

# 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

Columns 1-10: Similar valence structure

IA		IIA												IIIA	IVA	VA	VIA	VIIA	0																
1	H	4	Be										5	B	6	C	7	N	8	O	9	F	10	Ne											
3	Li	12	Mg										13	Al	14	Si	15	P	16	S	17	Cl	18	Ar											
11	Na	20	Ca	21	Sc	22	Ti	23	V	24	Cr	25	Mn	26	Fe	27	Co	28	Ni	29	Cu	30	Zn	31	Ga	32	Ge	33	As	34	Se	35	Br	36	Kr
37	Rb	38	Sr	39	Y	40	Zr	41	Nb	42	Mo	43	Tc	44	Ru	45	Rh	46	Pd	47	Ag	48	Cd	49	In	50	Sn	51	Sb	52	Te	53	I	54	Xe
55	Cs	56	Ba	Rare earth series		72	Hf	73	Ta	74	W	75	Re	76	Os	77	Ir	78	Pt	79	Au	80	Hg	81	Tl	82	Pb	83	Bi	84	Po	85	At	86	Rn
87	Fr	88	Ra	Acti-nide series		104	Rf	105	Db	106	Sg	107	Bh	108	Hs	109	Mt	110	Ds																

Metal

Nonmetal

Intermediate

accept 2e

accept 1e

inert gases

Adapted from  
Fig. 2.6,  
Callister 7e.

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

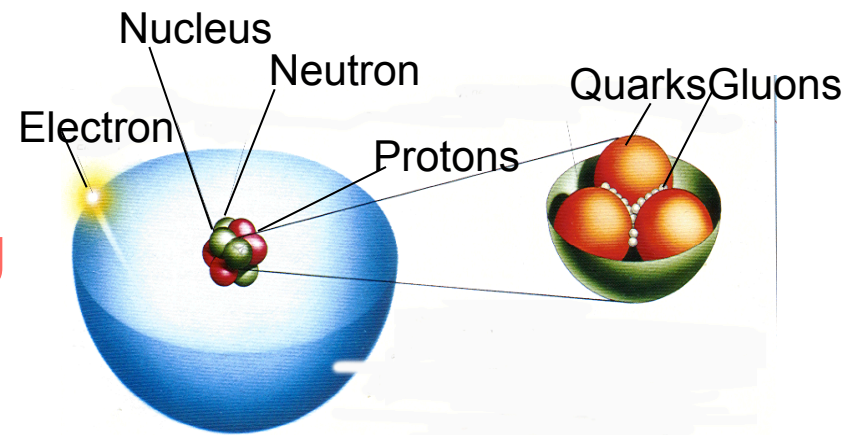
Electronegative elements:  
Readily acquire electrons  
to become - ions.



# Chapter 2: Atomic structure and interatomic bonding

## ❑ Fundamental concepts

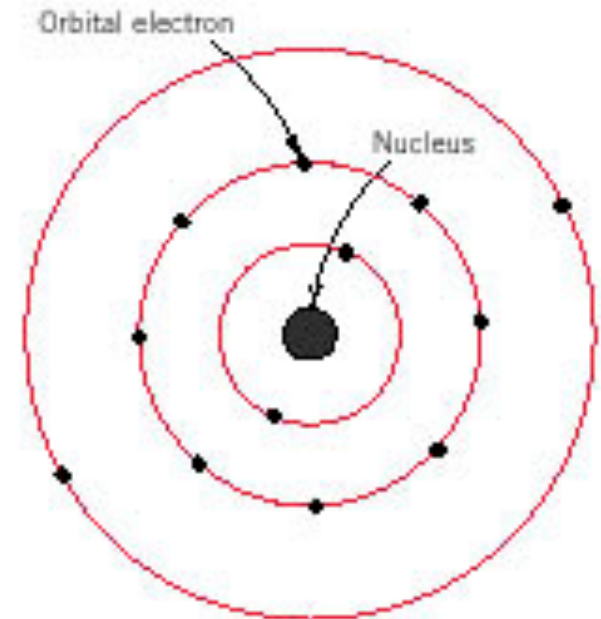
- Proton and electron, charged  $1.60 \times 10^{-19} \text{ C}$
- Mass of electron  $9.11 \times 10^{-31} \text{ kg}$
- Mass of protons and neutrons  
→  $1.67 \times 10^{-27} \text{ kg}$
- Atomic number: the number of protons
- Atomic mass = protons + neutrons
- Isotope
- Atomic mass unit (amu):  $1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



# Electrons in atoms

## ❑ Atomic models

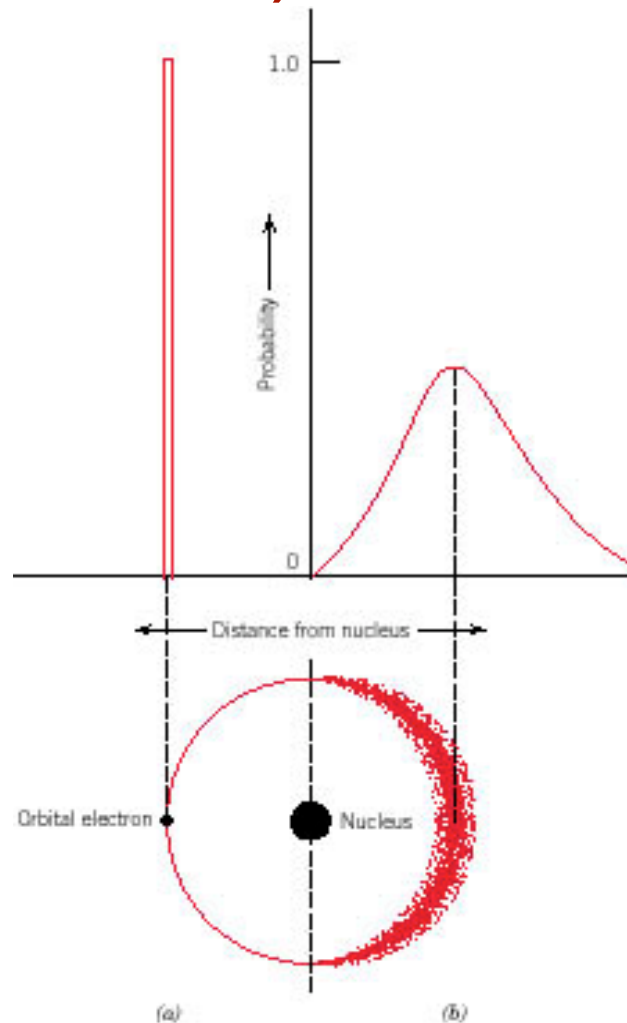
- Bohr atomic  
electrons revolve around the atomic nucleus in discrete orbital and the energies of electrons are quantized
- Wave-mechanical  
Electron exhibits both wavelike and particle-like characteristics, its position is considered to be a probability distribution



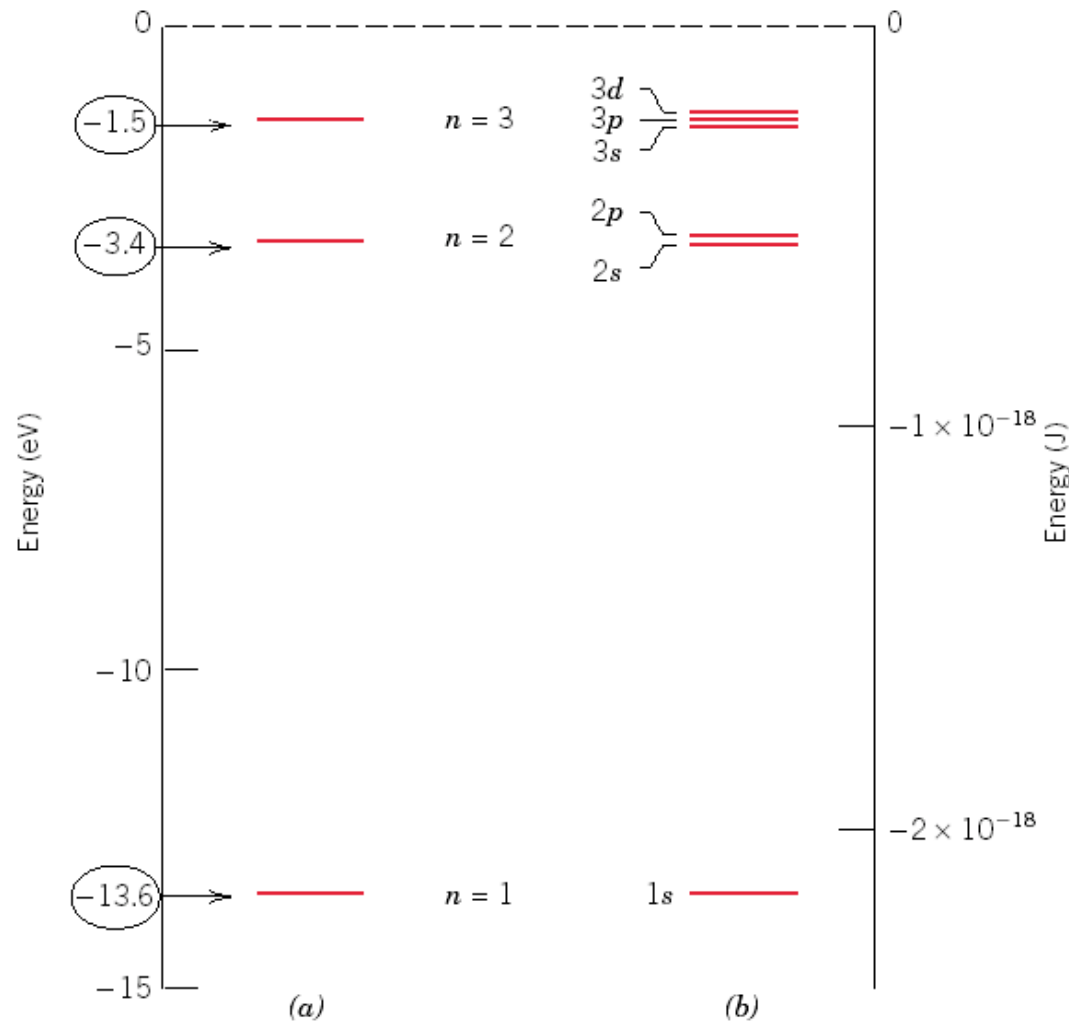
# Electrons in atoms (*continue*)

❑ 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  $n=1, 2 \dots$ ; K, L, M, N, O
- Orbital quantum number  $l=0, \dots, n-1$ ; subshell, s, p, d, or f; the shape of the electron subshell
- Spin moment  $m_s$   $1/2$  or  $-1/2$

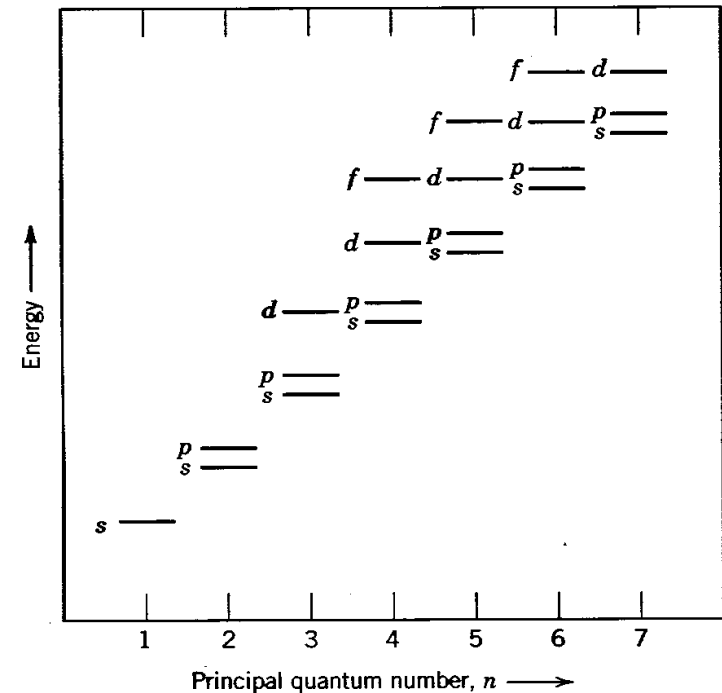
**Table 2.1** The Number of Available Electron States in Some of the Electron Shells and Subshells

<i>Principal Quantum Number <math>n</math></i>	<i>Shell Designation</i>	<i>Subshells</i>	<i>Number of States</i>	<i>Number of Electrons</i>	
				<i>Per Subshell</i>	<i>Per Shell</i>
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



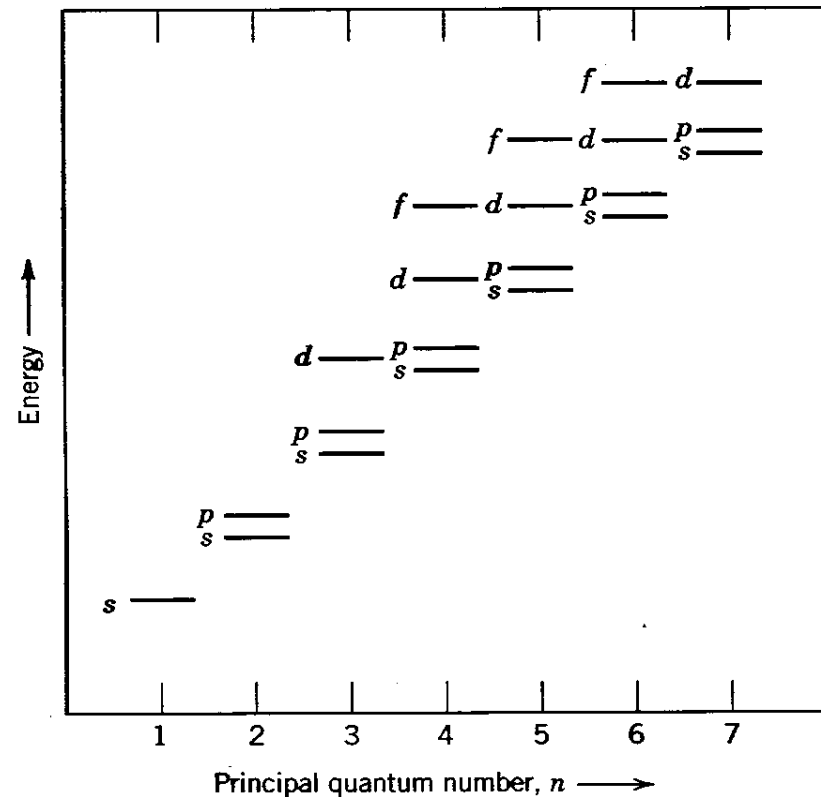
**Relative energies of the electrons for various shells and subshells**





# Electron configurations

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

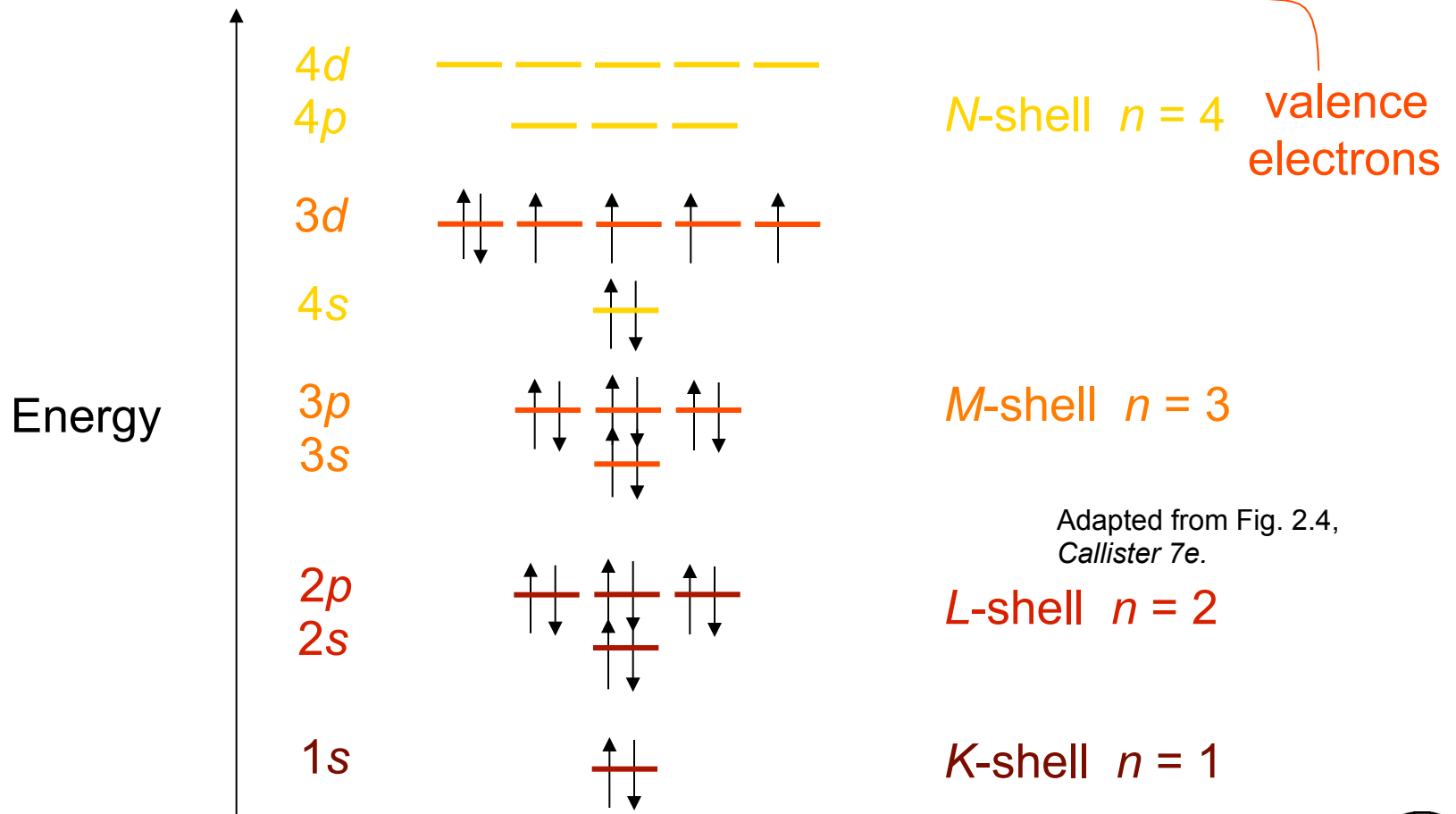


Relative energies of the electrons  
for various shells and subshells



# Electronic Configurations

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



Adapted from Fig. 2.4,  
Callister 7e.



# The Periodic Table

- Columns: Similar **Valence** Structure

Columns 1-3: Similar valence structure

IA	IIA											IIIA	IVA	VA	VIA	VIIA	0	
1	2											13	14	15	16	17	18	
H	He											B	C	N	O	F	Ne	
3	4											5	6	7	8	9	10	
Li	Be											Al	Si	P	S	Cl	Ar	
11	12	IIIB	IVB	VB	VIB	VIIA	VIII				IB	IIB	13	14	15	16	17	18
Na	Mg											Ga	Ge	As	Se	Br	Kr	
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
55	56	Rare earth series	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
87	88	Actinide series	104	105	106	107	108	109	110									
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds									

Metal

Nonmetal

Intermediate

accept 2e

accept 1e

inert gases

give up 1e

give up 2e

give up 3e

Adapted from  
Fig. 2.6,  
Callister 7e.

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

Electronegative elements:  
Readily acquire electrons  
to become - ions.



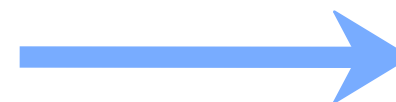
# Electronegativity

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

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

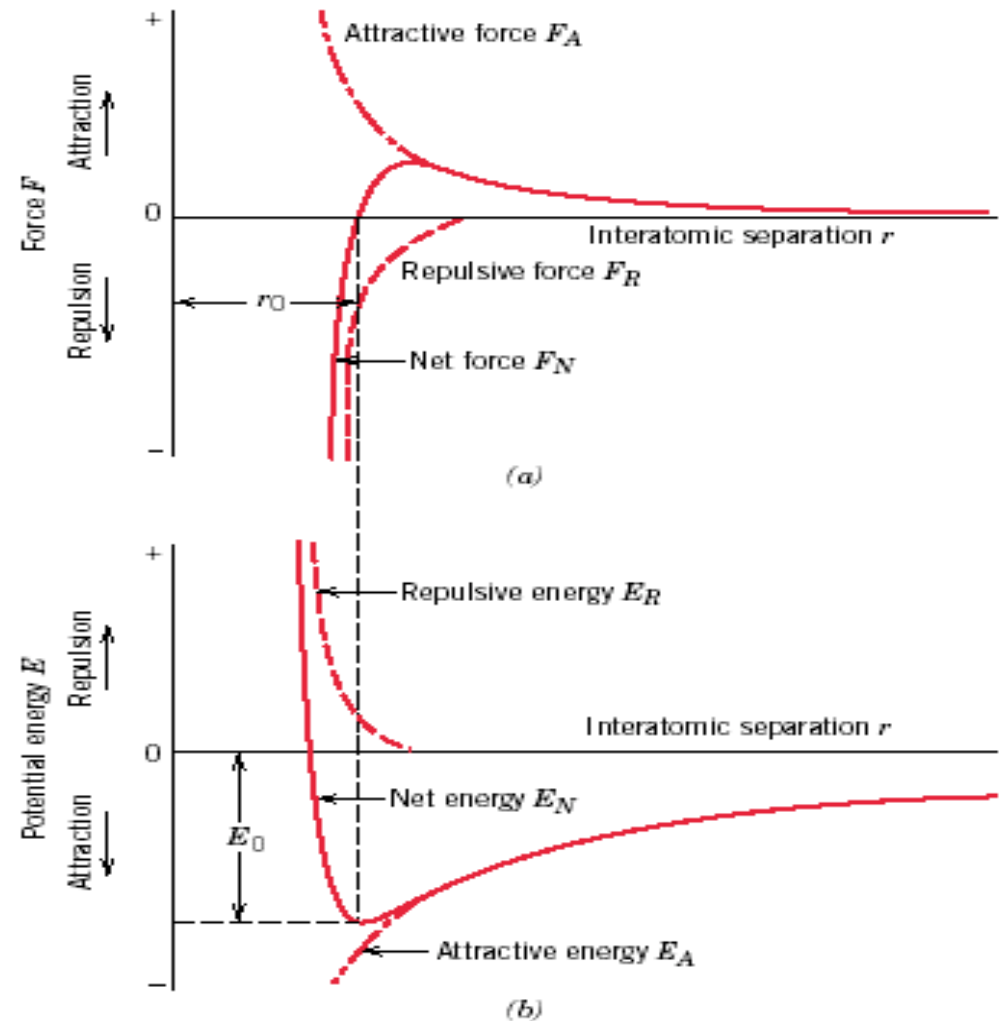
Adapted from Table 2.2,  
Callister 7e.

- 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

↑  
donates  
electrons

↑  
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<sup>2+</sup>  $1s^2 2s^2 2p^6$   
[Ne]

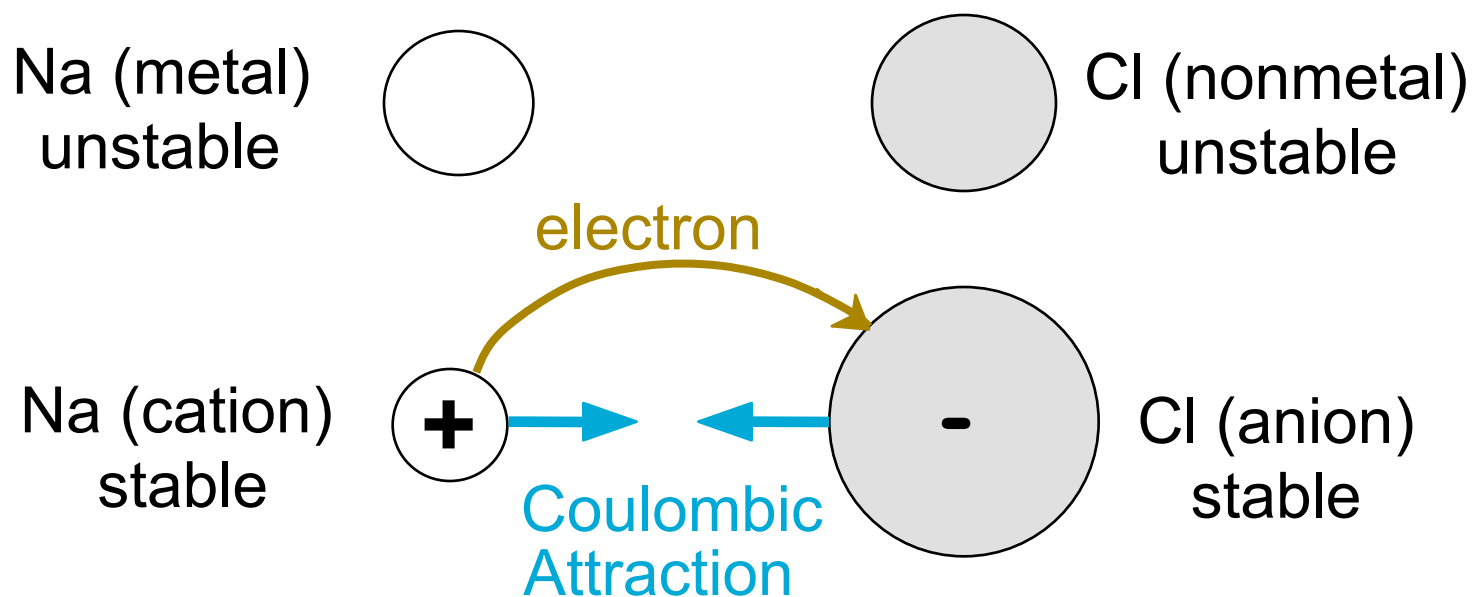
O<sup>2-</sup>  $1s^2 2s^2 2p^6$   
[Ne]





# Ionic Bonding

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



# Examples: Ionic Bonding

- Predominant bonding in **Ceramics**

Diagram illustrating the periodic table with arrows indicating the formation of ionic compounds:

- NaCl**: Arrow from Na (Group IA) to Cl (Group VIIA).
- MgO**: Arrow from Mg (Group IIA) to O (Group VIA).
- CaF<sub>2</sub>**: Arrow from Ca (Group IIA) to F (Group VIIA).
- CsCl**: Arrow from Cs (Group IA) to Cl (Group VIIA).

Below the periodic table, two large arrows indicate the direction of electron transfer:

- Give up electrons**: Red arrow pointing left (towards the left side of the periodic table).
- Acquire electrons**: Blue arrow pointing right (towards the right side of the periodic table).

IA																	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	IIIB	IVB	VB	VIB	VII B	VIII			IB	IIB	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar -				
K 0.8	Ca 1.0	Sc	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	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																			

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.)



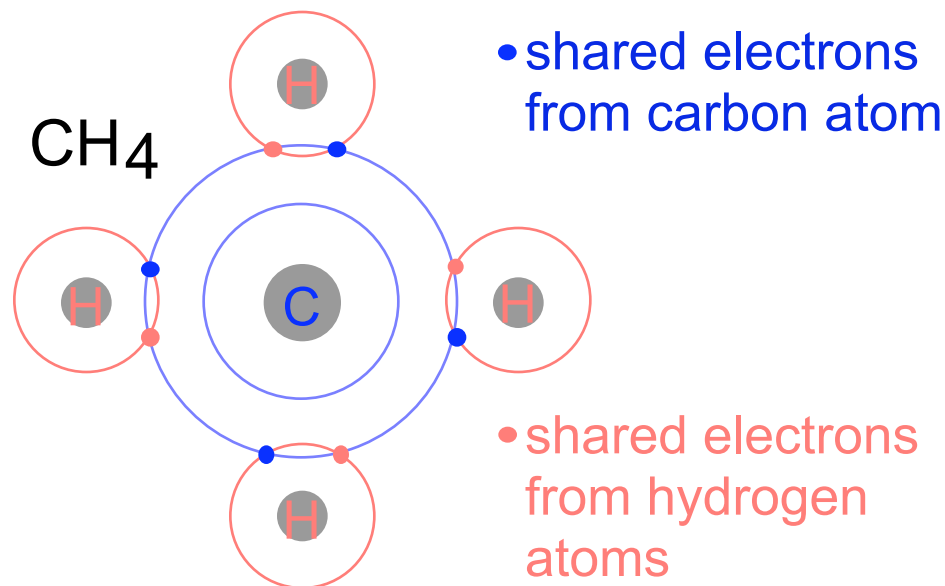
# Covalent Bonding

- similar **electronegativity**  $\therefore$  share electrons
- bonds determined by valence – *s* & *p* orbitals dominate bonding
- Example: CH<sub>4</sub>

C: has 4 valence e<sup>-</sup>,  
needs 4 more

H: has 1 valence e<sup>-</sup>,  
needs 1 more

Electronegativities  
are comparable.



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



# Primary Bonding

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

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

where  $X_A$  &  $X_B$  are Pauling electronegativities

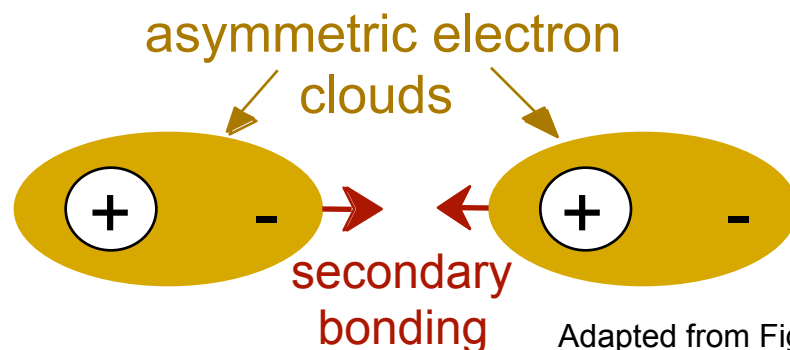
Ex: MgO

$$\begin{aligned} X_{\text{Mg}} &= 1.3 \\ X_{\text{O}} &= 3.5 \end{aligned}$$

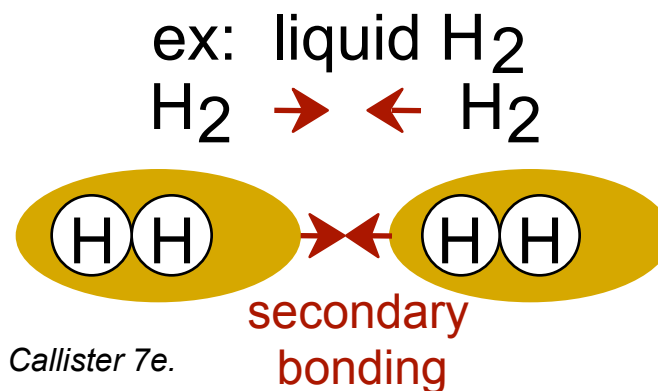
# SECONDARY BONDING

Arises from interaction between dipoles

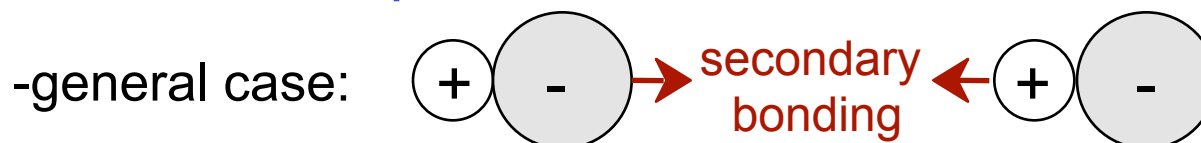
- Fluctuating dipoles



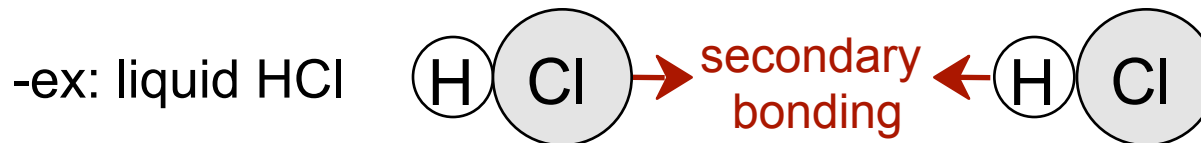
Adapted from Fig. 2.13, Callister 7e.



- Permanent dipoles-molecule induced



Adapted from Fig. 2.14, Callister 7e.



secondary bonding

# Summary: Bonding

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

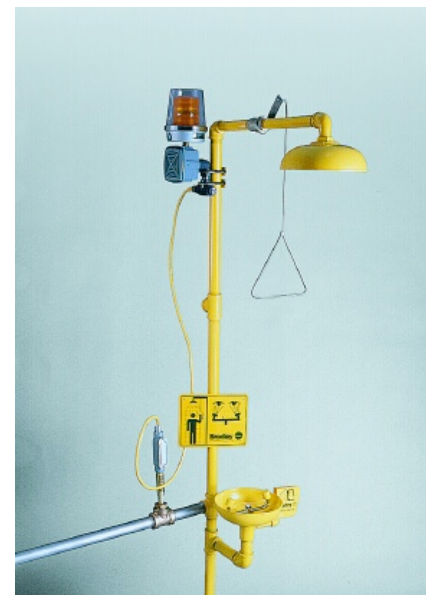
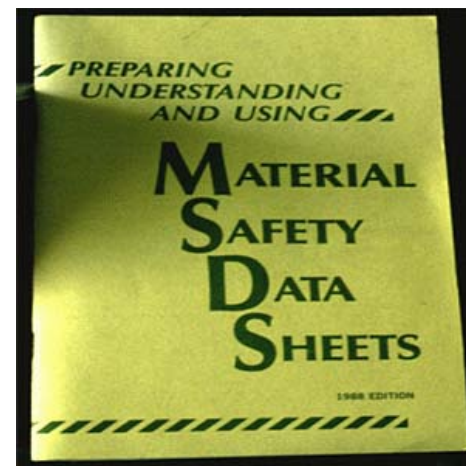
Tuesday Kuykendall MSE Dept. Safety Coordinator





# 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



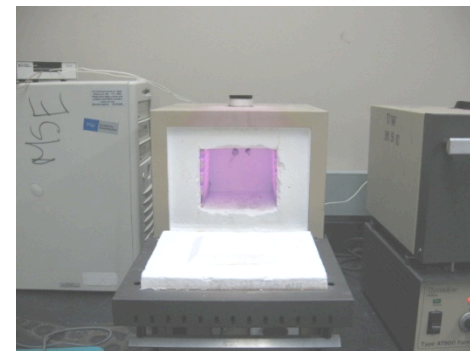
Cold  
Rolling



Instr  
on



Charpy

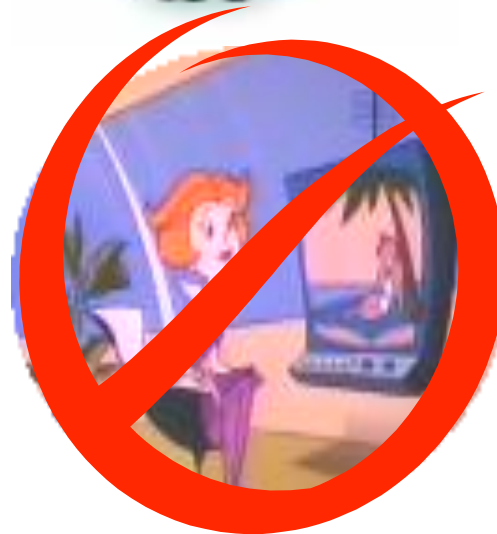


Furnac  
es



# 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

