MSE200

CHAPTER 2 Atomic Structure And Bonding

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Objectives: Structure of the atom, atomic numbers and atomic masses.

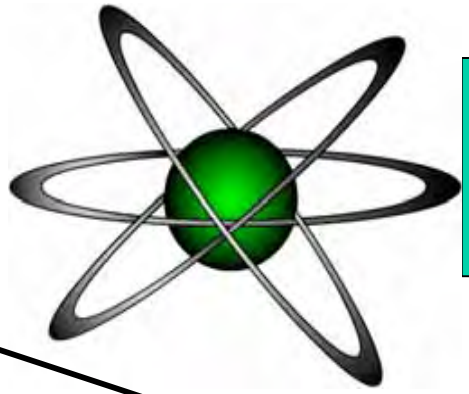
Electronic structure and electronic notations.

Interatomic forces and energies.

Types of atomic and molecular bonds: the ionic bond, the covalent bond, the metallic bond, and secondary bonds.

Structure of Atoms

ATOM
Basic Unit of an Element
Diameter : 10^{-10} m = 1Å
Neutrally Charged



Nucleus
Diameter : 10^{-14} m
Accounts for almost all mass
Positive Charge

Electron Cloud
Mass : 9.109×10^{-28} g
Charge : -1.602×10^{-19} C
Accounts for all volume

Proton
Mass : 1.673×10^{-24} g
Charge : 1.602×10^{-19} C

Neutron
Mass : 1.675×10^{-24} g
Neutral Charge

An atom is made of:

Atomic Number and Atomic Mass

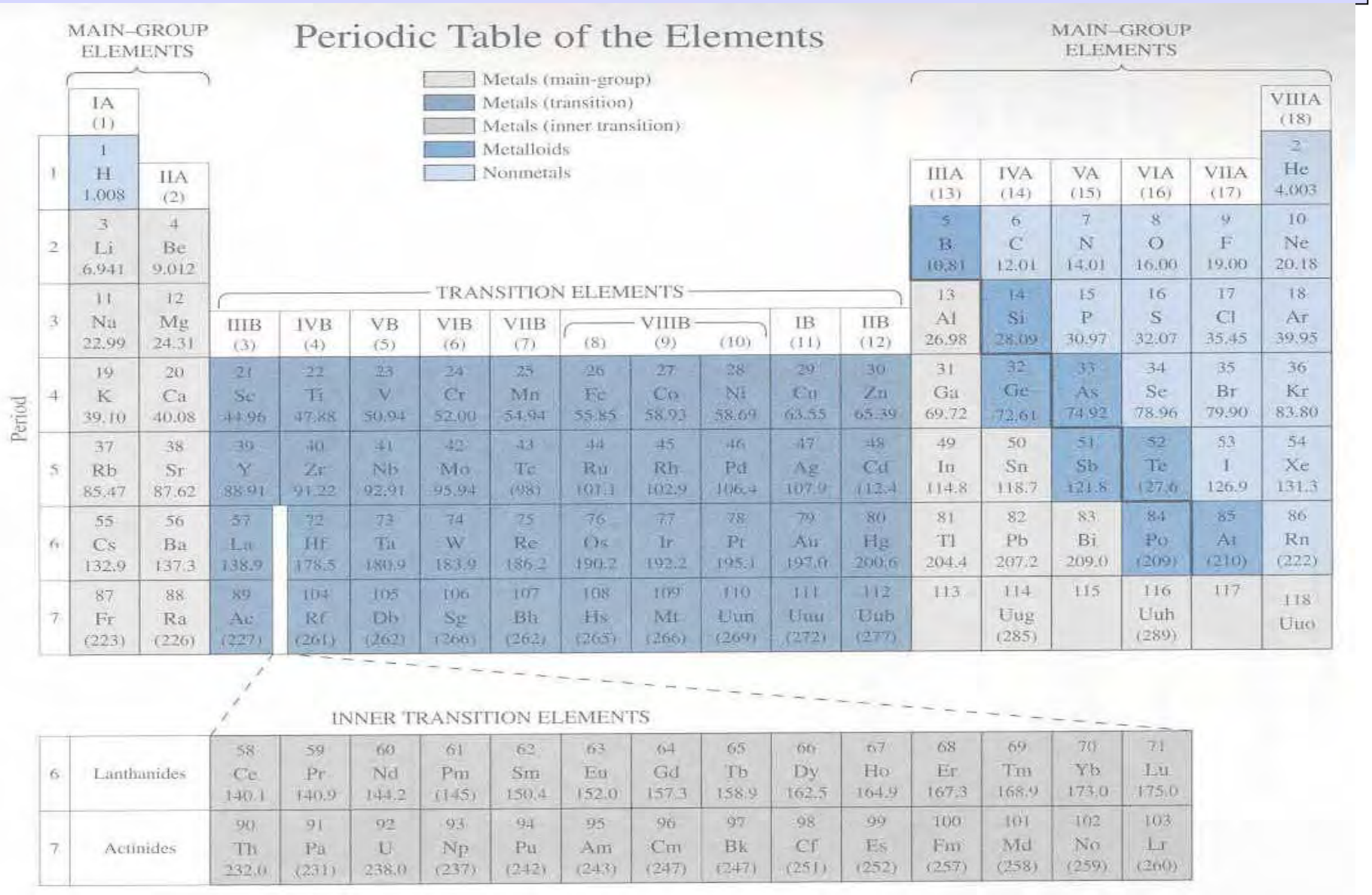
- **Atomic Number = Number of Protons in the nucleus**
  - **Examples:**

- **1 mole of atoms =** N_A = **6.023 x 10^{23} atoms (Avogadro's #)**

- **Meaning of the atomic mass in periodic table:**

Example: 2.1

Periodic Table

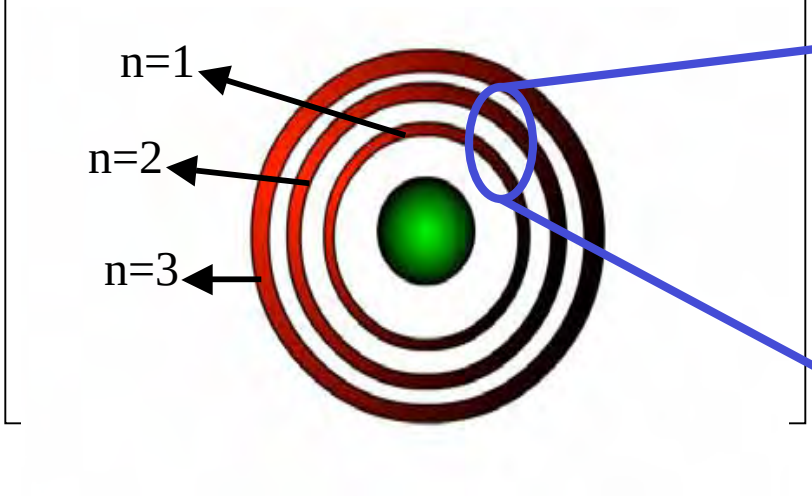


Source: Davis, M. and Davis, R., Fundamentals of Chemical Reaction Engineering, McGraw-Hill, 2003.

Quantum Numbers of Electrons of Atoms

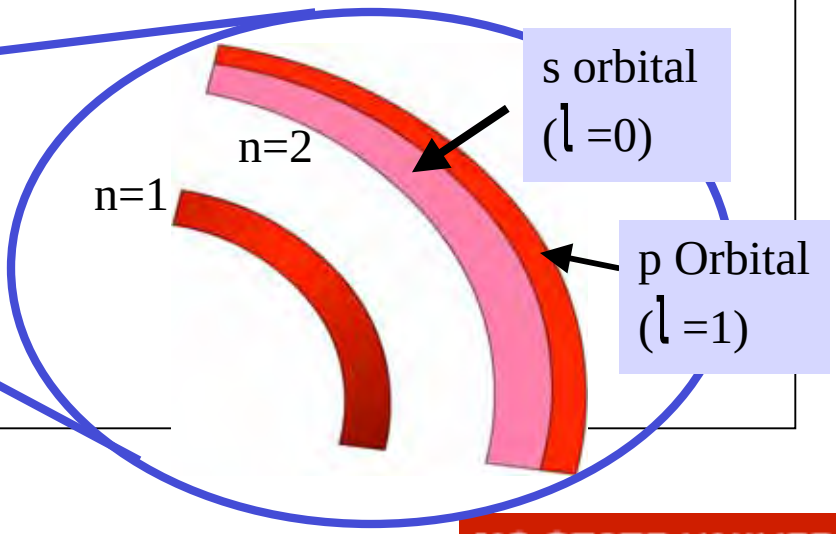
Principal Quantum Number (n)

- **Represents main energy levels.**
- **Range 1 to 7.**
- **Larger the 'n' higher the energy.**



Subsidiary Quantum Number l

- **Represents sub energy levels (orbital).**
- **l = 0, 1, 2, 3, 4…n-1.**
- **s, p, d, f, g……**



Quantum Numbers of Electrons of Atoms (Cont..)

Magnetic Quantum Number m_l.

- Represents spatial orientation of single atomic orbital.
- Permissible values are –l to + l.
- Example:- if l =1,

  m_l = -1,0,+1.

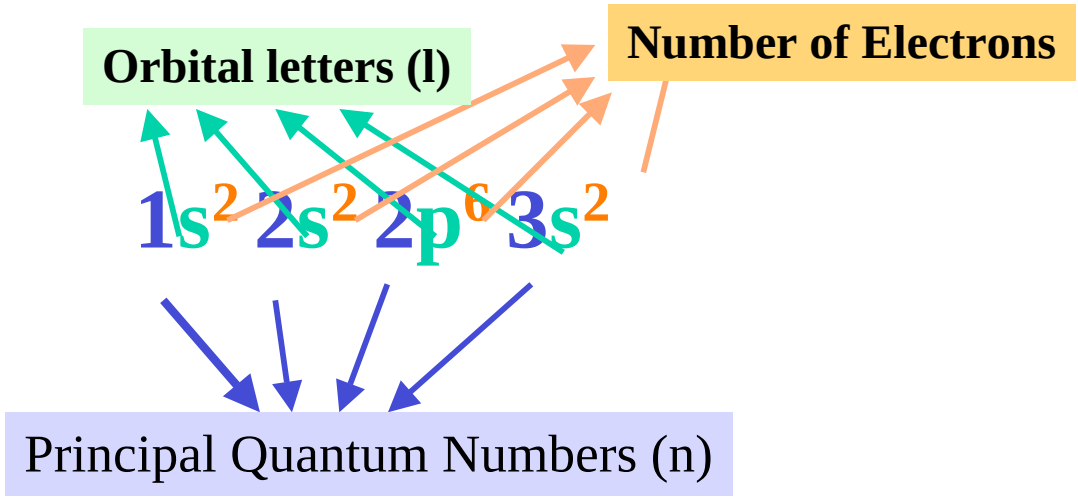
  i.e. 2 l+1 allowed values.
- No effect on energy.

Electron spin quantum number m_s.

- Specifies two directions of electron spin.
- Directions are clockwise or anticlockwise.
- Values are +1/2 or –1/2.
- Two electrons on same orbital have opposite spins.
- No effect on energy.

Electron Configuration

- **Electron Configuration lists the arrangement of electrons in orbits.**
  - ➢



Orbital energy levels and filling sequence

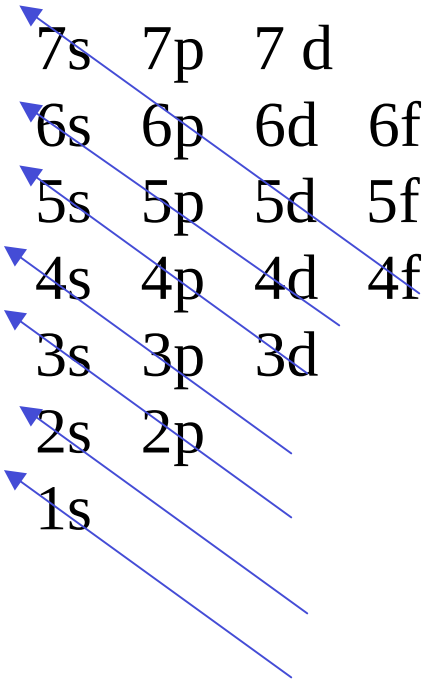
N = 1, 2, 3, 4, 5, 6, 7

l = 0, 1, 2, 3, 4…n-1.

s, p, d, f, g……

m_l = –l to + l, (2l + 1 total)

m_s = +1/2 or –1/2



l	s	p	d	f
# of orbits	1	3	5	7
max # of electrons	2	6	10	14

Electron Structure and Chemical Activity

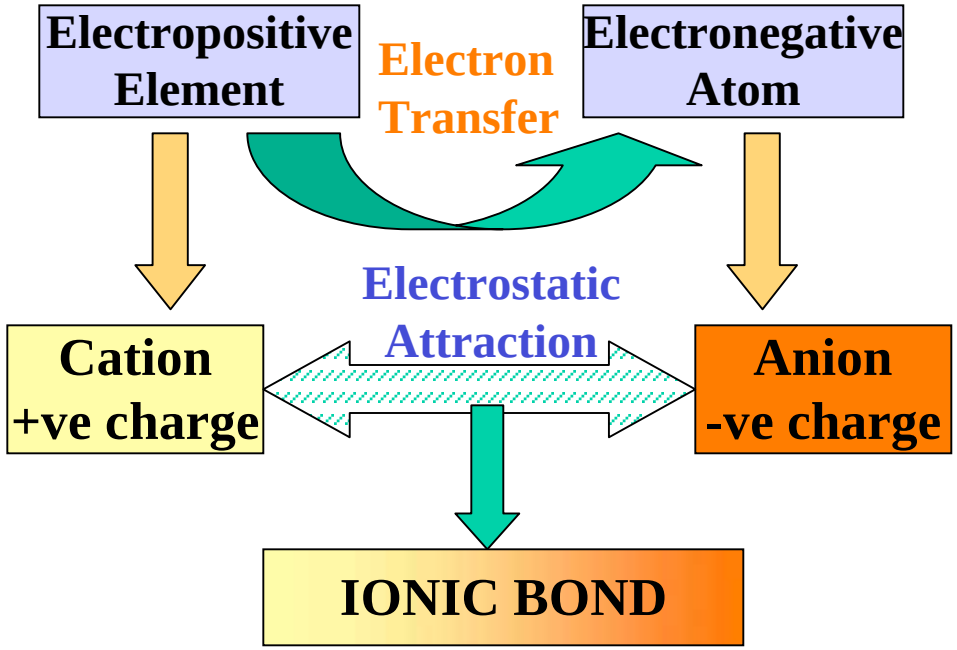
- **Except Helium, most *noble gasses* (Ne, Ar, Kr, Xe, Rn) are chemically very stable (outer shell filled)**
  - **All have s^2 p^6 configuration for outermost shell.**
  - **Helium has $1s^2$ configuration**
- **Electropositive elements give electrons during chemical reactions to form *cations***
  - **metals**
- **Electronegative elements accept electrons during chemical reaction to form anions**
  - **Non-metals**

Atomic and Molecular Bonds

- **Ionic bonds :- Strong atomic bonds due to transfer of electrons**
- **Covalent bonds :- Large interactive force due to sharing of electrons**
- **Metallic bonds :- Non-directional bonds formed by sharing of electrons**
- **Permanent Dipole bonds :- Weak intermolecular bonds due to attraction between the ends of permanent dipoles.**
- **Fluctuating Dipole bonds :- Very weak electric dipole bonds due to asymmetric distribution of electron densities.**

Ionic Bonding

- **It can form between metallic and nonmetallic elements.**
- **Electrons are transferred from electropositive to electronegative atoms**



Ionic Bonding - Example

- **Ionic bonding in NaCl**

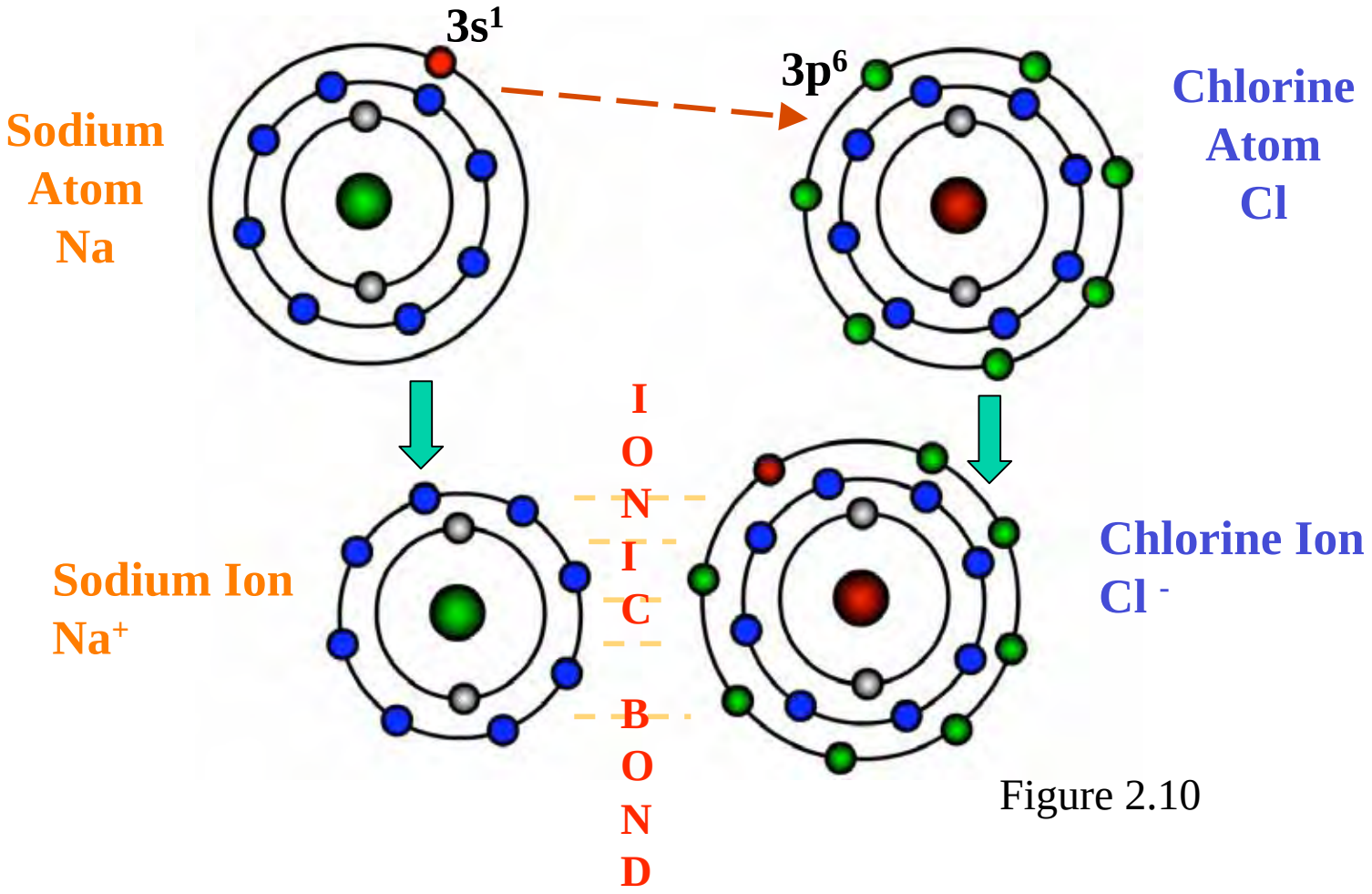
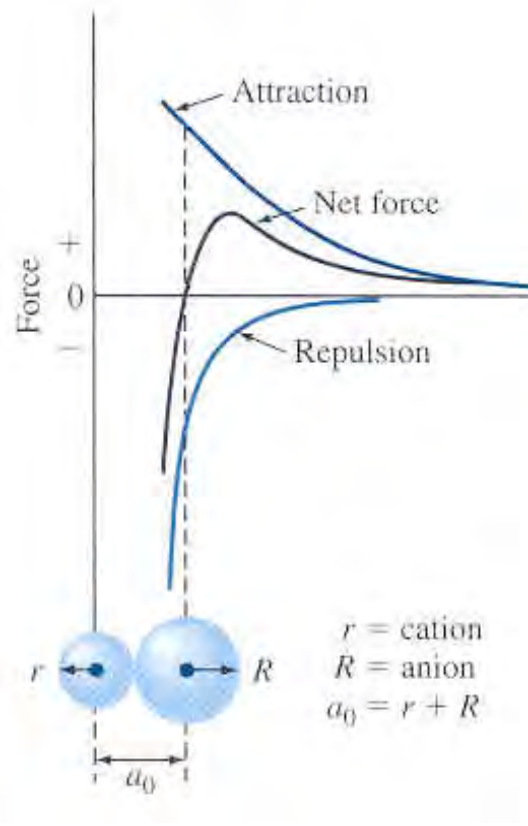
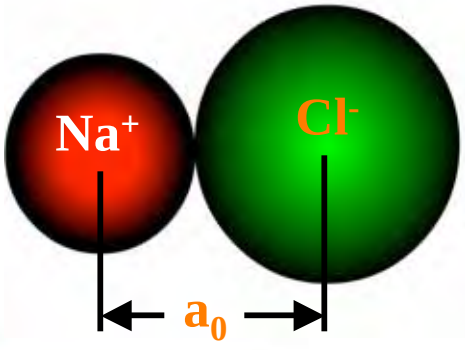


Figure 2.10

Ionic Force for Ion Pair

- **Nucleus of one ion attracts electron of another ion.**
- **The electron clouds of ion repulse each other when they are sufficiently close.**



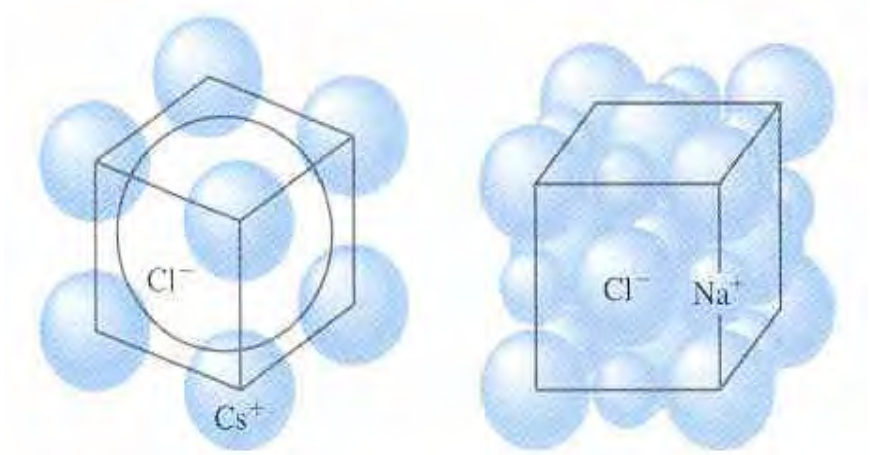


Force versus separation Distance for a pair of oppositely charged ions

Figure 2.11

Ion Arrangements in Ionic Solids

- **Ionic bonds are *Non Directional***
- **Geometric arrangements are present in solids to maintain electric neutrality.**
  - **Example:- in NaCl, six Cl- ions pack around central Na+**



CsCl **NaCl**

Ionic packing In NaCl and CsCl

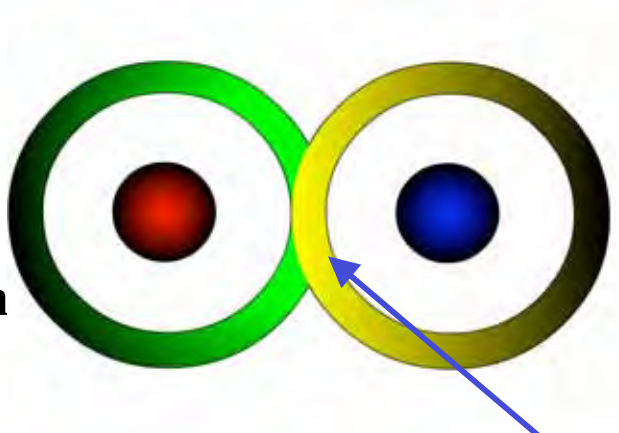
Figure 2.13

- **Lattice energies and melting points of ionically bonded solids are high**

http://video.google.com/videosearch?q=electron&hl=en&emb=0&aq=f#q=ionic&hl=en&emb=0

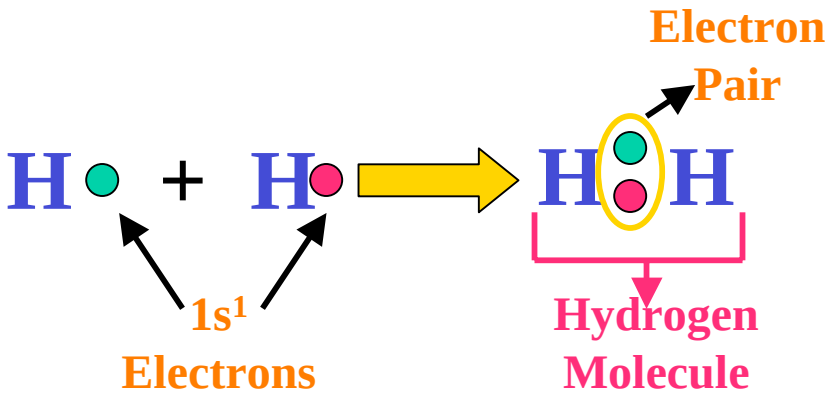
Covalent Bonding

- **In Covalent bonding, outer s and p electrons are shared between two atoms to obtain noble gas configuration.**
- **Takes place between elements with small differences in *electronegativity* and close by in periodic table.**
- **In Hydrogen, a bond is formed between $1s^1$ electrons**



Overlapping Electron Clouds

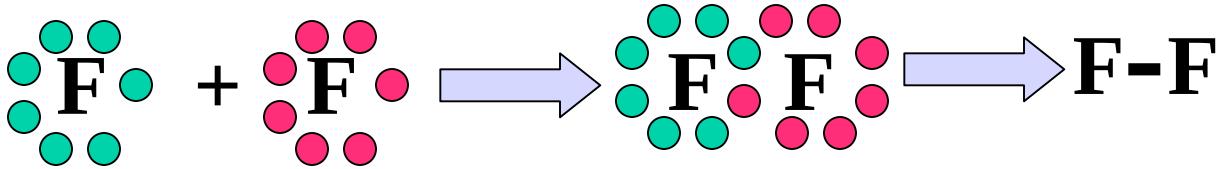
Directional



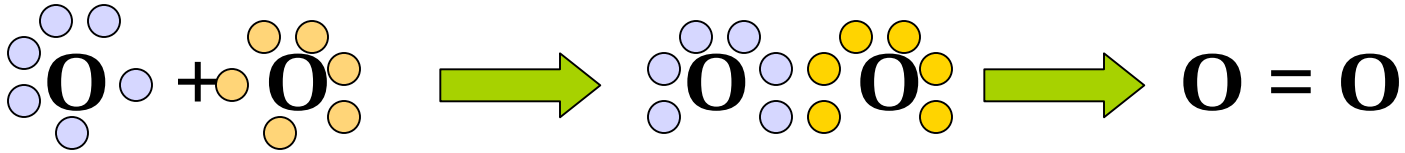
Determine the # of shared electrons

Covalent Bonding - Examples

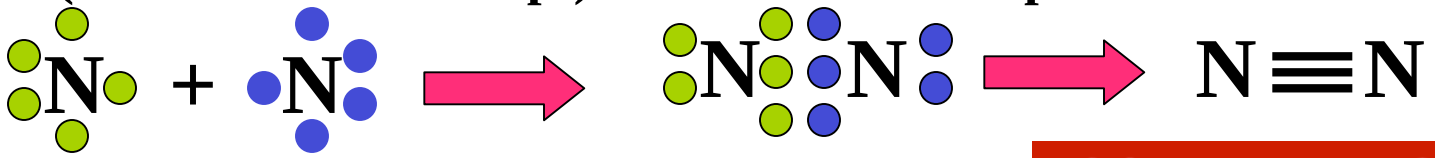
- **In case of F_2, O_2 and N_2, covalent bonding is formed by sharing p electrons**
- **Fluorine gas (Outer orbital – $2s^2\ 2p^5$) share one p electron to attain noble gas configuration.**



- **Oxygen (Outer orbital - $2s^2\ 2p^4$) atoms share two p electrons**



- **Nitrogen (Outer orbital - $2s^2\ 2p^3$) atoms share three p electrons**



Metallic Bonding

- **Atoms in metals are closely packed in crystal structure.**
- **Loosely bounded valence electrons are attracted towards nucleus of other atoms.**
- **Electrons spread out among atoms forming electron clouds.**
- **These free electrons are reason for electric conductivity and ductility**
- **Since outer electrons are shared by many atoms, metallic bonds are *Non-directional***

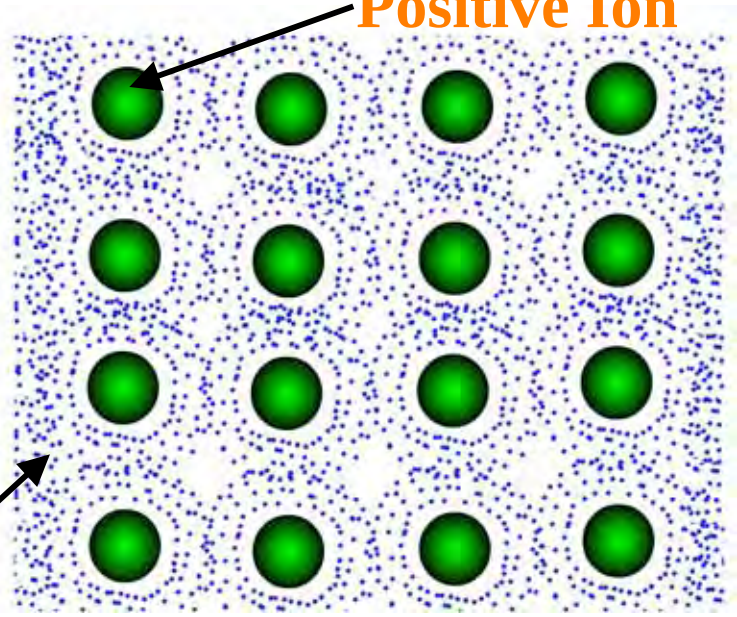


Figure 2.24

HW

- Example Problem: 2.2, 2.3, 2.6, 2.7
- Regular Problem, Chapter 2: 3, 5, 6, 12,
- Reading assignment for the next class: 3.1-3.5