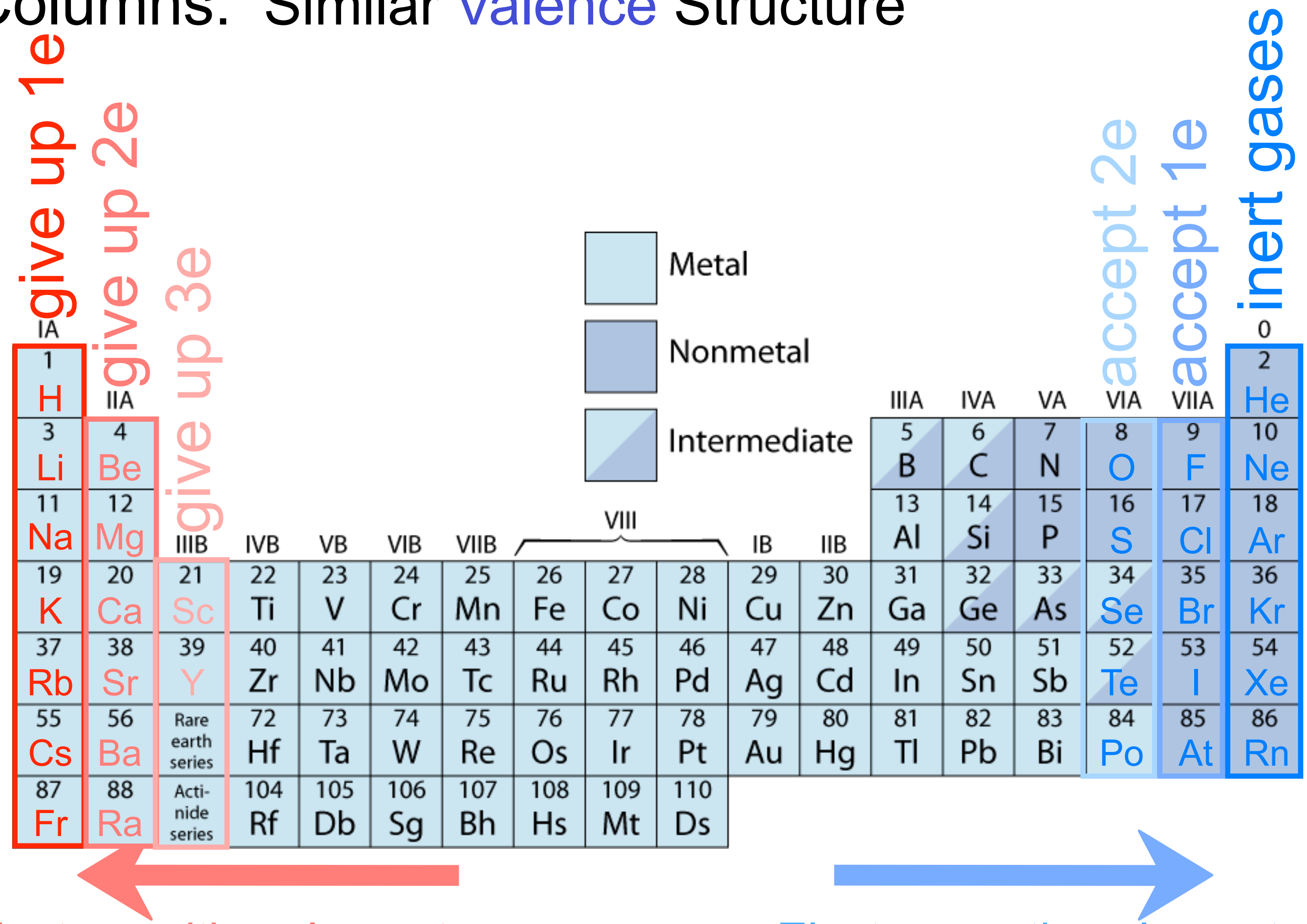
Chapter 2: Atomic structure and interatomic bonding

- Fundamental concepts
- Electrons in atoms
- Periodic table
- Bonding forces and energies

The Periodic Table

- Columns: Similar Valence Structure



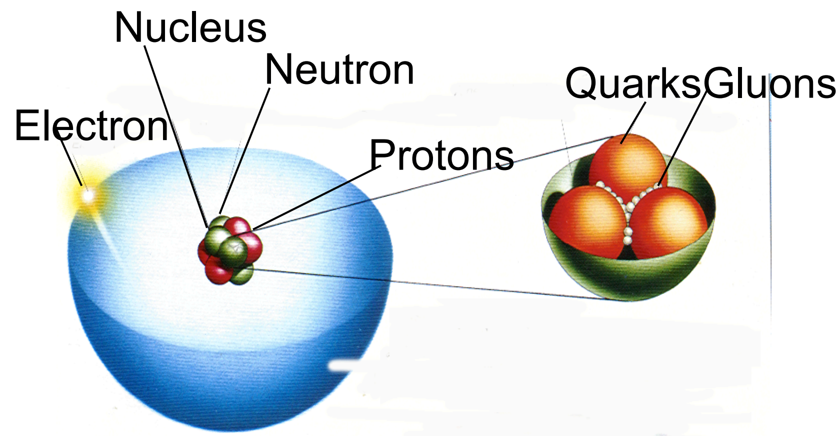
Adapted from Fig. 2.6, *Callister 7e.*

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

Electronegative elements: Readily acquire electrons to become - ions.

Chapter 2: Atomic structure and interatomic bonding

- Fundamental concepts
  - Proton and electron, charged 1.60×10^{-19} C
  - Mass of electron 9.11×10^{-31} kg
  - Mass of protons and neutrons
    ➡ 1.67×10^{-27} kg
  - Atomic number: the number of protons
  - Atomic mass =protons+neutrons
  - Isotope
  - Atomic mass unit(amu): 1amu=1/12 C
  - One mole = 6.023×10^{23} atoms(Avogadro’s)



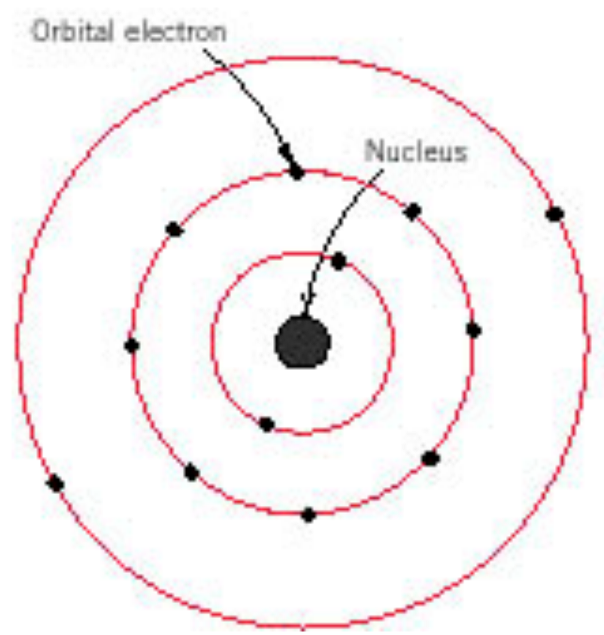
Electrons in atoms

- Atomic models
  - Bohr atomic

    electrons revolve around the atomic nucleus in discrete orbital and the energies of electrons are quantized

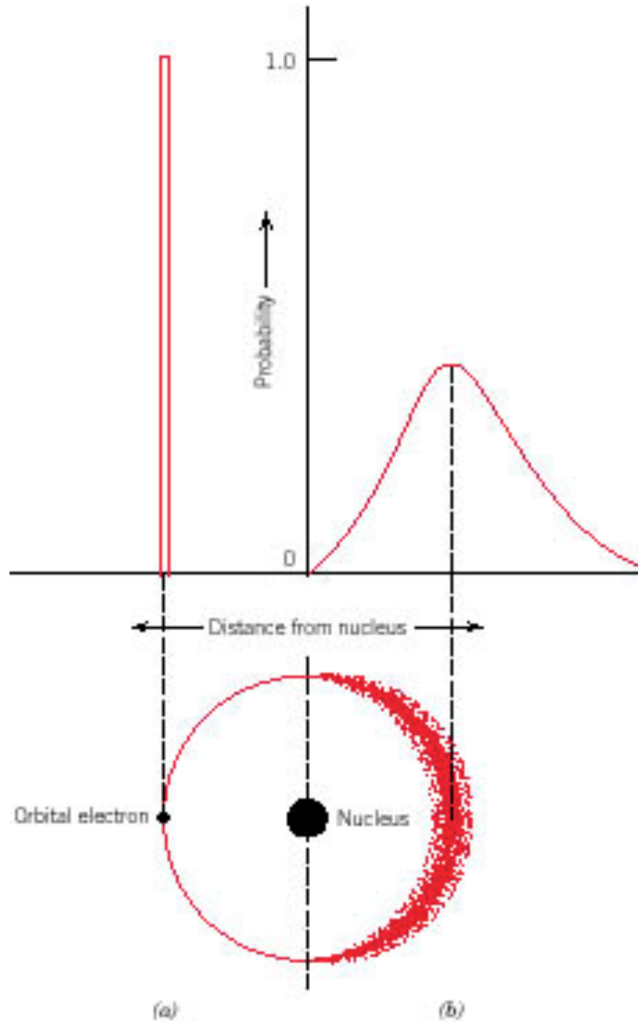
  - Wave-mechanical

    Electron exhibits both wavelike and particle-like characteristics, its position is considered to be a probability distribution



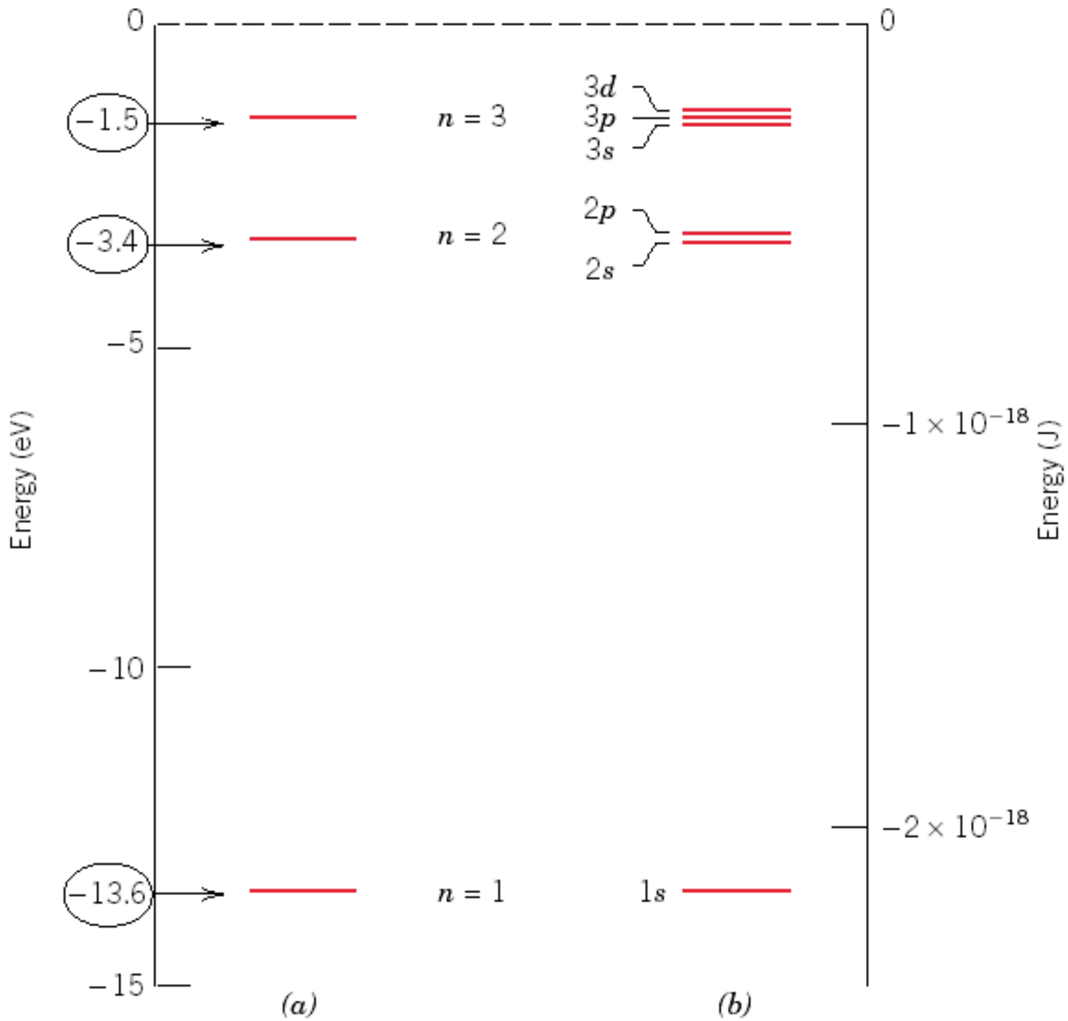
Electrons in atoms (*continue*)

❑ **Comparison of the (a) Bohr and (b) wave-mechanical atom models**



In terms of electron distribution

Electron energy states



Bohr hydrogen model

Wave-mechanical hydrogen

Quantum numbers

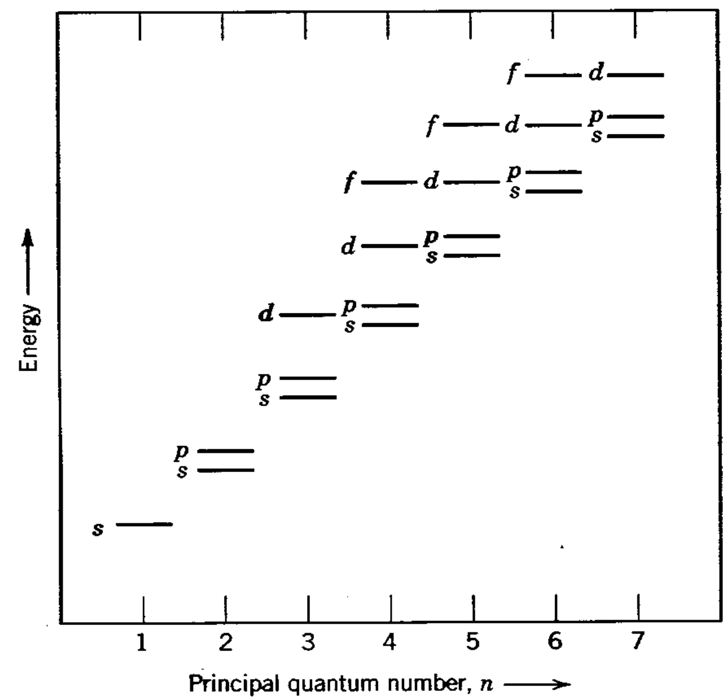
- Principal quantum number n=1, 2 ..; K, L, M, N, O
- Orbital quantum number l=0, ..n-1; subshell, s, p, d, or f; the shape of the electron subshell
- Spin moment ms 1/2 or -1/2

Table 2.1 The Number of Available Electron States in Some of the Electron Shells and Subshells

Principal Quantum Number n	Shell Designation	Subshells	Number of States	Number of Electrons: Per Subshell	Number of Electrons: Per Shell
1	K	s	1	2	2
2	L	s	1	2	8
		p	3	6	
3	M	s	1	2	18
		p	3	6	
		d	5	10	
4	N	s	1	2	32
		p	3	6	
		d	5	10	
		f	7	14	

Quantum Numbers

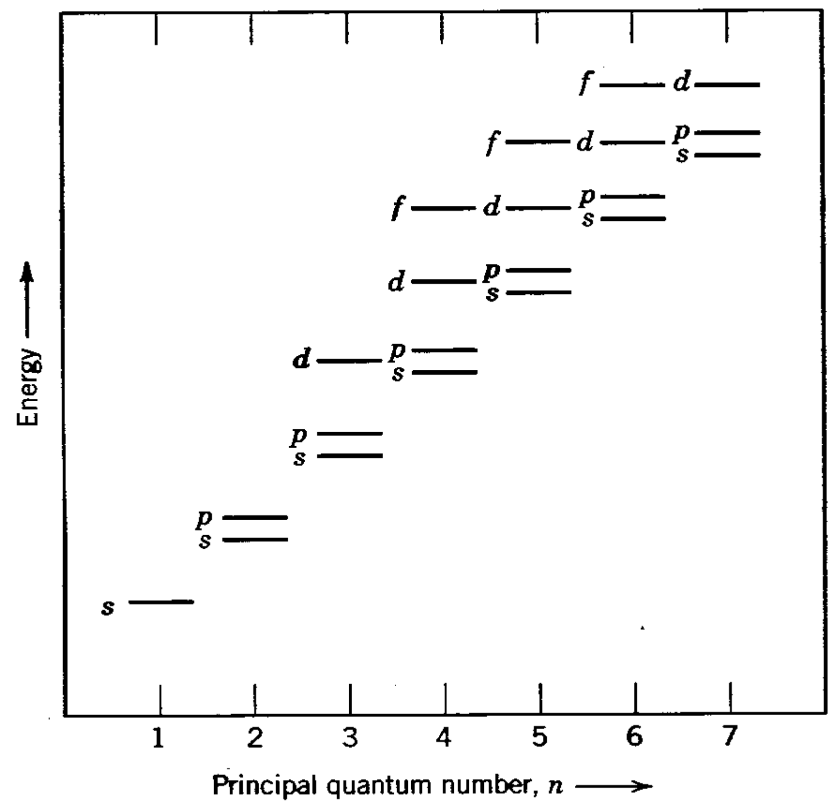
- The smaller n, the lower energy
- The smaller l, the lower energy
- There are some overlaps in energy, especially for d and f states



Relative energies of the electrons for various shells and subshells

Electron configurations

- Energy minimum rule
- Pauli exclusion
- Hund's rule: as many unpaired electrons as possible
- Ground state
- Valence electrons

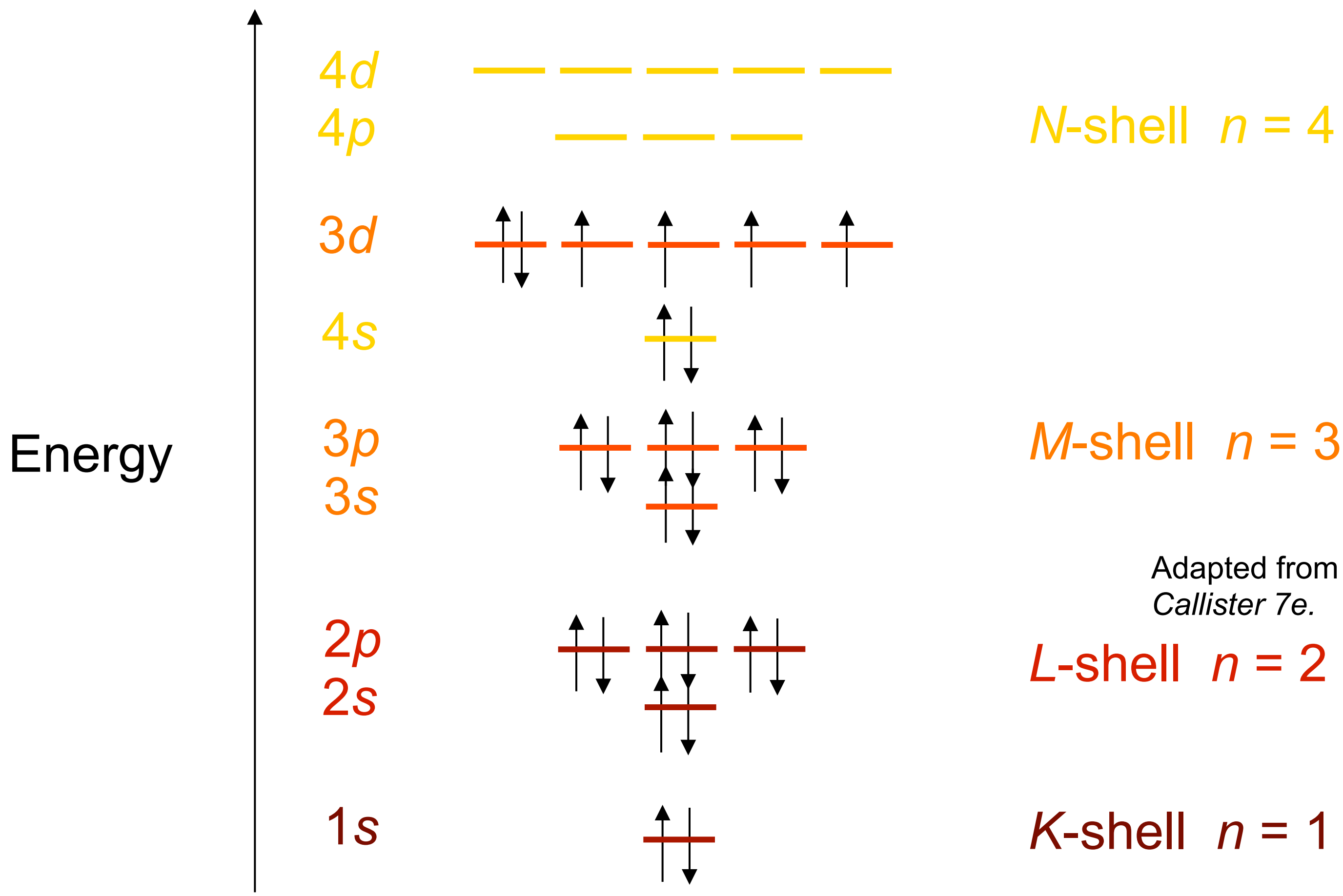


Relative energies of the electrons for various shells and subshells

Electronic Configurations

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

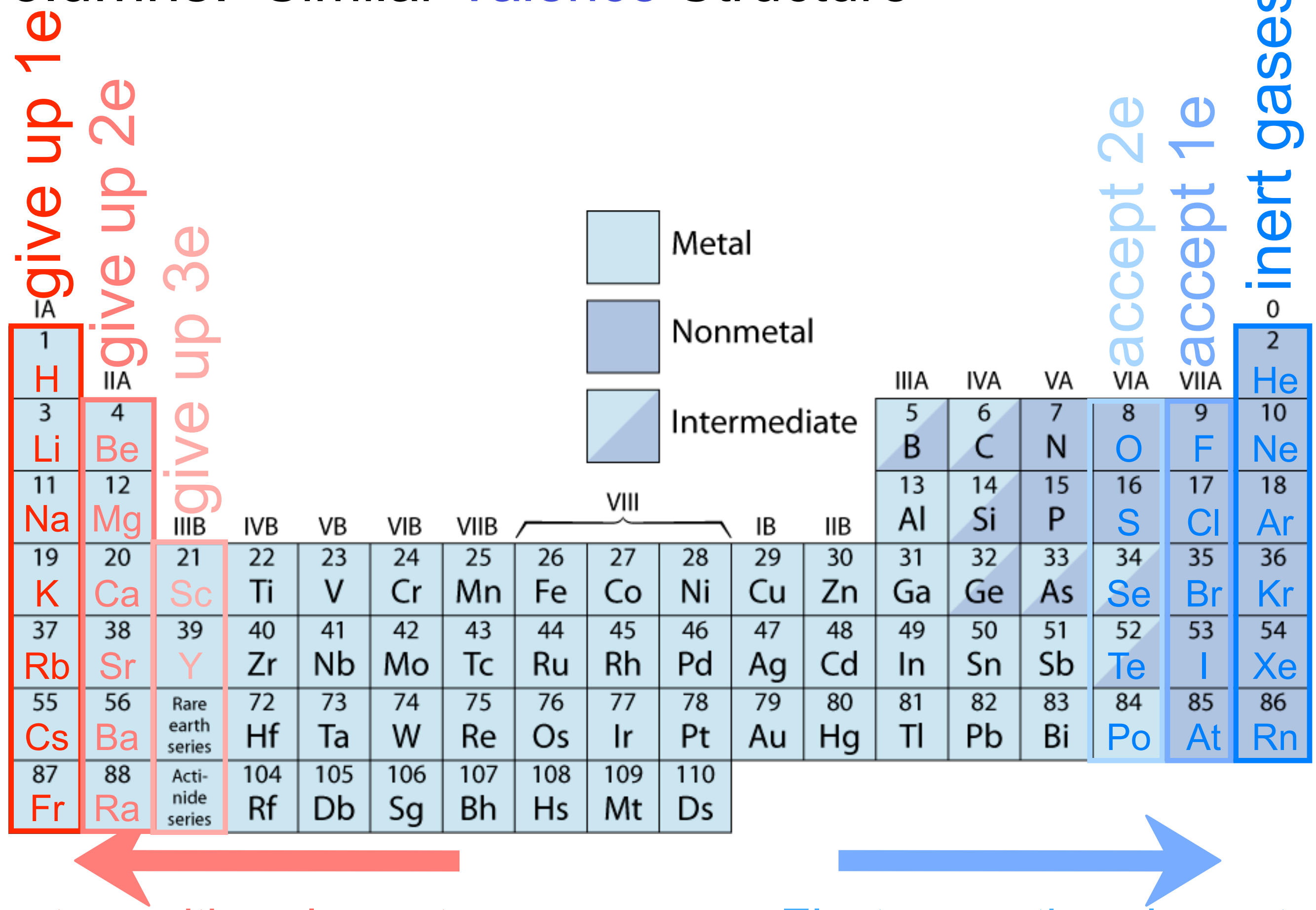
valence electrons



Adapted from Fig. 2.4, *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			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.

The periodic table(*continued*)

- Period: horizontal rows
- Group and column
  - Same group, same valence electrons, similar properties
  - Group 0, inert gas
  - Group IA, IIA, 1 or 2 excess electrons from stable structure
  - Transition metals (IVB and IIB).
  - III A, IVA and VA, semiconductor

- Electropositive and electronegative
- Electronegativity

SURVEY OF ELEMENTS

- Most elements: Electron configuration not stable.

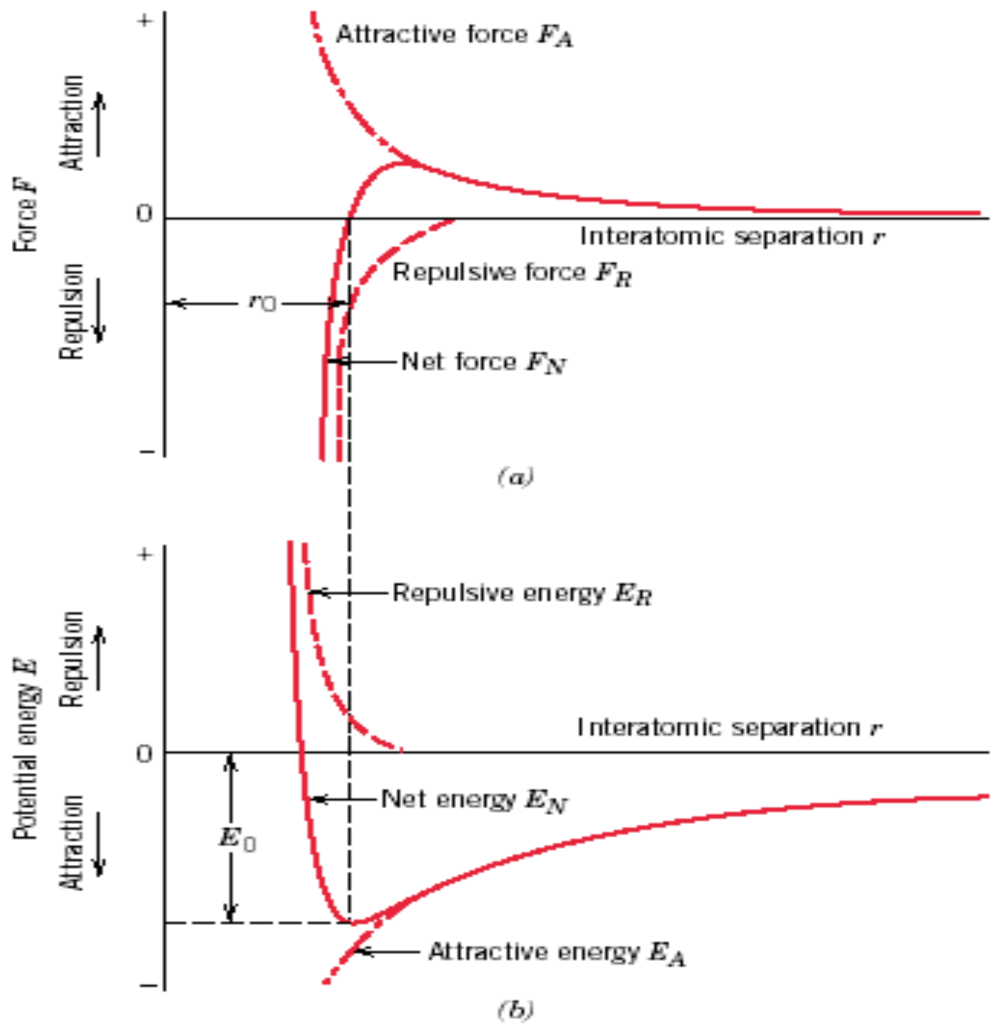
Element	Atomic #	Electron configuration	
Hydrogen	1	$1s^1$	
Helium	2	$1s^2$	(stable)
Lithium	3	$1s^2 2s^1$	
Beryllium	4	$1s^2 2s^2$	
Boron	5	$1s^2 2s^2 2p^1$	
Carbon	6	$1s^2 2s^2 2p^2$	
...		...	
Neon	10	$1s^2 2s^2 2p^6$	(stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$	
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$	
Aluminum	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 7e.*

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

Atomic bonding in solids

- Bonding forces and energies
  - $F_n = F_A + F_R$
  - E_0 -- bonding energy
  - large bonding E, high melting point
  - stiffness -- shape of f-r curve
  - thermal expansion --E-r curve



Ionic bond – metal + nonmetal

metal: donates electrons

nonmetal: accepts 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+} $1s^2\ 2s^2\ 2p^6$

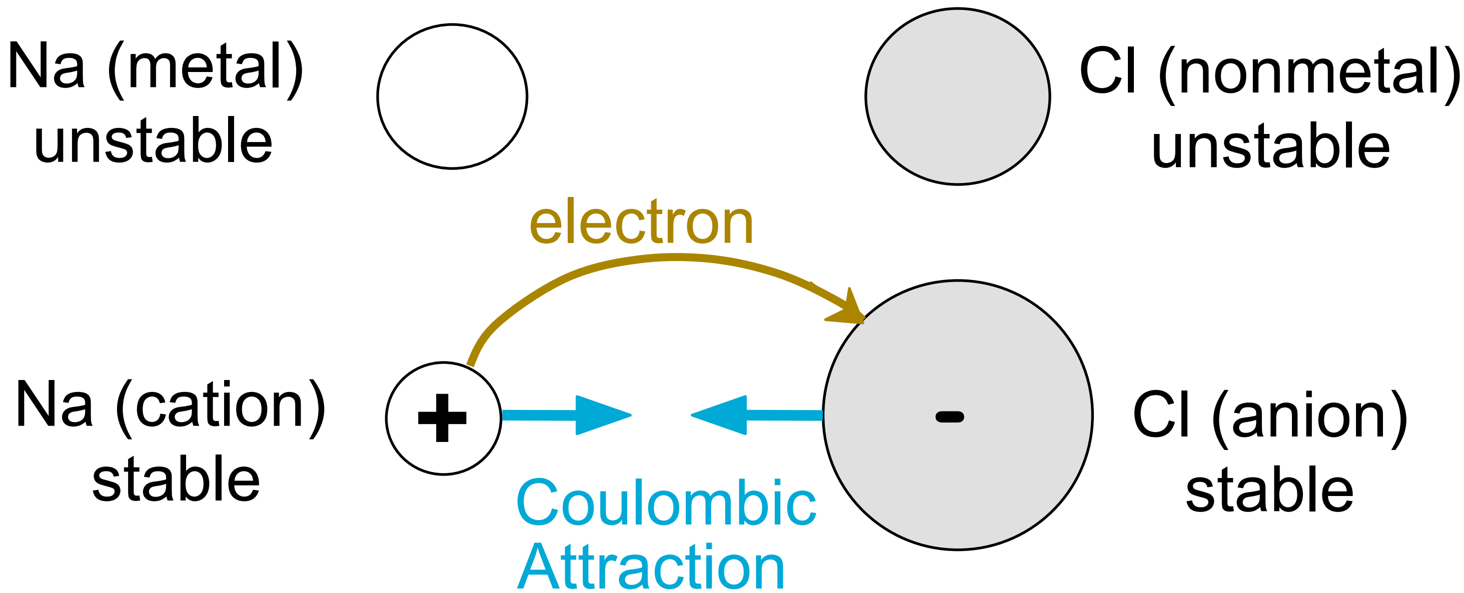
[Ne]

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

[Ne]

Ionic Bonding

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



Examples: Ionic Bonding

- Predominant bonding in Ceramics

NaCl

MgO

CaF_2

CsCl

IA	IIA	IIIB	IVB	VB	VIB	VIIB	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															

Give up electrons

Acquire electrons

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.

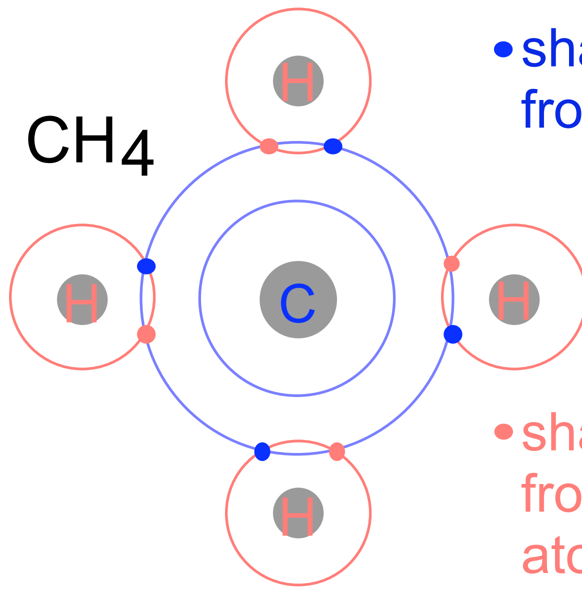
Covalent Bonding

- similar electronegativity ∴ share electrons
- bonds determined by valence – *s* & *p* orbitals dominate bonding
- Example: CH_4

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

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

Electronegativities are comparable.



- shared electrons from carbon atom
- shared electrons from hydrogen atoms

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

Primary Bonding

- Metallic Bond -- delocalized as electron cloud

- Ionic-Covalent Mixed Bonding

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

where X_A & X_B are Pauling electronegativities

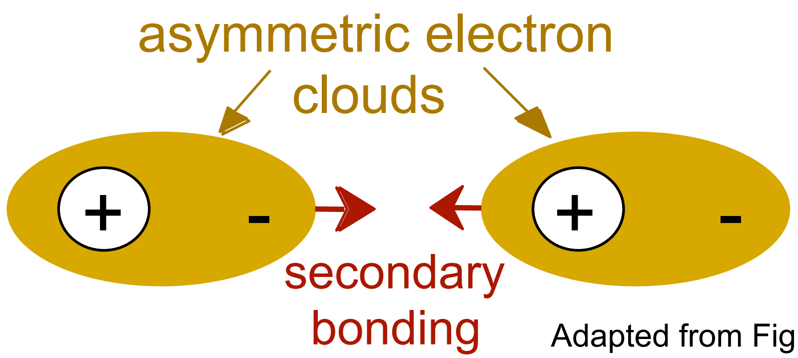
Ex: MgO $\quad X_{Mg} = 1.3$

$X_O = 3.5$

SECONDARY BONDING

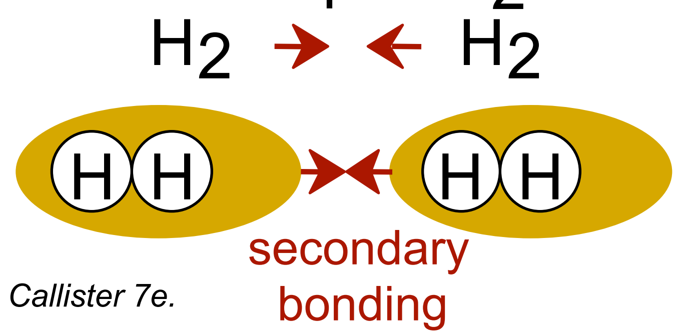
Arises from interaction between dipoles

- Fluctuating dipoles



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

ex: liquid H_2



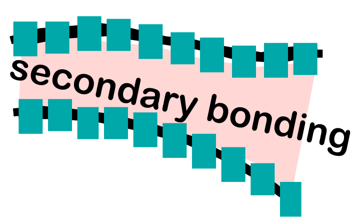
- Permanent dipoles-molecule induced

-general case:

Adapted from Fig. 2.14, *Callister 7e.*

-ex: liquid HCl

-ex: polymer



secondary bonding

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

Summary

- Atomic structure
- Electrons in atoms:
  - Bohr atomic and wave-mechanical model
  - Quantum numbers
  - Electron configuration
- Periodic table
- Bonding forces and energies
- Bondings

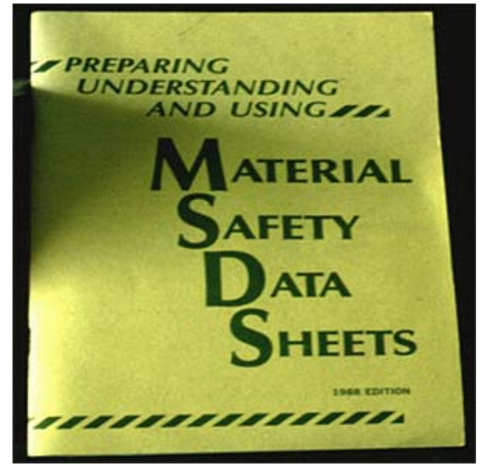
MSE LAB SAFETY POLICIES

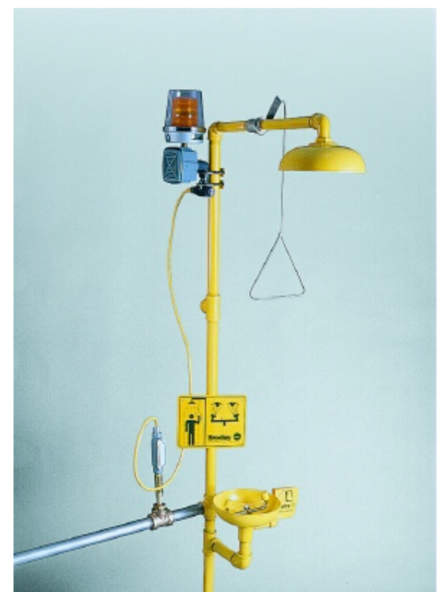
Fall 2009

Tuesday Kuykendall   MSE Dept. Safety Coordinator

YOUR PERSONAL SAFETY IS IMPORTANT

- Wear goggles & gloves and/or any other safety wear required for your project.
- Wear long pants and closed toed shoes.
- Know where the MSDS's are located and **read** them for the chemicals you use.
- Know where the chemical emergency wash and Fire extinguishers are located.





What's the big deal?

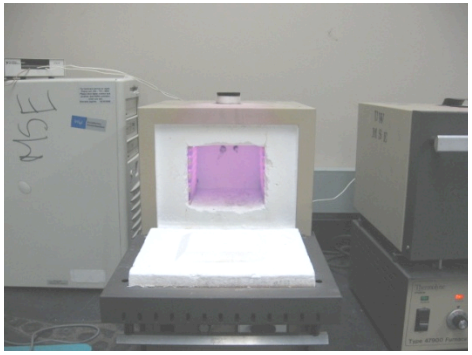
- Injuries occur when you least expect it.
- The safety glasses are required to prevent you from experiencing this:

EQUIPMENT SAFETY

Cold Rolling

Instr
on

Charpy



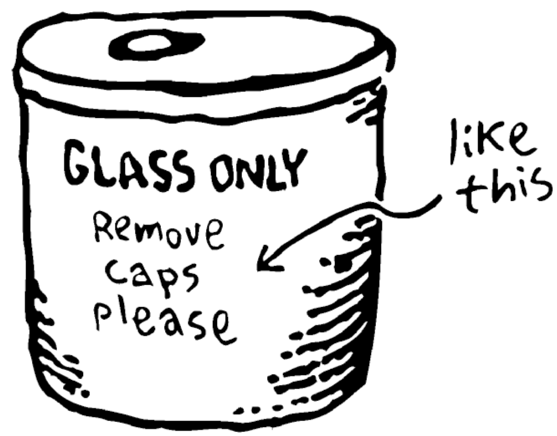
Furnac
es

General Housekeeping

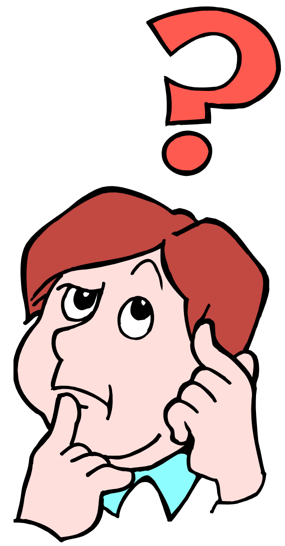
- **Clean up after yourself.**
- **Wash, Dry, and put away your glassware or any supplies.**
- **Put trash in the trash receptacles.**
- **Broken glass or sharps do not go in the trash.**
- **Don’t leave completed experiments or projects for someone else to pick up.**
- **Have the proper tools and materials before you start.**

SEWER,GLASS,& TRASH

- Be aware of what can and cannot go in the sink.
- Put glass waste in glass waste containers only
- Be aware of what can and cannot go in the trash. Razors and other sharp objects must go in a sharps container, not the trash.
- Lists are available in the lab safety notebook and online.



- If you don't know, ASK!



- No eating or drinking in the labs.
- Especially MUE 166