Chapter 2: Atomic Structure & Interatomic Bonding

ISSUES TO ADDRESS...

- What promotes bonding?
- What types of bonds are there?
- What properties are inferred from bonding?

Chapter 2 - 1

Atomic Structure (Freshman Chem.)

- atom – electrons – 9.11 x 10^{-31} kg
  ____
  neutrons } ___________
- atomic number = # of protons in nucleus of atom
  = # of electrons of _______ species
- A [=] atomic mass unit = ____ = 1/12 mass of ^{12}C

  Atomic wt = wt of ___________ molecules or atoms

  1 amu/atom = 1g/mol

  C 12.011
  H 1.008 etc.

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Atomic Structure

- Valence electrons determine all of the following properties
  1) Chemical
  2) ________
  3) Thermal
  4) ________

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Electronic Structure

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

Quantum #	Designation
n = ________ (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 = __________	1, 3, 5, 7 (-l to +l)
m_s = spin	½, -½

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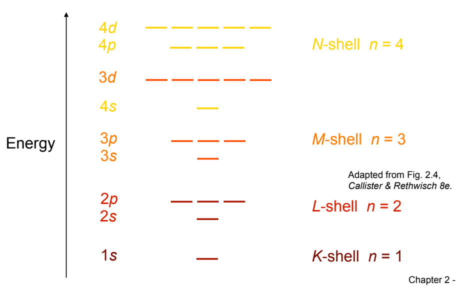
Electron Energy States

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



Adapted from Fig. 2.4, *Callister & Rethwisch 8e.*

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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)

Adapted from Table 2.2, *Callister & Rethwisch 8e.*

- Why? Valence (outer) shell usually not filled completely.

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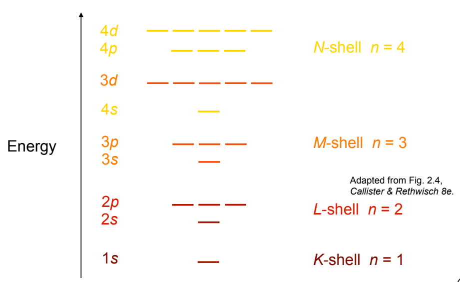
Electron Configurations

- Valence electrons – those in unfilled shells
- ______________________
- Valence electrons are most available for bonding and tend to control the chemical properties
  - example: C (atomic number = 6)

$1s^2$ $2s^2\ 2p^2$ ← valence electrons

Electronic Configurations

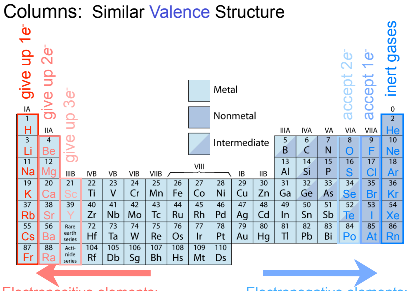
ex: Fe - atomic # = 26 $1s^2\ \ 2s^2 2p^6\ \ 3s^2 3p^6\ \ 3d^6\ \ 4s^2$



Adapted from Fig. 2.4, *Callister & Rethwisch 8e.*

The Periodic Table

- Columns: Similar Valence Structure



Adapted from Fig. 2.6, *Callister & Rethwisch 8e.*

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 & Rethwisch 8e.* (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 bond – metal + nonmetal

metal ↑ ______ electrons

nonmetal ↑ ______ electrons

Dissimilar electronegativities

ex: MgO

Mg $1s^2\ 2s^2\ 2p^6\ 3s^2$
[Ne] $3s^2$

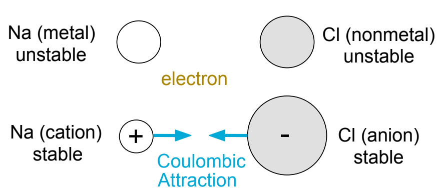
O $1s^2\ 2s^2\ 2p^4$

Mg^{2+} $1s^2\ 2s^2\ 2p^6$
[Ne]

O^{2-} $1s^2\ 2s^2\ 2p^6$
[Ne]

Ionic Bonding

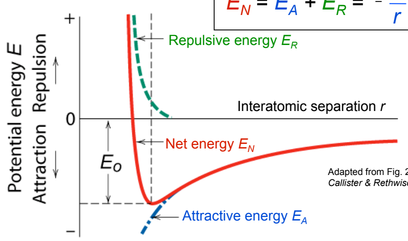
- Occurs between + and - ions.
- Requires ______________.
- Large difference in ________________________
- Example: NaCl



Ionic Bonding

- Energy – _________ energy most stable
  - Energy balance of attractive and ________ terms

$$E_N = E_A + E_R = -\frac{A}{r} + \frac{B}{r^n}$$



Adapted from Fig. 2.8(b), *Callister & Rethwisch 8e.*

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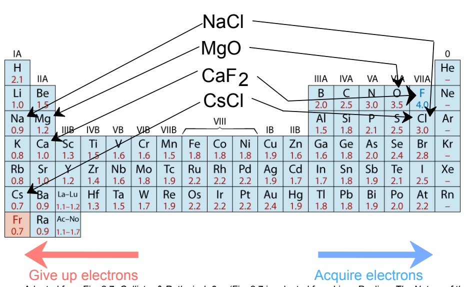
Examples: Ionic Bonding

- Predominant bonding in _________



Adapted from Fig. 2.7, *Callister & Rethwisch 8e.* (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.

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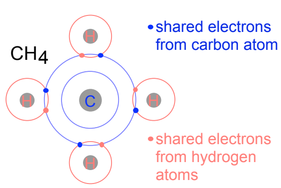
Covalent Bonding

- similar ______________ ∴ share electrons
- bonds determined by _______ – *s* & *p* _______ dominate bonding
- Example: CH_4

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

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

________________ are comparable.



Adapted from Fig. 2.10, *Callister & Rethwisch 8e.*

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Primary Bonding

- Metallic Bond -- delocalized as electron cloud
- Ionic-Covalent Mixed Bonding

$$\text{\% ionic character} = \left(1 - e^{-\frac{(X_A - X_B)^2}{4}}\right) \times (100\%)$$

where X_A & X_B are _________electronegativities

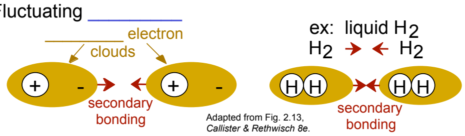
Ex: MgO $X_{Mg} = 1.2$, $X_O = 3.5$

$$\text{\% ionic character} = \left(1 - e^{-\frac{(3.5-1.2)^2}{4}}\right) \times (100\%) = 73.4\% \text{ ionic}$$

SECONDARY BONDING

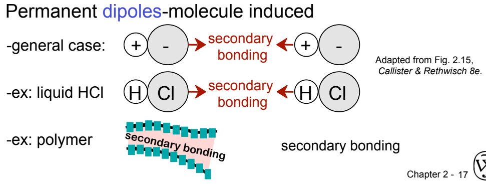
Arises from interaction between _________

- Fluctuating _________



Adapted from Fig. 2.13, *Callister & Rethwisch 8e.*

- Permanent dipoles-molecule induced



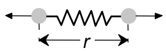
Adapted from Fig. 2.15, *Callister & Rethwisch 8e.*

Summary: Bonding

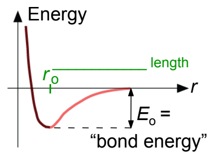
Type	Bond Energy	Comments
Ionic	Large!	Nondirectional (_________)
Covalent	Variable large-Diamond small-Bismuth	Directional (_____________, _________ polymer chains)
Metallic	Variable large-Tungsten small-Mercury	Nondirectional (______)
Secondary	smallest	Directional inter-chain (________) inter-molecular

Properties From Bonding: T_m

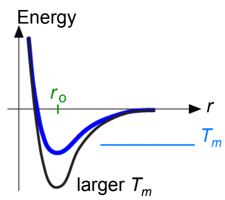
- Bond length, r



- _____ energy, E_o



- Melting Temperature, T_m



__________ if E_o is larger.

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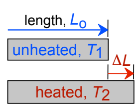
Properties From Bonding : α

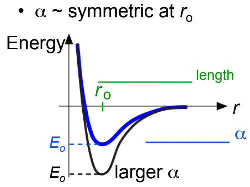
- Coefficient of thermal expansion, α



coeff. ________ expansion

$$\frac{\Delta L}{L_o} = \alpha (T_2 - T_1)$$

- α ~ symmetric at r_o



________ E_o is smaller.

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Summary: Primary Bonds

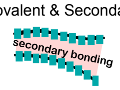
Ceramics
(Ionic & covalent bonding):

Large bond energy
large T_m
large E
_____ α

Metals
(Metallic bonding):

Variable bond energy
________ T_m
________ E
moderate α

Polymers
(Covalent & Secondary):



Directional Properties
Secondary bonding dominates
small T_m
________ E
large α

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