)
Covalent	Variable large-Diamond small-Bismuth	Directional (semiconductors, ceramics polymer chains)
Metallic	Variable large-Tungsten small-Mercury	Nondirectional (metals)
Secondary	smallest	Directional inter-chain (polymer) inter-molecular