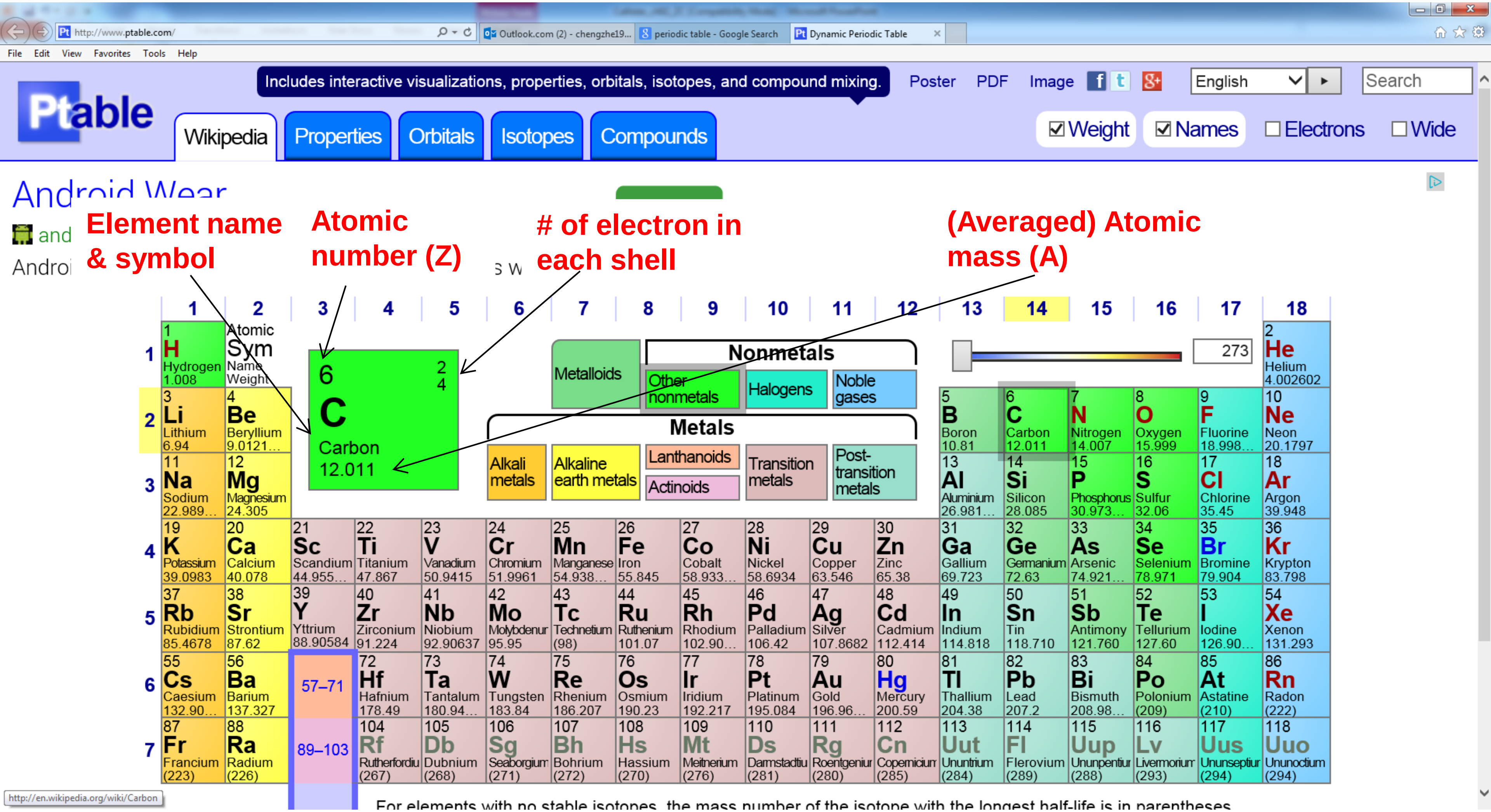
Chapter 2: Atomic Structure & Interatomic Bonding

Review…

- Atom and related basics
- Atom electron configuration and valence electrons
- Bonding between atoms and types of bonds in materials

Class Exercise: Review of Basics for Atom



- Element name? **Carbon**
- # of electrons in a **neutral** atom? **=Z=6**
- # protons in such an atom? **=Z=6**
- Atomic number (Z)? **Z=6**
- (Averaged) Atomic mass (A) and Unit? **A=12.011 g/mol**

Atomic Structure

- 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 for a **neutral** atom
- Isotope: same Z, different number of neutrons
- Atomic mass unit (amu), 1/12 mass of ^{12}C
- Atomic mass (or weight) A = averaged mass with respect to natural isotopes for an element

  Unit of atomic mass: **g/mol** **(preferred)** or amu/atom
  - 1 mole of atoms: Avogadro number $N_A = 6.022 \times 10^{23}$ of atoms
  - Examples:
    - For C, atomic mass = 12.011 g/mol, i.e., 12.011 g for 6.022×10^{23} of C atoms
    - For H, atomic mass = 1.008 g/mol, i.e., 1.008 g for 6.022×10^{23} of H atoms

Class Exercise – Periodic Table

Given information on right from periodic table for aluminum,

13	2 8 3
Al	
Aluminium	
26.9815385	

•What is the atomic number ***Z***

13

•What is the number of proton in Al nucleus

13

•What is the atomic weight ***A*** and the unit for atomic weight ***A***

26.98 g/mol

•On average, one gram of Al will contain how many Al atoms? (Knowing Avogadro's number N_A=6.02x10^{23} mol^{-1}

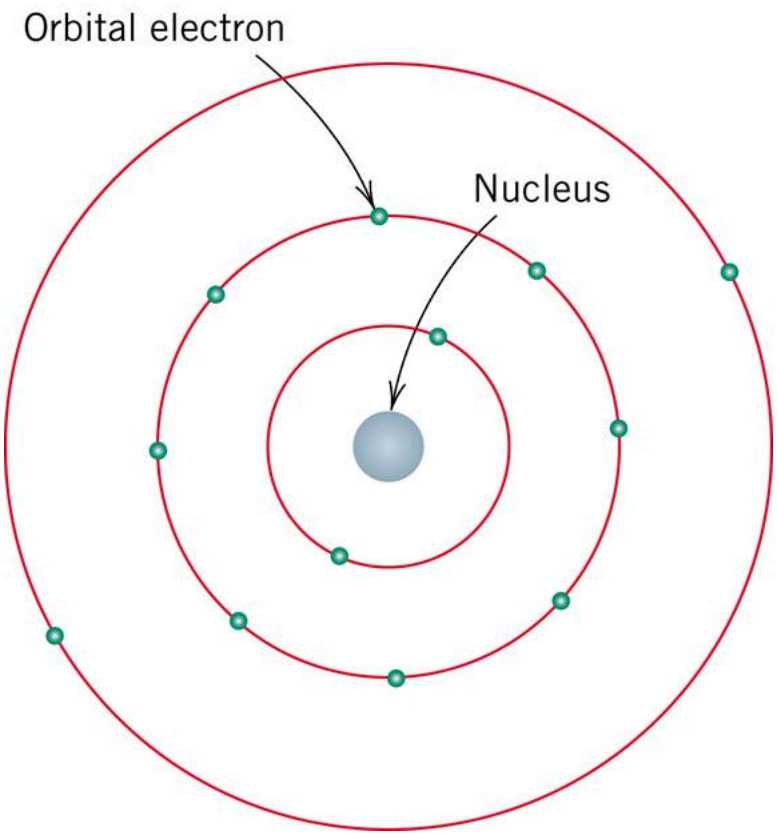
$$\frac{1}{A}\cdot N_A = \frac{1g}{26.98\ g/mol}\cdot 6.02\times 10^{23}/mol = 2.23\times 10^{22}$$

•What is the averaged (over naturally occurring isotope) mass (weight) for one aluminum atom?

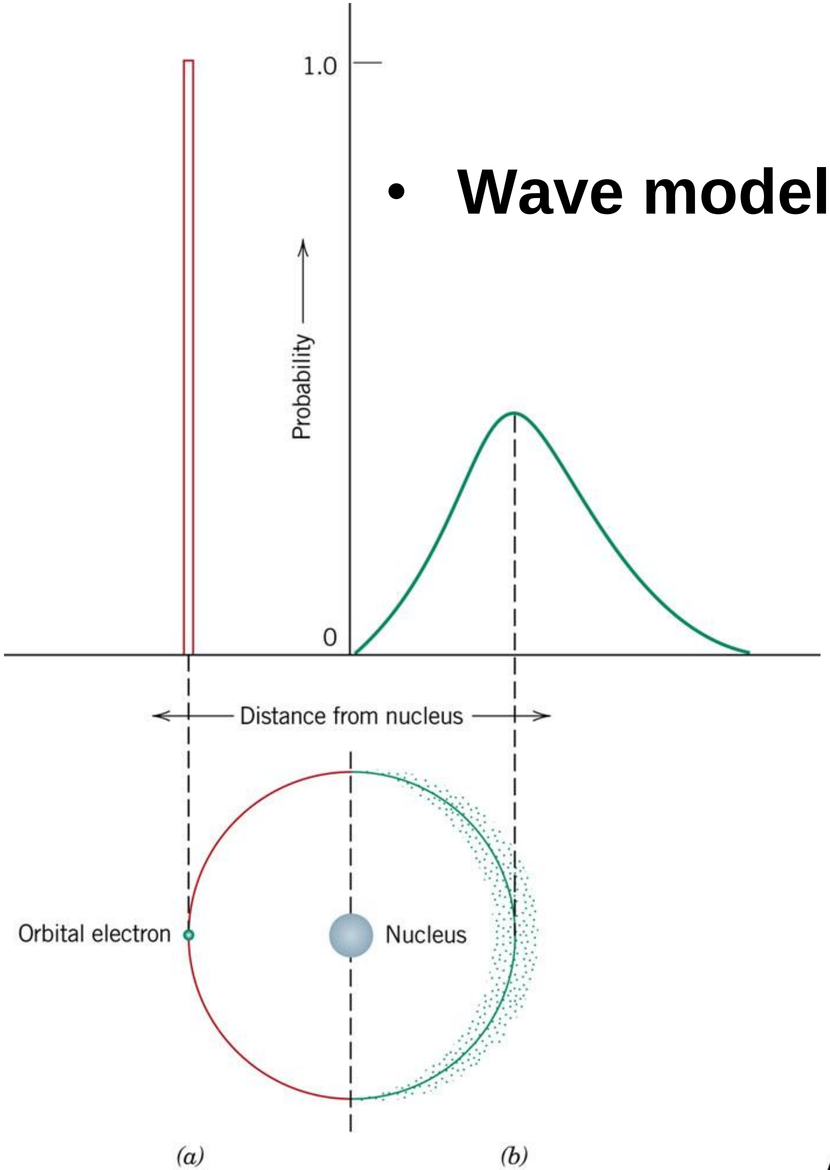
$$\frac{A}{N_A} = \frac{26.98\ g/mol}{6.02\times 10^{23}/mol} = 4.48\times 10^{-23}\ g$$

Atomic (or Electron) Orbital Models

- **Bohr model**



- **Wave model**



Electronic Structure for Atoms

In an atom, electrons have certain arrangement/structure:

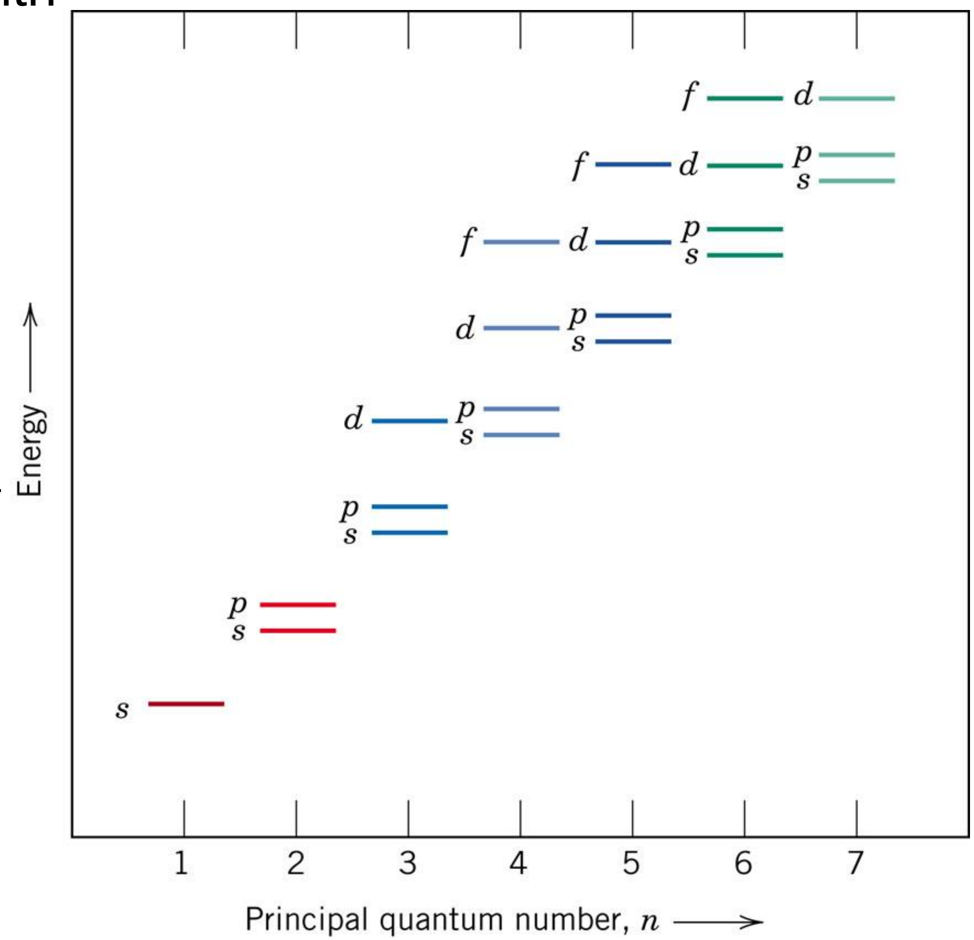
•Electrons are in a series of orbitals with different, discrete energy states following certain rules

•Electrons occupy lower available energy states (orbitals) first

– Shell: K, L, M, (or 1, 2, 3) etc. from low to high energy

– Subshell: s, p, d, f, etc. within a shell from low to high energy

– Different orientations (orbits) of same energy within each subshell (for an isolated single atom)

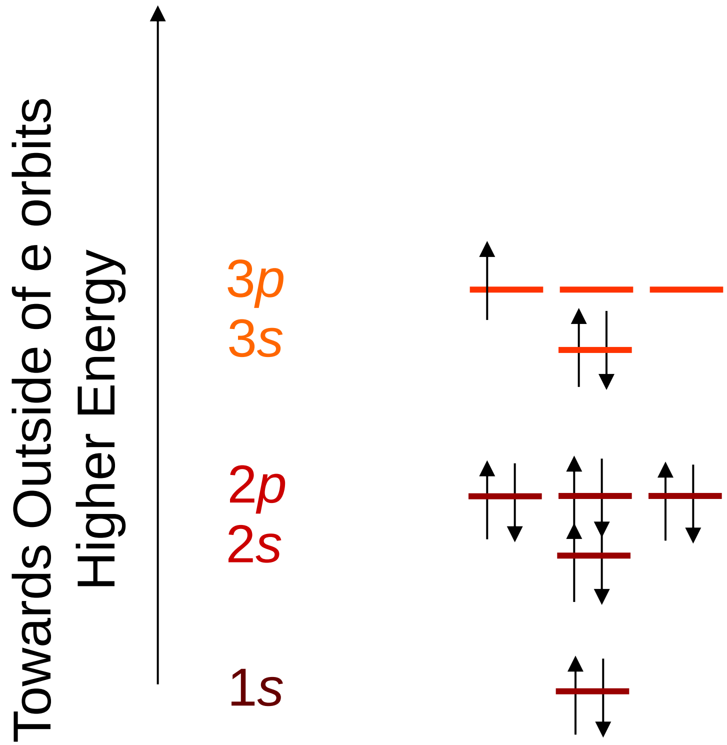


•Follow Pauli exclusion principle: no more than two electrons in the same orbit, with one spin up & one spin down

Electron Configuration

13 2 8 3
Al
Aluminium
26.9815385

ex: Aluminum, Al - atomic # Z = 13



M-shell $n = 3$

L-shell $n = 2$

K-shell $n = 1$

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

Electron configuration for a neutral Al atom

$1s^2 \quad 2s^2\, 2p^6 \quad 3s^2\, 3p^1$

valence electrons

Examples of Electron Configuration

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.*

Valence Electrons

- Valence electrons – those electrons occupy outmost **shells** (and, for transition metals, a few of of inner shell electrons in the d-orbits)
- Valence electrons are most available for bonding and tend to control the chemical properties for the atom/element

– example: Neutral Cl atom - atomic number Z = 17

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

valence electrons

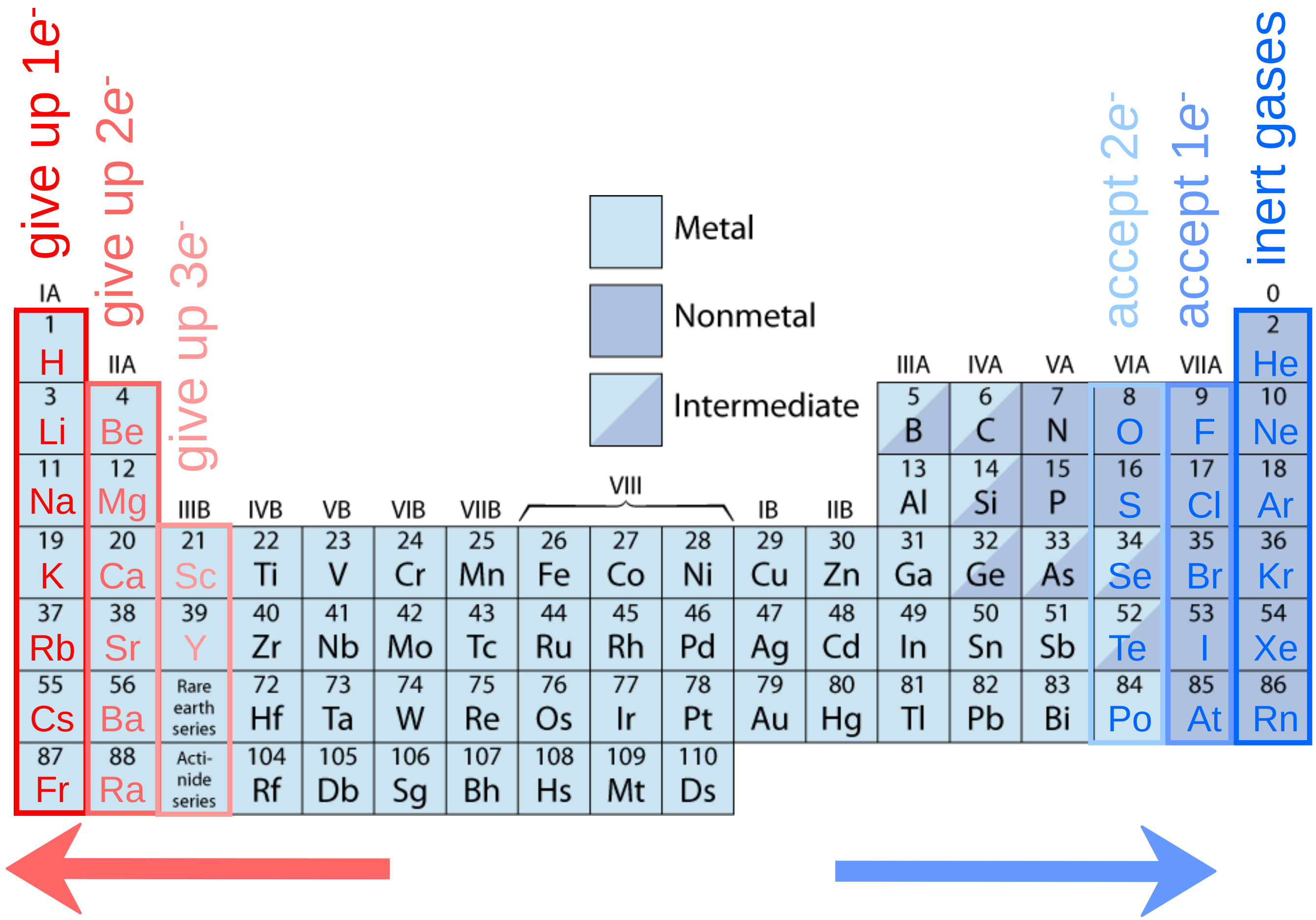
- Valence electrons determine the following properties

1) Chemical
2) Electrical
3) Thermal
4) Optical

- **Atoms/ions with filled outmost shell will be stable:**
  For H, He, Li, Be: two(2) e^- for *1s* as the outmost shell is stable
  For others: outmost shell with eight (8) e^- is stable

The Periodic Table

- **Columns**: Similar valence electron structure – **Group**
- **Row**: Same number of electron shells (not subshells) – **Period**



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

Readily give up electrons to become cations or + ions

Readily acquire electrons to become anions or - ions

Electronegativity

- A number representing the tendency for an atom to **acquire** electrons
- Right side of periodic table & fewer number of shells → HIGHER electronegativity, easier to GET electron(s)
- Left side of periodic table & more number of shells → LOWER electronegativity, easier to GIVE OUT electron(s)

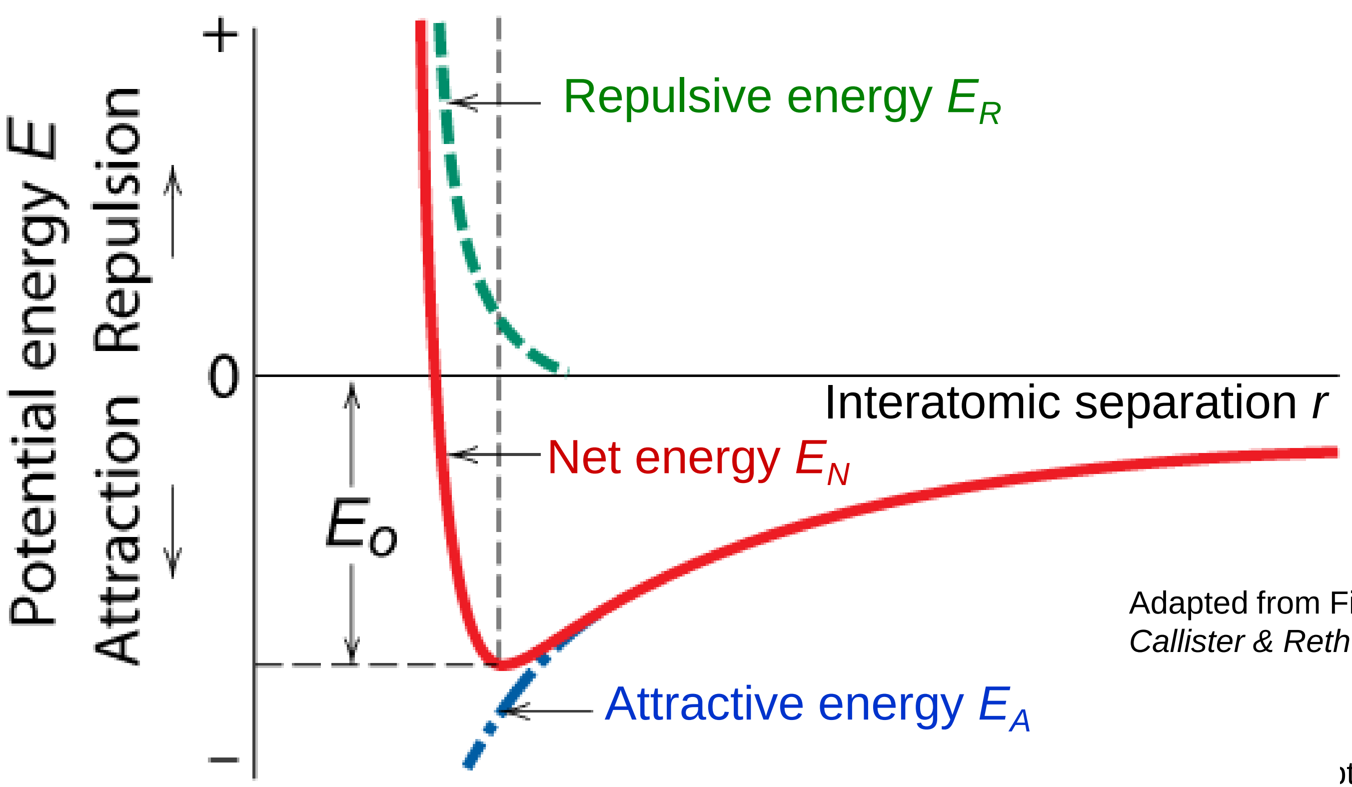
HIGHER electronegativity

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															

LOWER electronegativity

Bonding Energy

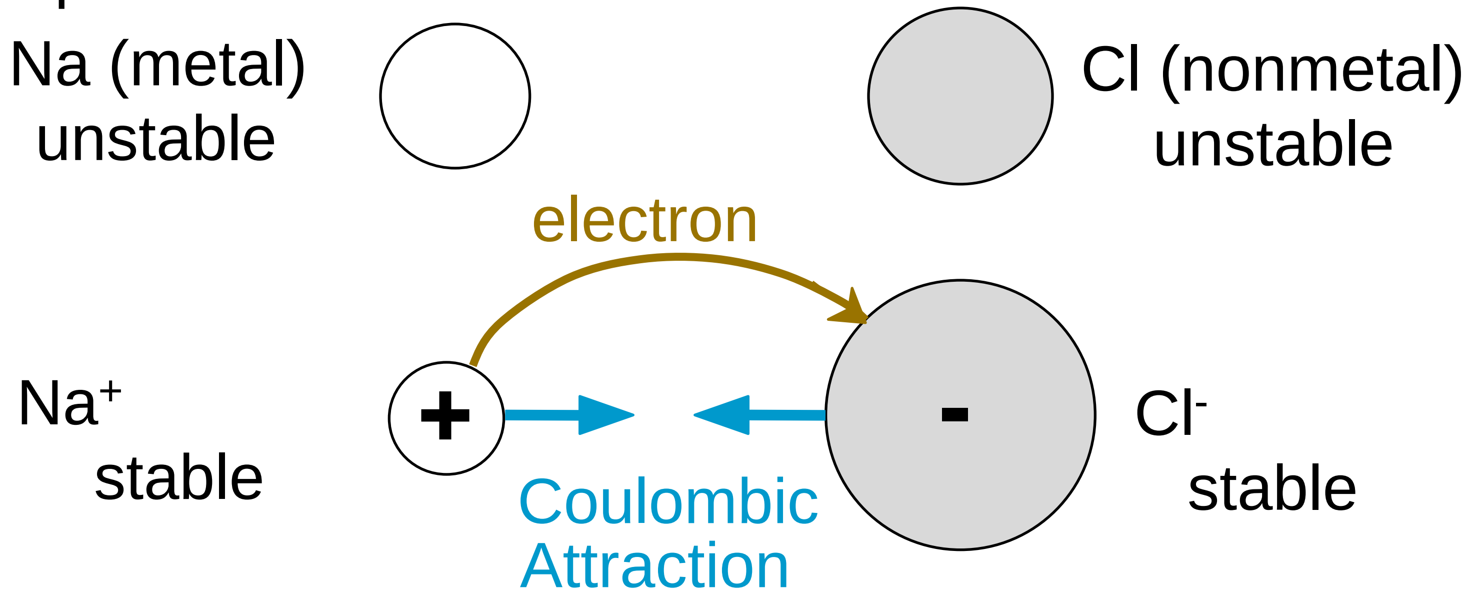
- In materials, atoms are bonded together in certain ways
- Bonding energy - energy required to **break** the bonds between atoms
- Result of balance of attractive and repulsive forces
  - minimum energy → most stable → stable inter-atomic distance



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

Primary Bond (1) - Ionic Bond

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



- Large bond energy

Ionic bond – metal + nonmetal

metal: donates electrons

nonmetal: accepts electrons

ex: NaCl

$\chi = 0.9$

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

$[Ne]\ 3s^1$

$\chi = 3.0$

Cl $1s^2 2s^2 2p^6 3s^2 3p^5$

$[Ne] 3s^2 3p^5$

Na^+ $1s^2\ 2s^2\ 2p^6$

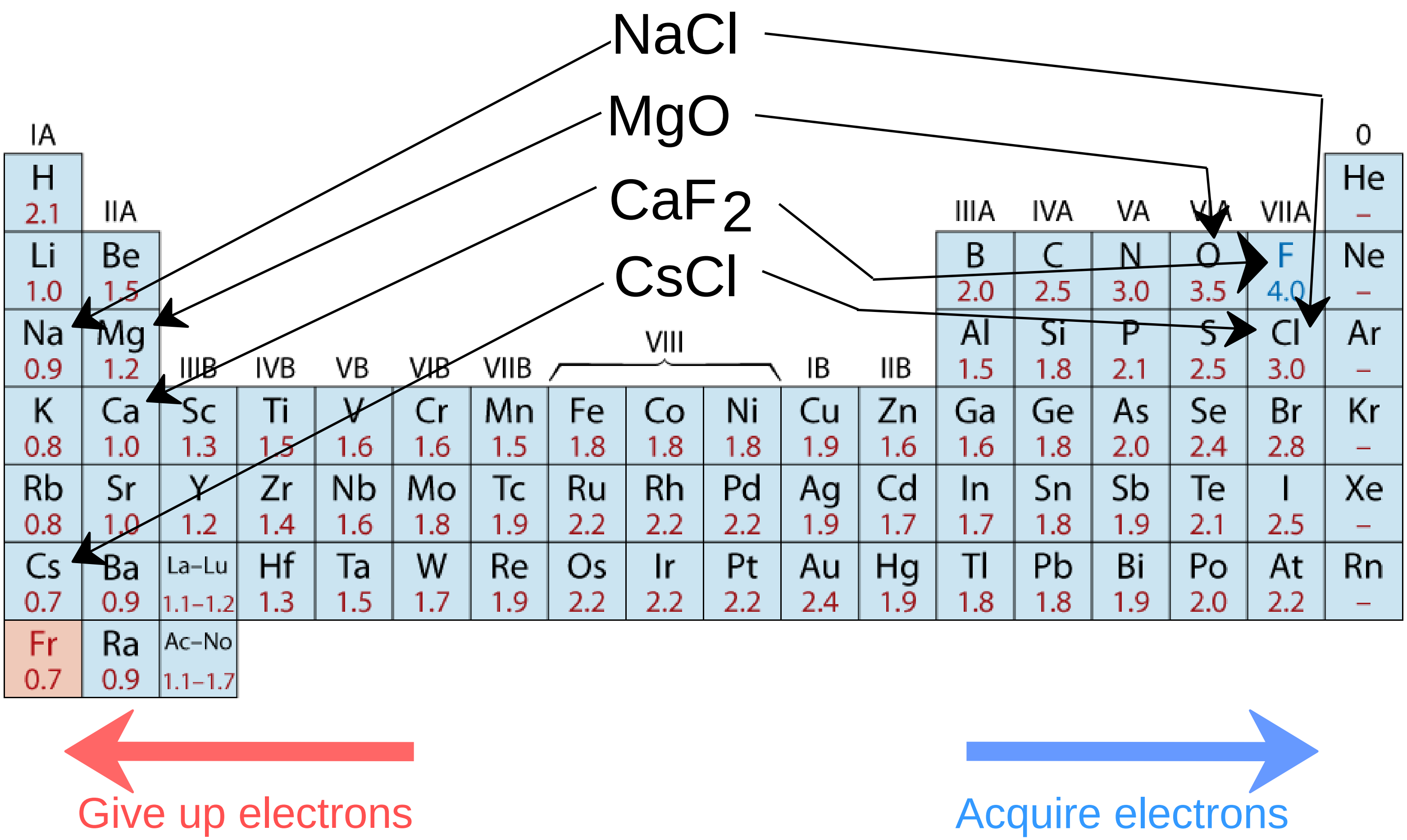
$[Ne]$

Cl^- $1s^2\ 2s^2 2p^6\ 3s^2 3p^6$

$[Ar]$

Examples: Ionic Bond

- Often found in Ceramics



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.

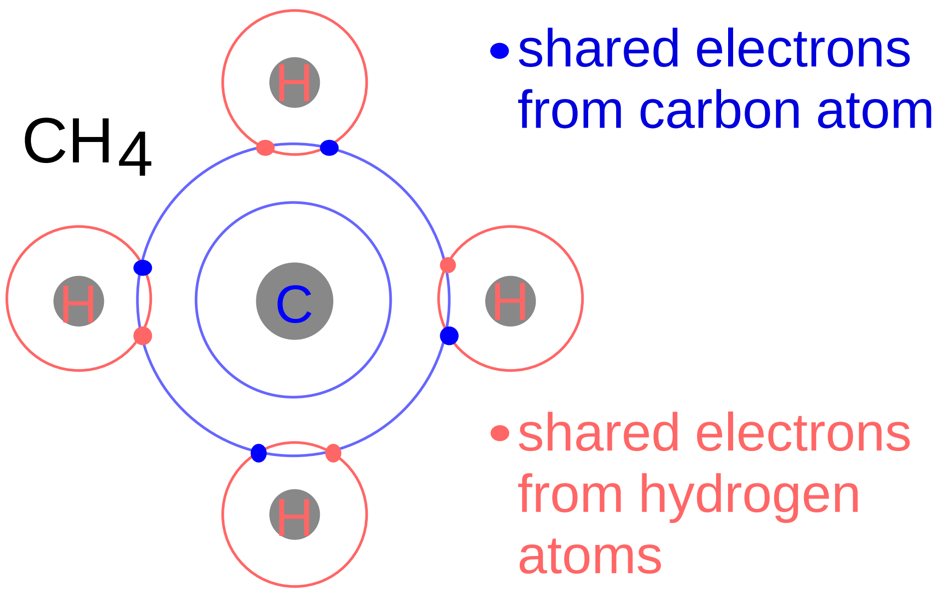
Primary Bond (2) - Covalent Bond

- Between non-metals with similar electronegativity → share electrons
- Bonds determined by valence – often *s* & *p* orbitals dominate bonding
- Example: CH_4

C: has 4 valence e^-, needs 4 more to be stable

H: has 1 valence e^-, needs 1 more to be stable

Electronegativities χ are **comparable**: 2.1 for H and 2.5 for C

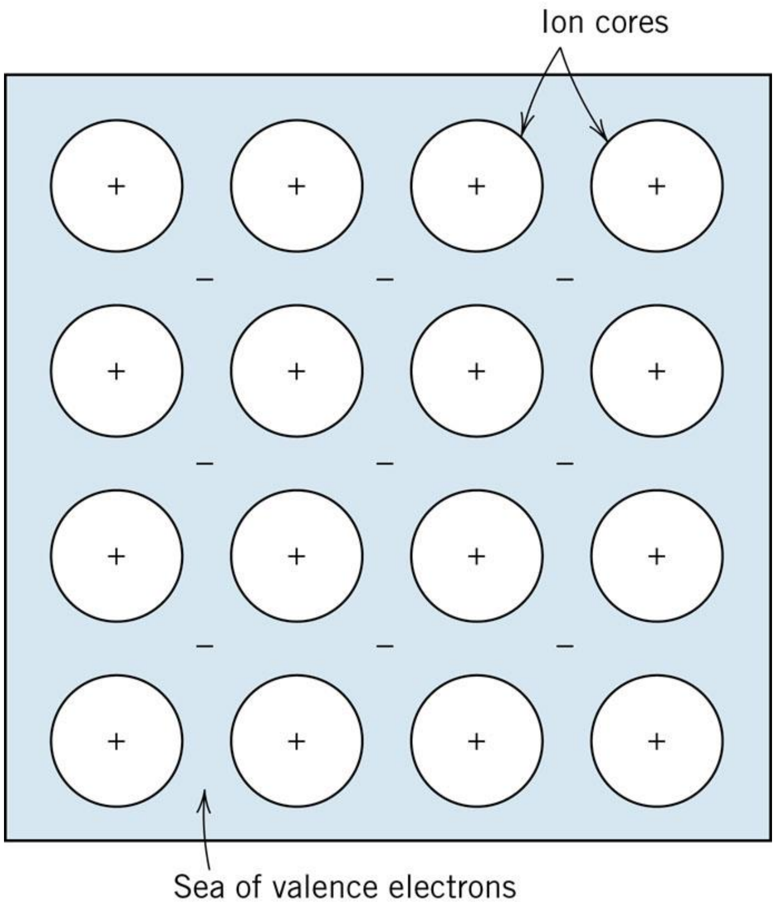


Adapted from Fig. 2.10, *Callister & Rethwisch 8e.*

- Bond energy: usually large

Primary Bond (3) - Metallic Bond

- Metallic Bond -- Bonds between metal cations and **delocalized** electron cloud

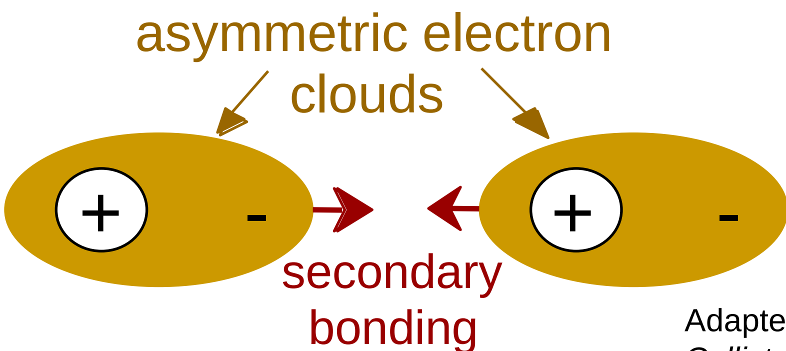


- Bond energy usually large

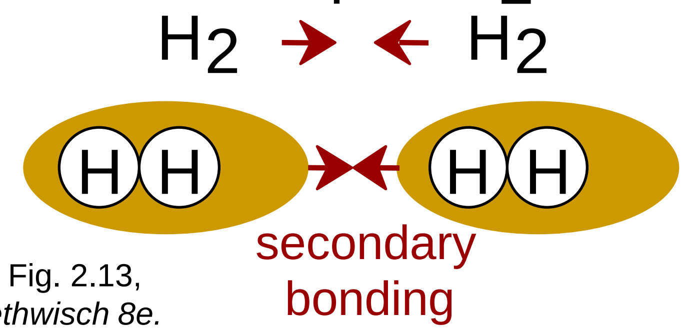
<u>**Secondary**</u> Bonds

"Bond" arising from interactions between **dipoles** in **molecules**

Case 1: Between <u>fluctuating (induced)</u> dipoles (e.g., for H_2, Cl_2)



ex: liquid H_2



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

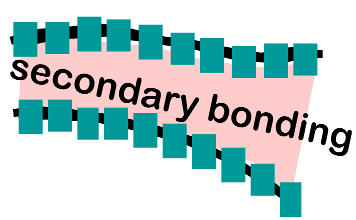
Case 2: Between <u>permanent</u> dipoles (e.g., for HCl, H_2O)

-general case:

-ex: liquid HCl

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

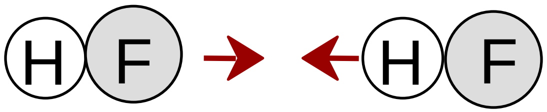
-ex: polymer



secondary bonding between individual polymer molecules

Hydrogen Bond – A Special Type of **Secondary** Bond

- Strongest among all secondary bonds
- A special case of permanent dipole induced bonding
- **Between individual molecules** in which H is covalently bonded to F (e.g., HF), O (e.g., H_2O), and N (e.g., NH_3)



- Hydrogen bond bonding energy is much higher than other types of secondary bonding but still much weaker than bonding energy for primary bonds (i.e., covalent, ionic, or metallic bonds)

Summary: Bond Type (1)

Type		Bonding Energy
Primary bonds	Ionic	Large
	Covalent	Variable Large-Diamond Small-Bismuth
	Metallic	Variable Large-Tungsten Small-Mercury
Secondary bonds (between molecules or even particles) e.g., hydrogen bond		Generally small

Bond Type & Materials Physical Properties

Table 2.3 Bonding Energies and Melting Temperatures for Various Substances

Bonding Type	Substance	Bonding Energy kJ/mol	Bonding Energy eV/Atom, Ion, Molecule	Melting Temperature (°C)
Ionic	NaCl	640	3.3	801
	MgO	1000	5.2	2800
Covalent	Si	450	4.7	1410
	C (diamond)	713	7.4	>3550
Metallic	Hg	68	0.7	−39
	Al	324	3.4	660
	Fe	406	4.2	1538
	W	849	8.8	3410
van der Waals	Ar	7.7	0.08	−189
	Cl_2	31	0.32	−101
Hydrogen	NH_3	35	0.36	−78
	H_2O	51	0.52	0

- Higher bonding energy → Higher melting point

Materials Class & Bonding Type

Ceramics

Ionic & covalent bonding

Generally large bonding energy

High T_m
High *E (Elastic modulus, see Chapter 6)*

Metals

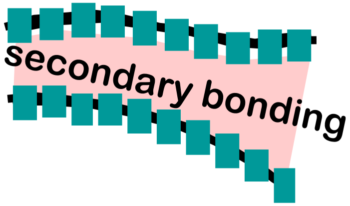
Metallic bonding

Generally large bonding energy

High T_m
High *E*

Polymers

Covalent/secondary bond



Generally low bonding energy

- Secondary bonds dominate interaction between molecules
  small T_m
  small *E*

Class Exercise - Bonds

- Given the following electronegativity numbers
  - χ (Na)=0.9;
  - χ (F)=4.0;
  - χ (Si)=1.8;
  - χ (C)=2.5;
  - χ (Mg)=1.2;

Determine the predominant primary bond type in the follow materials

- Sodium fluoride (NaF) Ionic bond
- Silicon carbide (SiC) Covalent bond
- Pure magnesium (Mg) Metallic bond

Class Exercise – Bonds (2)

- What is the bonding type between Oxygen and Oxygen atoms WITHIN a single oxygen molecule?

Covalent bond

- Is the bonding between different oxygen molecules in liquid oxygen primary bonding or secondary bonding?

Secondary bond

- What is the bonding type between Hydrogen (H) and oxygen WITHIN a single water molecule?

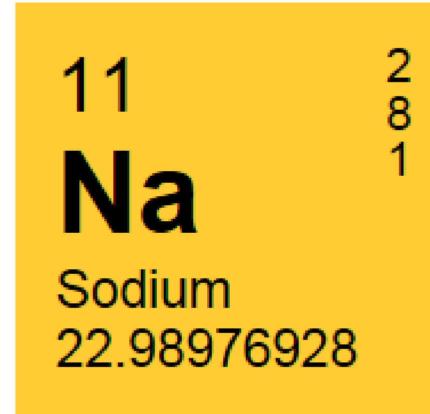
Covalent bond

- What is the bonding type BETWEEN different water molecules in ice?

Secondary bond (Hydrogen bond, in particular)

Class Exercise

Given information on right from periodic table for sodium,



•What is the atomic number Z

11

•What is the number of proton in Na nucleus

11

•What is the atomic weight A and the unit for atomic weight A

22.99 g/mol

•On average, one gram of Na will contain how many Na atoms?

1g/(22.99 g/mol) x (6.02×10^{23}/mol) = 2.62×10^{22}

•What is the averaged (over naturally occurring isotope) mass (weight) for one sodium atom?

(22.99 g/mol) / (6.02×10^{23}/mol) = 3.82×10^{-23} g

•Knowing F has electron configuration of $1s^2 2s^2 2p^5$ and atomic weight of 19.0, give the chemical formula for the stable compounds between Na and F and calculate the mass for one mole of that compound

Na has 1 valence e ([Ne]$3s^1$), F has 7 valence e ([Ne]$2s^2 2p^5$)

One Na atom gives one e to one F atom, both become stable → NaF

Mass for one mole of NaF: 19.0g + 23.0g = 42.0 g

Chapter 2 homework

- Read chapter 2 and give an honor statement confirm reading
- Calister 8ed, hw 2.7, 2.22, and one additional problem

- Calister 8ed, 2.7

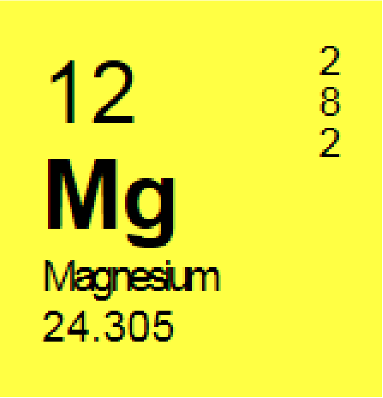
Give the electron configurations for the following ions: Fe^{2+}, Al^{3+}, Cu^{+}, Ba^{2+}, Br^{-}, and O^{2-}.

- Calister 8ed, 2.22

What type(s) of bonding would be expected for each of the following materials: brass (a copper-zinc alloy), rubber, barium sulfide (BaS), solid xenon, bronze, nylon, and aluminum phosphide (AlP)?

- One additional problem see attached

Homework



Given information on right from periodic table for magnesium,

•What is the atomic number Z

•What is the number of proton in Mg nucleus

•What is the atomic weight A and the unit for atomic weight A

•On average, one gram of Mg will contain how many Mg atoms?

•What is the averaged (over naturally occurring isotope) mass (weight) for one magnesium atom?

•Knowing F has electron configuration of $1s^2 2s^2 2p^5$ and atomic weight of 19.0, give the chemical formula for the stable compounds between Mg and F and calculate the mass for one mole of that compound