#### **METALLURGY AND MATERIALS ENGINEERING (ME210)**

# Module 1

What is the difference between matter and material?

"Matter" is a broad word that applies to anything perceived or known to be occupying space (solid matter; gaseous matter; vegetable matter).

"Material" usually means some definite kind, quality, or quantity of matter, especially as intended for use (cotton material; explosive materials; a house built of poor materials)

#### What is Engineering materials?

There is a wide variety of materials available which have shown their potential in various engineering fields ranging from aerospace to house hold applications. The materials are usually selected after considering their characteristics, specific application areas, advantages and limitations.

a) Ferrous Metals

- b) Non-ferrous Metals (aluminum, magnesium, copper, nickel, titanium)
- c) Plastics (thermoplastics, thermosets)
- d) Ceramics and Diamond
- e) Composite Materials
- f) Nano-materials

#### **Universe-image**

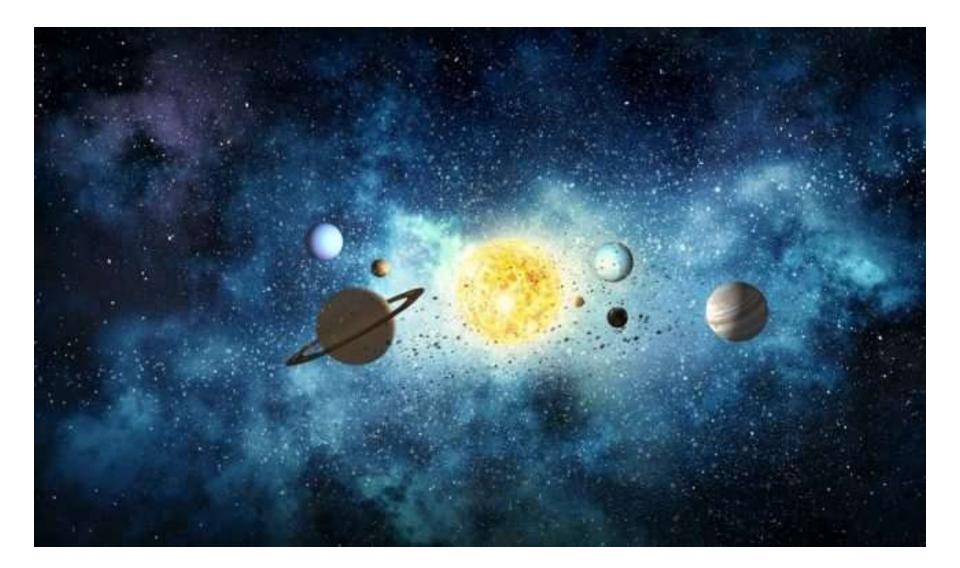


This NASA/ESA Hubble Space Telescope image shows the spiral galaxy NGC 3021 which lies about 100 million light-years away in the constellation of Leo Minor (The Little Lion)

#### Galaxy-Image



#### **Solar System-Artistic impression**

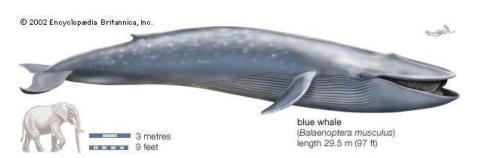


#### **Planet Earth**





#### Living and Non-Living





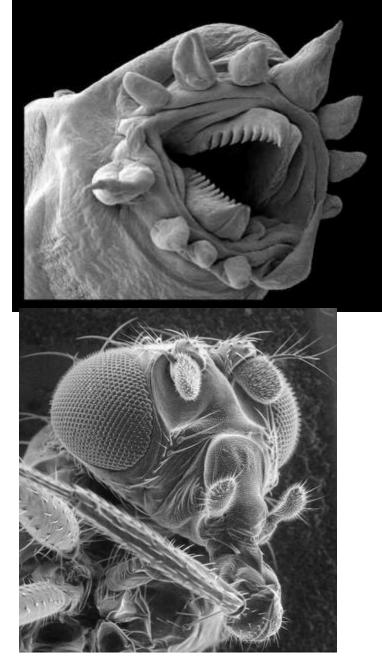


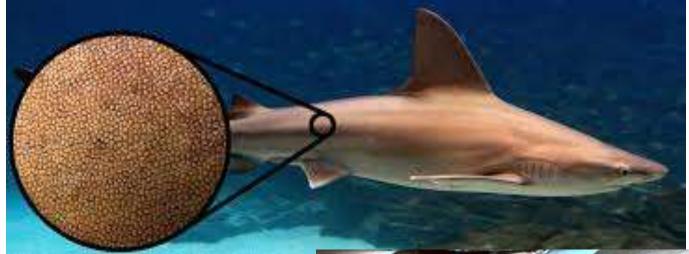


#### Micro level image

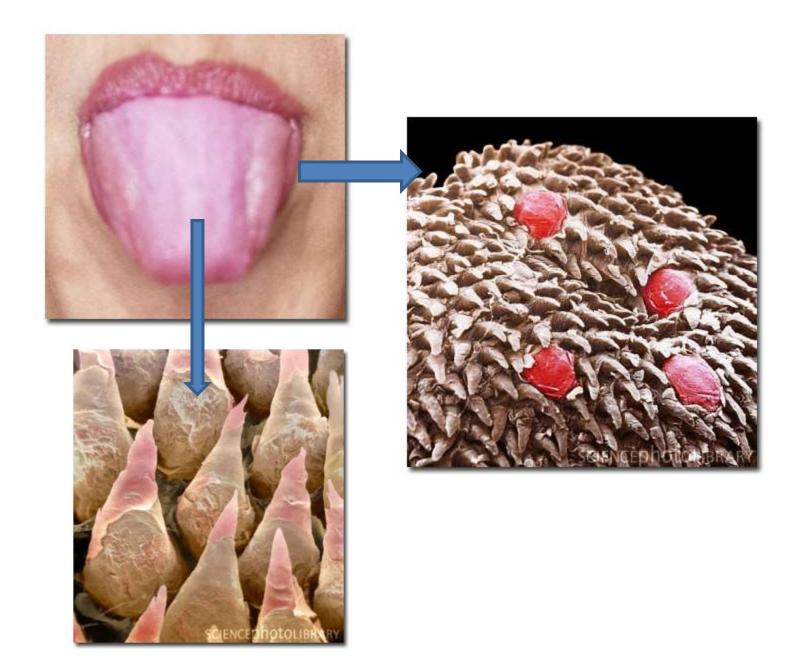






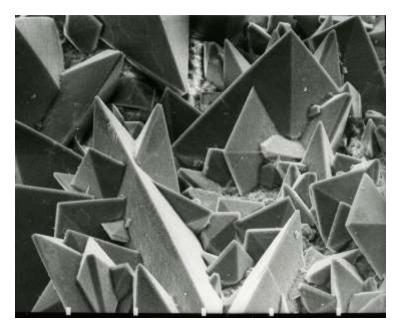


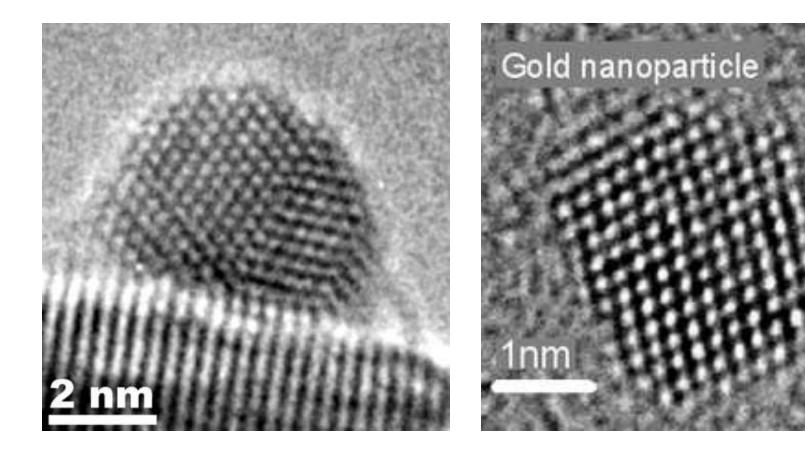


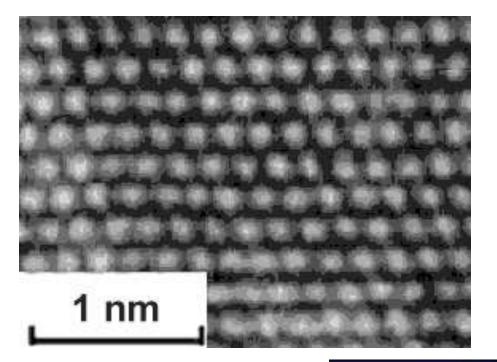






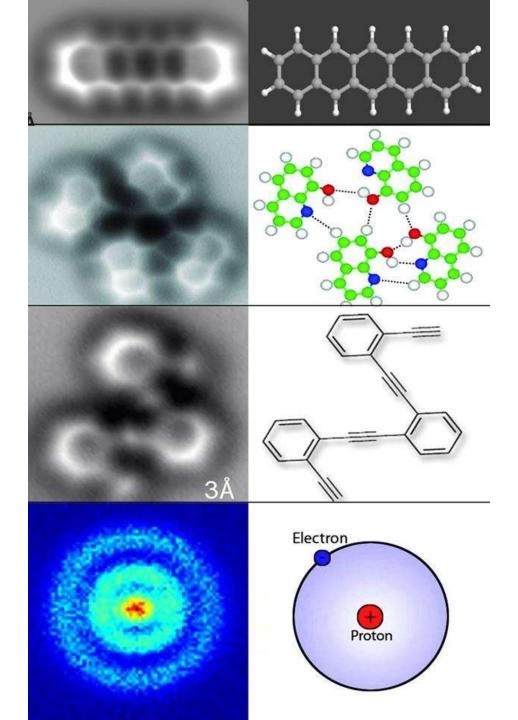


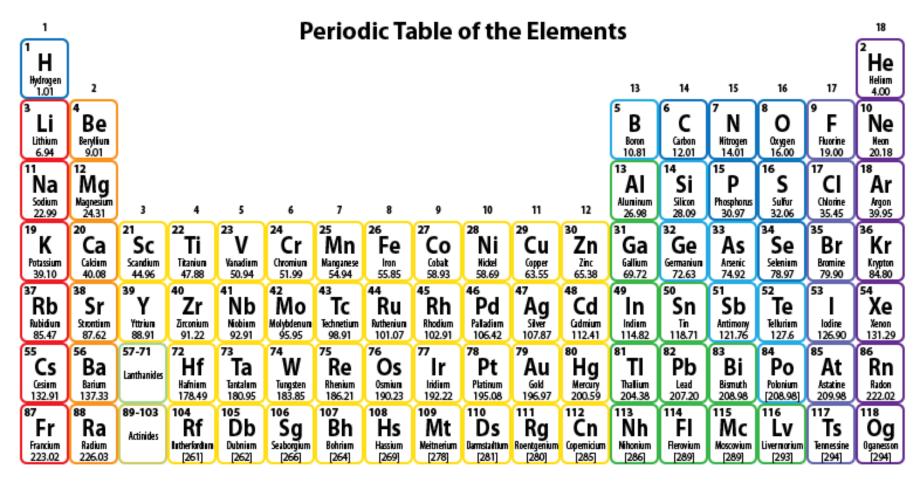




# This is a hydrogen atom.

This photograph shows the atom's electron orbital - the first time we have ever been able to observe the wave function of an atom. To capture this image scientists used a quantum microscope, a device capable of seeing into the quantum realm.





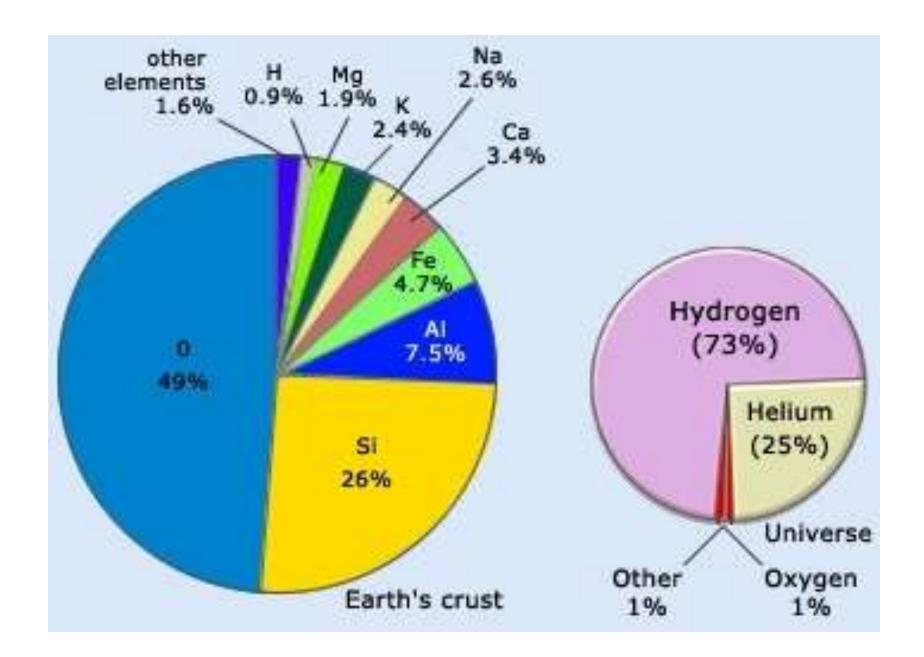
57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Lanthanum	Cerium	Praseodymium	Neodymium	Pronethiun	Samarium	Erropiun	Gadolinism	Tertiun	Dysprosium	Holmium	Erbium	Thuiun	Ytterbium	Lutetium
138.91	140.12	140.91	144.24	144.91	150.36	151.96	157.25	158.93	162.50	164.93	167.26	168.93	173.06	174.97
89	90	91	92	93	94	95	96	97	98	99	100	101	102	103
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
Actinium	Thorium	Potactinium	Uranium	Neptunium	Plutoniun	Americium	<sup>Curium</sup>	Berkelium	Californium	Einsteiniun	Fermiun	Mendelevium	Hobelium	Lawrencium
227.03	232.04	231.04	238.03	237.05	244.06	243.06	247.07	247.07	251.08	[254]	257.10	258.10	259.10	[262]

Noble Gas

Lanthanide

Alkali Metal	Alkaline Earth

id Konmetal Halogen



## **Atomic Structure**

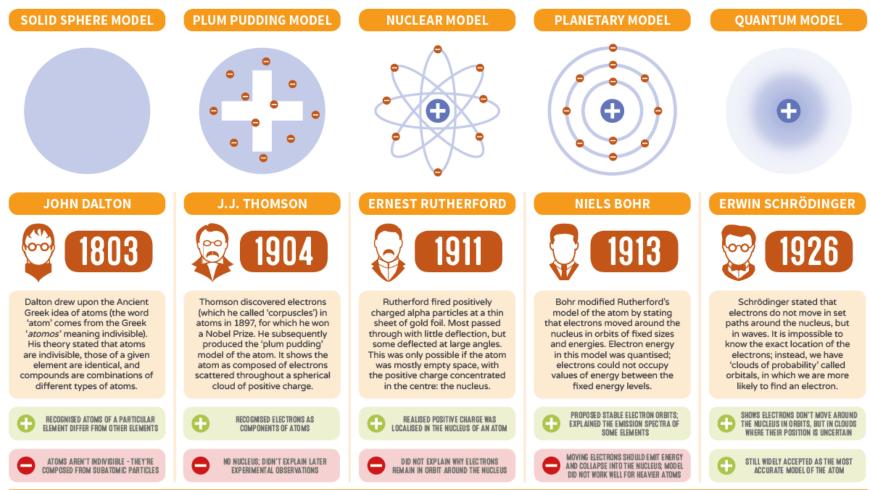
- Implies the system of electrons, protons, neutrons, etc., making up an individual atom.
- Every atom consists of a small nucleus composed of protons and neutrons, which is encircled by moving electrons in their orbitals, specific energy levels.
- The top most ortibal electrons, valence electrons, affect most material properties that are of interest to engineer. E.g.: chemical properties, nature of bonding, size of atom, optical/magnetic/electrical properties.

- Electrons and protons are negative and positive charges of the same magnitude being 1.60x10<sup>-19</sup> coulombs.
- > Neutrons are electrically neutral.
- Protons and neutrons have approximately the mass, 1.67x10<sup>-27</sup> kg, which is larger than that of an electron, 9.11x10<sup>-31</sup> kg.
- Atomic number (Z) is the number of either electrons or protons.
- Atomic weight is the total weight of protons and neutrons within the nucleus.
- Atomic weight is expressed in grams per gram-atom. One gramatom always contains 6.02 x 10<sup>23</sup> atoms (Avogadro's number).

# Atom models

#### **A HISTORY OF THE ATOM: THEORIES AND MODELS**

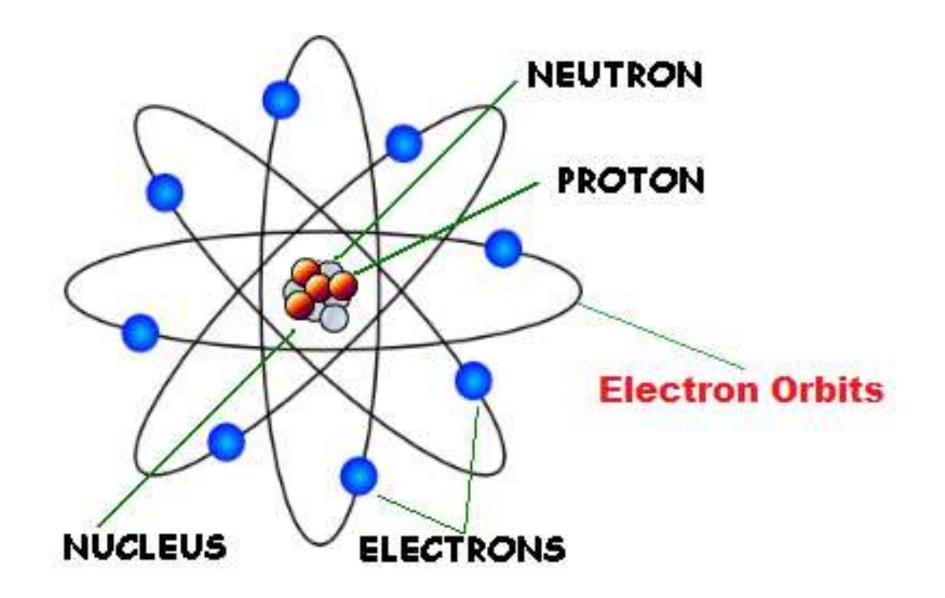
How have our ideas about atoms changed over the years? This graphic looks at atomic models and how they developed.



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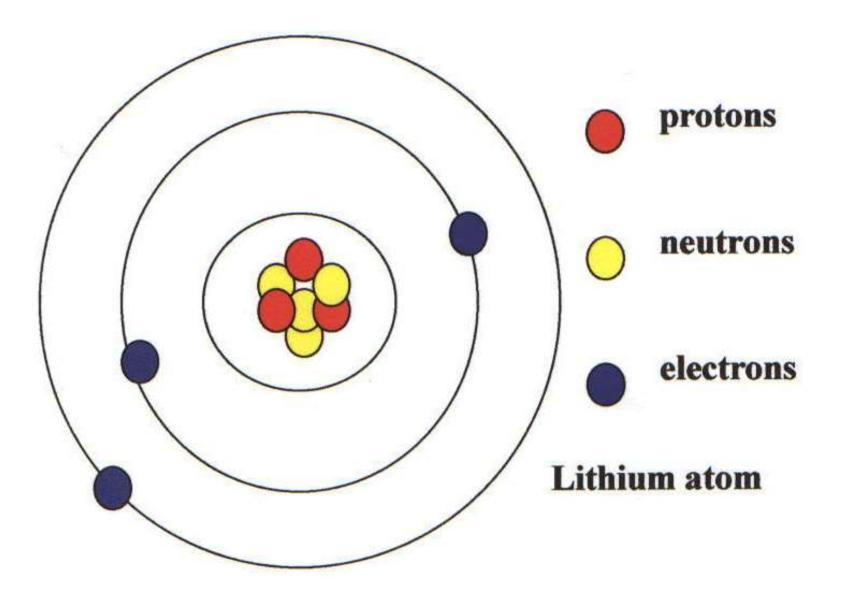
## Rutherford's Atomic Model

- Devised by Ernest Rutherford
- Proposed his atomic model by differential scattering experiments
- An atom consists of a nucleus of radius 10<sup>-12</sup> cm surrounded by planetary electrons of radius 10<sup>-13</sup> cm at distances relatively greater as compared to the diameter of the electrons
- he assumed that force of attraction between the electrons and the nucleus was balanced by the centrifugal force attained by electrons due to their rotational motion
- He suggested that electrostatic attraction between two opposite charges was responsible for holding the atoms together



## **Bohr Atomic Model**

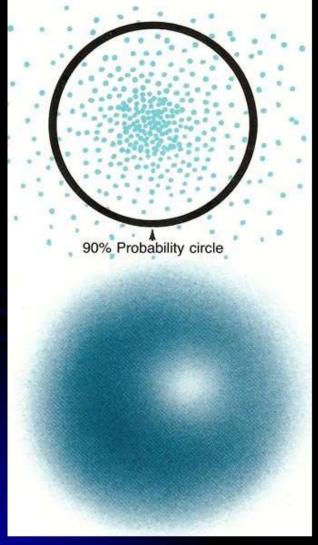
- Electrons are assumed to revolve around the atomic nucleus in discrete orbitals or quantum states
- > Each quantum state represents discrete level of energy
- Electrons may shift from shell to shell from a lower energy shell to a higher energy shell with absorption of energy and from higher to a lower with emission of energy



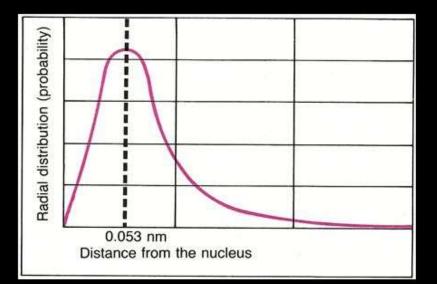
## Wave – Mechanical Atomic Model

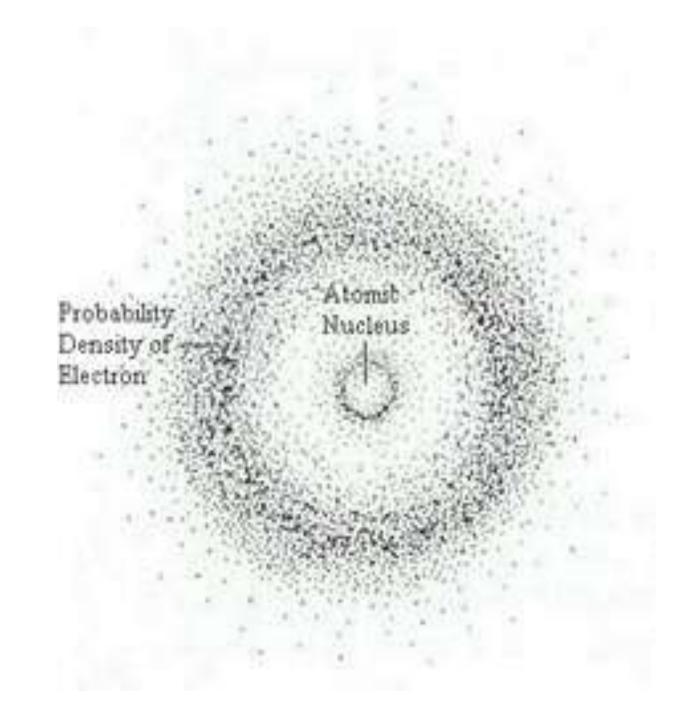
- An electron is considered to exhibit both particle like and wave like characteristics
- ➤The position of an electron is specified not in terms of the discrete orbitals but the position is considered to be the probability of an electron being at various locations around the nucleus

# Wave Mechanical Model



The location of the electron in a hydrogen atom is a probability distribution.





#### **Quantum numbers**

➢ Using the principles of wave mechanics every electron in an atom is characterised by four parameters called quantum numbers designated as n, l, m₁ and m₅

➤ n - principal quantum no.

- Related to the energy of an electron in a particular state
- Defines the place of an electron orbital or the size of the electron probability density
- Can take values 1,2,3,4,5 etc.
- Larger the values of n, the farther away is the orbital from the nucleus

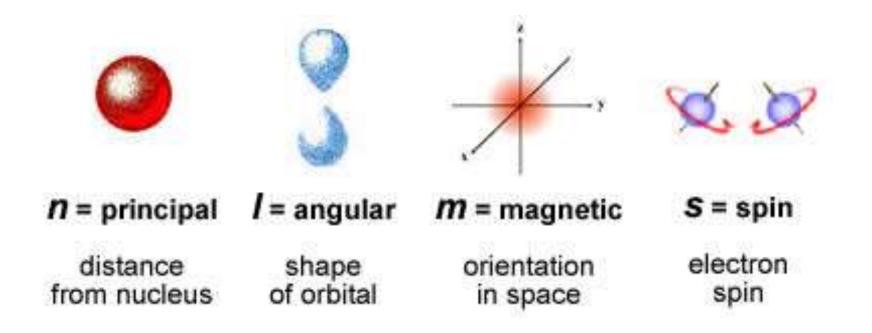
➤ I – orbital angular momentum quantum no.

- Related to the shape of an electron orbital
- Can take values 0 to n-1
- Letters s, p, d, f,g and h to represent the values of I
  = 0,1,2,3,4 and 5
- They defines the suborbital and their energy levels
- ➤ m<sub>I</sub> magnetic quantum no.
  - Defines the spacial orientation of the electron probability density cloud
  - Can take values I to +I including zero
  - So there will be 2 l +1 values for m<sub>l</sub>

#### $\succ$ m<sub>s</sub> - spin quantum no.

- Defines the spin of the electron on its own axis
- Two possible spins spin up and spin down

• 
$$m_s = + \frac{1}{2}$$
 and  $m_s = -\frac{1}{2}$ 



## **Electron Configuration**

- ➢ Pauli exclusion principle is used
  - No two electrons can have the same set of quantum numbers

> For an element having one electron in its atom

• 
$$n=1$$
,  $\ell=0$ ,  $m_l=0$ ,  $m_s=+\frac{1}{2}$  or  $-\frac{1}{2}$ 

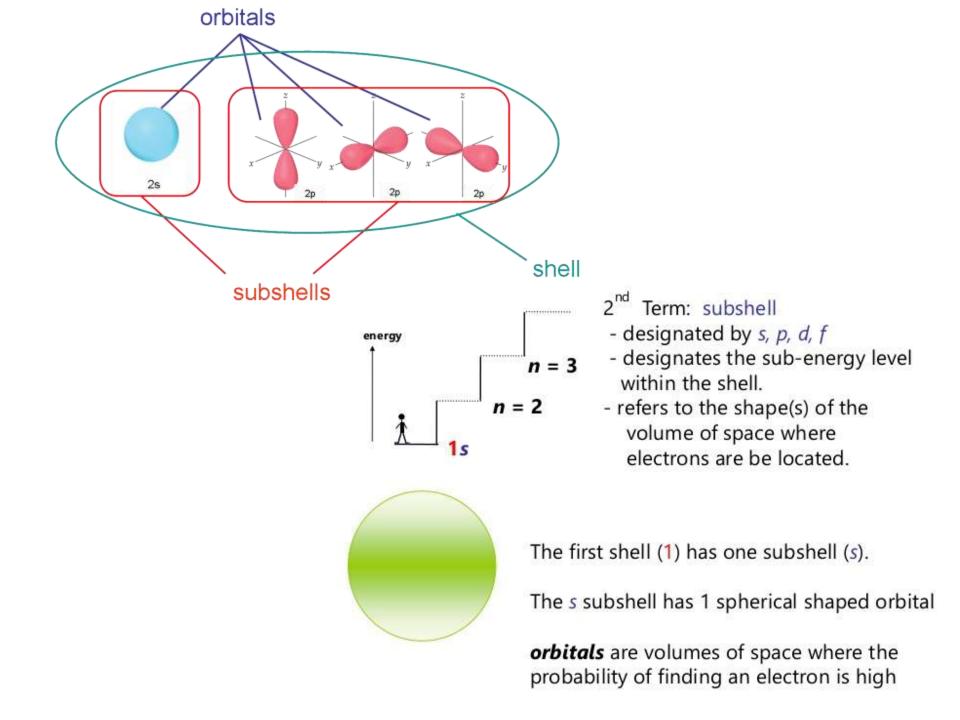
- For Hydrogen  $1s^1$
- For Lithium  $-1s^2 2s^1$
- For Neon  $1s^2 2s^2p^6$

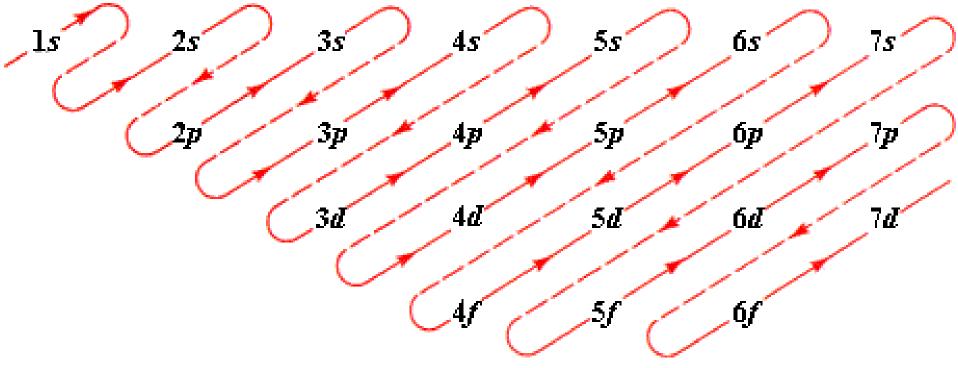
#### In Bohr atomic model the main electron shells

are designated by letters K,L, M, N, O, P, and Q

with principal quantum nos., n = 1,2,3,4,5,6

and 7

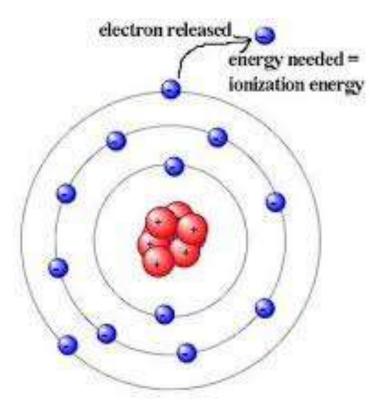




1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d 6p 7s 5f 6d 7p

# **Ionization Energy**

The **ionization energy** (IE) is qualitatively defined as the amount of **energy** required to remove the most loosely bound electron, the valence electron, of an isolated gaseous atom to form a cation.



malleability, ductility, good conduction of heat and electricity and tendency to produce positive ions are all ascribable to the presence of free electrons in the metals.

More easily a metal atom releases electron, greater is its metallic character.

The smaller the ionization energy, the greater the metallic character.

## Electronegativity

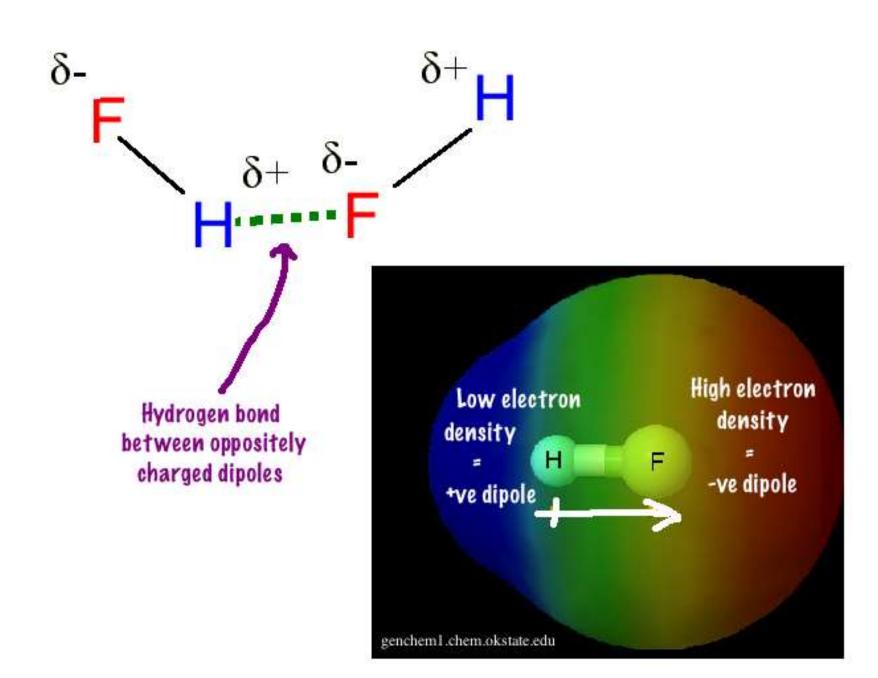
- Electronegativity is a property of atoms within molecules rather than free atoms.
- It measures the tendency of that atom to draw bonding electrons towards itself.
- ➤ In HF, the fluorine atom is much more electronegative than the hydrogen atom. The electrons in the H-F bond are not equally distributed between the atoms. The electron density is greater around the fluorine atom.

#### Electronegativity

increase

0

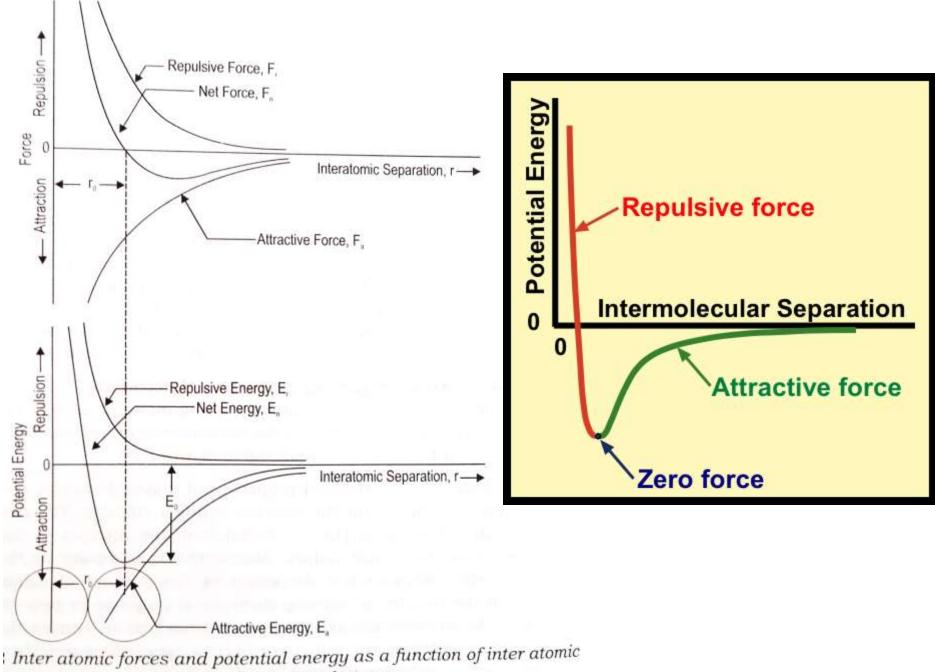
Electronegativity is the measure an atom's tendency to attract electrons toward itself. Electronegativity tends to increase across a period because of decreasing atomic radii. In a smaller atom, a positive nucleus is closer to the valence electrons of nearby atoms, so it is easier to attract those electrons. Electronegativity tends to decrease down a group because of increasing atomic radii. In a larger atom, a positive nucleus is farther away from electrons of nearby atoms, so it is harder to attract those electrons.



## **Atomic Radius**

- The distance which is of the order of A<sup>o</sup> units (1 A<sup>o</sup> = 10<sup>-10</sup> m) from the nucleus to the outer shell
- Atomic radius increases as the no. of occupied shells increases and decreases as the no. of valence electrons increases
- If the number of valence electrons is one or two, they being far away from the nucleus are loosely attracted towards it
- ➤ As the no. of electrons increases they are pulled in closer to the nucleus tending to shrink the atom and there by reducing the atomic radius
- Materials with shorter bond lengths are stronger compared to those with larger bond length

## **Deep & Shallow Energy Well Bonds**



separation for two isolated atoms

 $\succ$  The value of E<sub>o</sub> is known as bond energy

> Bonds with larger values of  $E_o$  is called deep energy well bonds

> Bonds with smaller values are called shallow

energy well bonds

### > Melting and Boiling Temperature

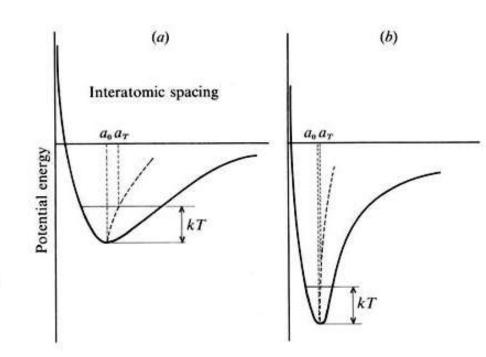
- Atoms have minimum energy at a temperature of absolute zero
- Increased temperature raises the energy until the atoms are able to separate themselves one from the other
- Materials with deep energy well bonds have higher melting and boiling temperature compared to shallow energy wells
- ionic solids have higher melting and boiling points

### > Thermal Expansion

- The equilibrium distance of separation r<sub>o</sub> applies to absolute zero degree temperature
- At higher temperatures under the influence of thermal energy atoms vibrate about their equilibrium positions
- If the potential energy curve were symmetrical the mean value would remain the same as r<sub>o</sub> at all time and there would not be any thermal expansion
- If its not symmetrical as in the case of shallow energy well bonds the mean value changes from r<sub>o</sub> to r<sub>1</sub> at temperature T1 and from r<sub>o</sub> to r<sub>2</sub> at T2
- ie bond length increases on heating, thermal expansion takes place

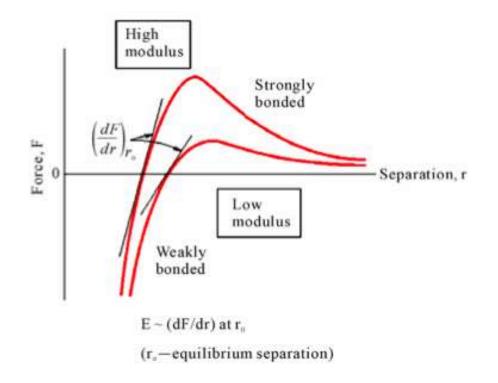
### Correlation of Thermal Expansion with structure

- Materials expand by their average bond length increasing
- Glasses are disordered, so expansion is isotropic
- Expansion is governed by the interatomic potential well that binds the atoms and ions together
- Tightly bound atoms reside in deep energy wells that are only slightly affected by temperature
- More weakly bound atoms reside in shallow energy wells that are more affected by temperature



### **Modulus of Elasticity**

- Related to the slope of the net force curve
- For very small values of strain, modulus of elasticity remains constant
- Extreme compression raises and extreme tension lowers the values of modulus of elasticity



## **Primary Bonds**

➢ Is an inter atomic bond

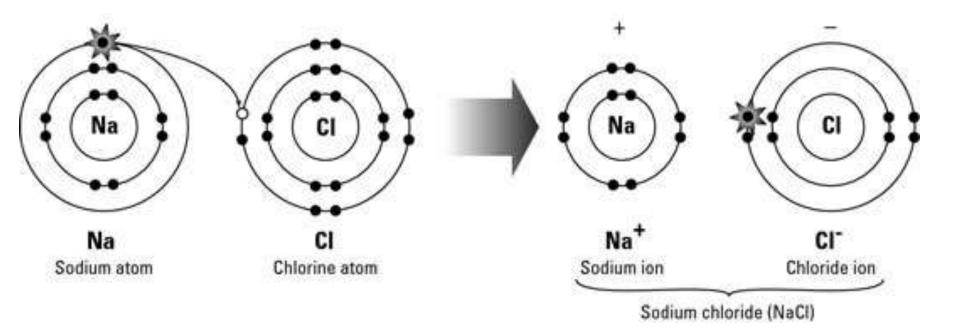
➢ Its strong and more stable

➤ 3 types

- Ionic bond
- Covalent bond
- Metallic bond

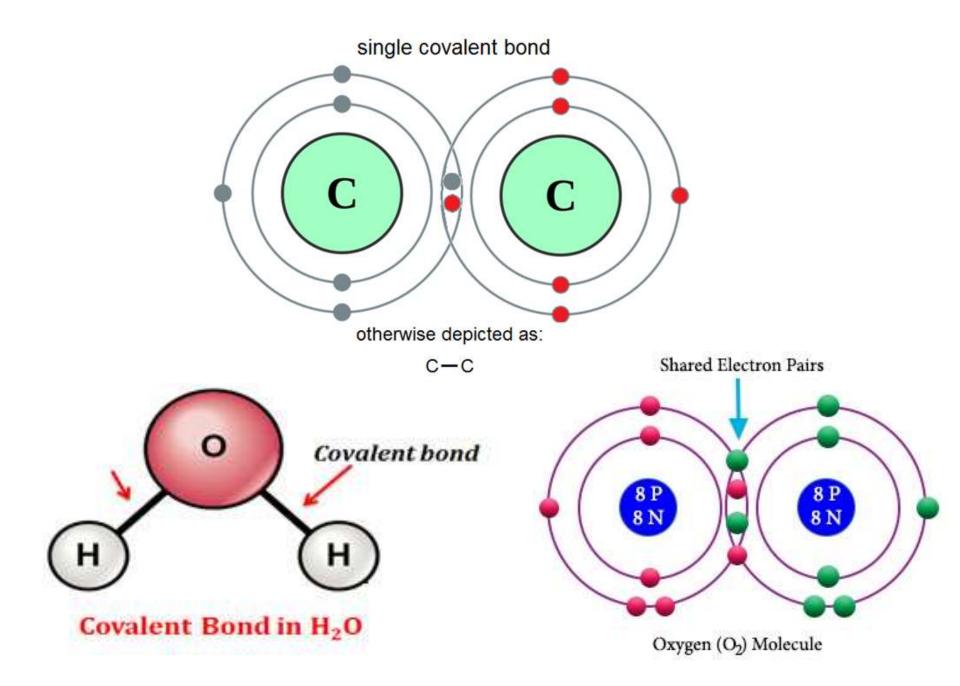
#### Ionic bond

- Ionic bonding is a type of chemical bond that involves the electrostatic attraction between oppositely charged ions
- Found in compounds that are composed of both metallic and non metallic elements
- Found at the horizontal extremities of the periodic table
- Eg.: alkali metals like Li, Na, K, Rb and F, Cl, Br, I
- Metallic elements easily give up their valence electrons to the non metallic atoms
- Eg.: NaCl



#### **Covalent Bond**

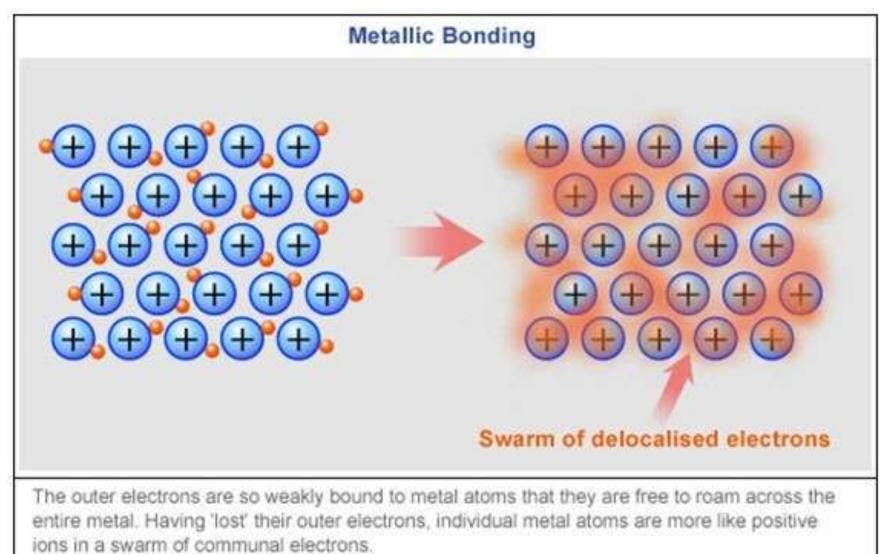
- Elements from the central group of the periodic table are not readily reducable to a closed shell electronic configuration because the energy required to remove all the valence electrons is too large
- Sharing electrons with its neighbours
- The shared electron may be considered to belong to both atoms
- Most common in liquids and gases
- Eg.: H<sub>2</sub>, Cl<sub>2</sub>, F<sub>2</sub>, HF, H<sub>2</sub>O etc.



### **Metallic Bond**

- Found in metals and their alloys
- Metallic materials have one, two or at the most three valence electrons
- They are more or less free to drift throughout the entire material
- They require only small amount of energy to detach themselves from their nuclei
- The free electrons then form what is known as electron cloud around the remaining non valence electrons and the nuclei
- Positive ion surrounded by a large no of free electrons forming a electron cloud

- Electrostatic attraction between the +ve ions and –ve electron cloud forms a bond known as metallic bond
- Metallic solids have opaque nature and bright lusture



Ionic Bond	Covalent Bond	Metallic Bond
Forms due to electrostatic force of attraction between +ve and -ve ions of different elements.	Forms due to electrostatic force of attraction between atoms of same or different materials by <i>sharing</i> electron pairs.	Forms due to electrostatic force of attraction between +ve ions and -ve electron cloud of same or different metals.
<i>Non-directional</i> because each +ve ion attracts all the neighbouring -ve ions and vice-versa.	Directional because, the electrostatic attraction is more localised. Also the centers of +ve and -ve charges are dispersed.	Non-directional because all the ion cores and electron cloud as a whole take part in the formation of the bond.

Ionic Bond	Covalent Bond	Metallic Bond
Ionic solids are bad conductors of electricity in the solid state, because the ions are held tightly together by the force of attraction and are not free to move.	Covalent solids are bad conductors, since the bond is formed due to sharing and not by transfer of electrons. Hence no ions are formed and no mobility.	Metallic bonded solids are good conductors, because the electrons are free to move within the material, and this movement gets enhanced under the influence of the applied electrical field.
Very low thermal conductivity.	Very low thermal conductivity.	Good thermal conductivity.
High melting point since the atoms are tightly held together. Considerable energy is needed to dislodge them.	Low melting point because the electrostatic force of attraction is lower (except for bonds having diamond structure).	Lower melting points than ionic solids. (except higher valent metallic elements).

Generally <i>crystalline</i> in nature. Rigid and hard.	Generally non-crystalline Low hardness and less rigid. Soft and elastic.	Crystalline in nature. Soft and less rigid (except special alloys).
Exists in the solid state only.	Exists as solids, liquids and gases.	Exists in the solid state only (except Hg).
Not malleable and ductile, because the ions are not free to move.	Not malleable and ductile, because the ions or molecules are not free to move over large distances.	Malleable and ductile, since the +ve ion core slides (or slips) over each other within the electron cloud under the influence of an external force,
lonic solids are soluble in water.	Covalent solids are soluble in organic solvents.	Not soluble in water or organic solvents.

## **Secondary Bonds**

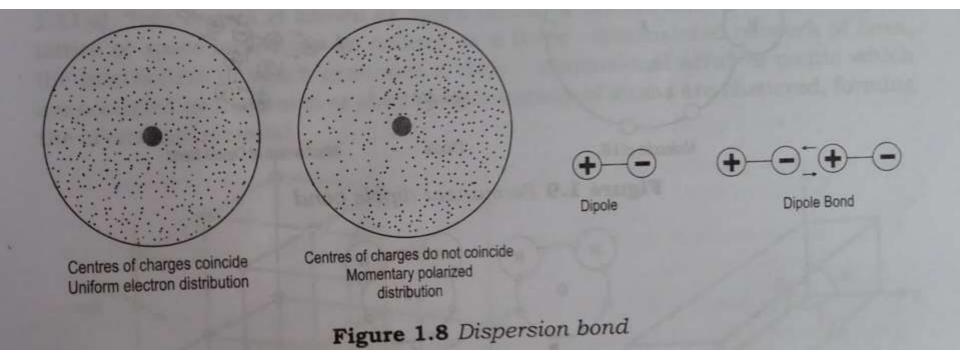
> Weak in comparison to the primary bond

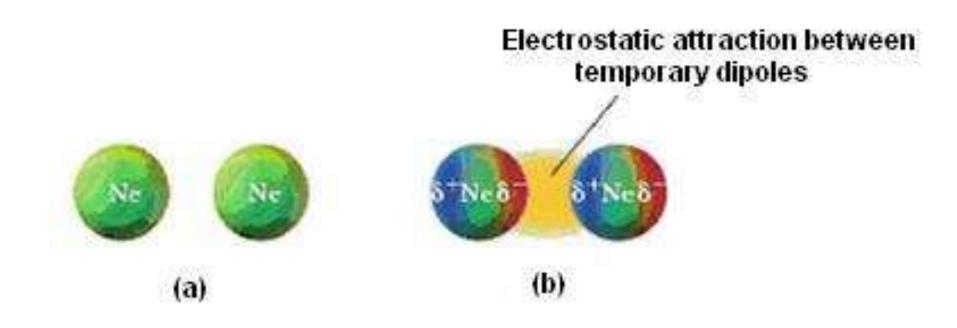
- They exists between virtually all atoms or molecules
- > They are termed as intermolecular bonding

### Dispersion Bonds

- In symmetric molecules and in all noble gas atoms, the overall spacial distribution of electrons is symmetric with respect to the positively charged nucleus
- Hence centres of positive and negative charge coincide
- As a result of random movement of electrons there may be a momentary change in the symmetric spacial distribution of atoms resulting in a momentary shift in the centres of positive and negative charges
- Thus an electric dipole is created

- This random fluctuating polarization is called dispersion effect
- One of these dipoles can in turn produce a displacement of electron distribution in an adjacent molecule or atom. A second dipole is created
- Bonding due to electrostatic force of attraction
  between +ve end of one dipole and -ve end of
  adjacent dipole
- Dispersion bonds are non directional





(a) The distribution of electron density averaged over time in neon is symmetrical and there is no net polarity.

(b) Temporary polarization of one neon atom induces temporary polarization in adjacent atoms. Electrostatic attraction between temporary dipoles are called dispersion forces.

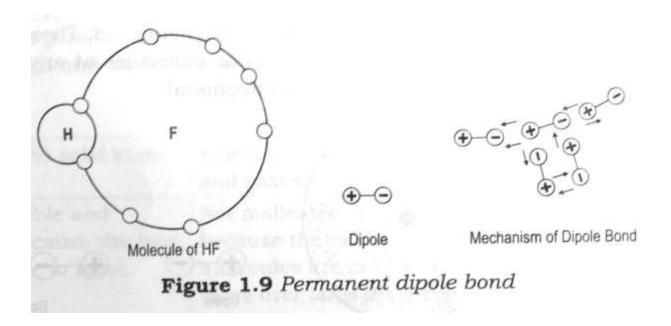
### Permanent dipole bond

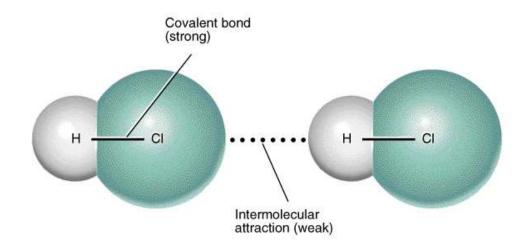
Exist in some molecule because of asymmetrical

arrangement of positively and negatively charged

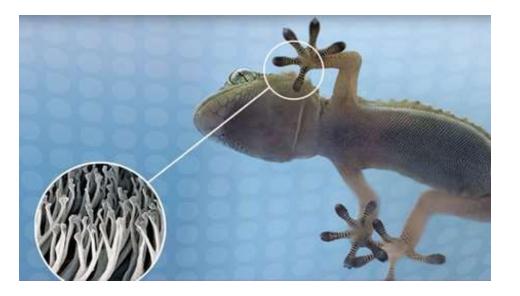
regions

- Such molecules are termed polar molecules
- Directional in nature
- Eg.: hydrogen fluride molecule





### Vander waals Force

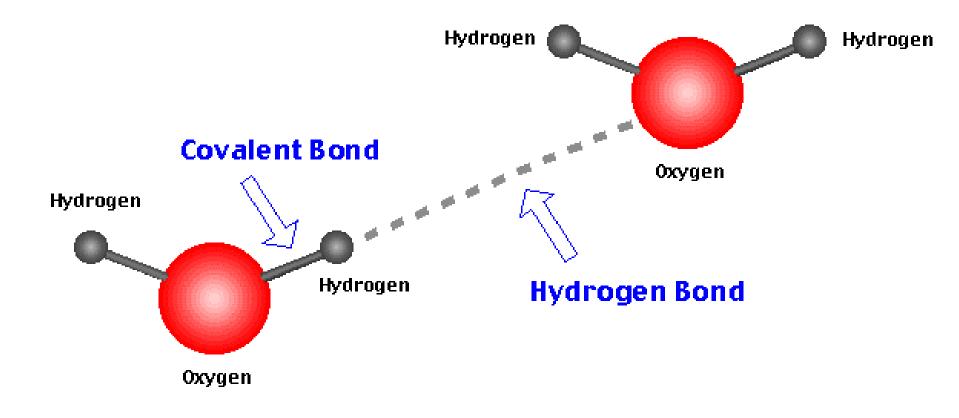






### Hydrogen bond

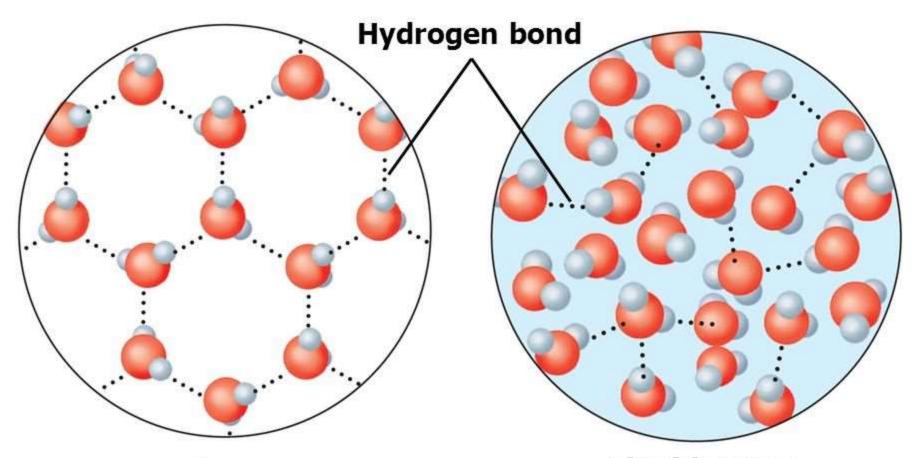
- Is a special case of polar molecular bonding
- Occurs between molecules in which hydrogen is covalently bonded to another element



# **Anomalous Properties Of Water**

- No other material is commonly found as solid, liquid and gas.
- Although it is an apparently simple molecule (H<sub>2</sub>O), it has a highly complex and anomalous character due to its inter-molecular hydrogen bonding
- As a gas, water is one of lightest known, as a liquid it is much denser than expected and as a solid it is much lighter than expected when compared with its liquid form.
- It can be extremely slippery and extremely sticky at the same time; and this 'stick/slip' behavior is how we recognize the feel of water

- When water freezes at 0 °C its volume increases by about 9% under atmospheric pressure; therefore ice floats on water (see above). If the melting point is lowered by increased pressure, the increase in volume on freezing is even greater
- The structure of ice is open with a low packing efficiency where all the water molecules are involved in four straight tetrahedrally-oriented hydrogen bonds;



Ice Hydrogen bonds are stable Liquid water Hydrogen bonds constantly break and re-form

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 $\blacktriangleright$  Ice is less dense than water because of its intermolecular forces. Water contains hydrogen bonds (a type of intermolecular force of attraction) between the H (hydrogen) of one atom and the O (oxygen) of another atom. As the water gets colder and the kinetic energy of the molecules decreases, the hydrogen bonds keep the water molecules apart, forming hexagonal structures with water molecules at each vertex. In between the water molecules is nothing. In liquid water, the molecules of water can be much closer together; the hydrogen bonds are more flexible. Therefore, the solid ice, with its molecules kept at a fairly fixed distance and the crystals holding lots of "nothing" among the water molecules, is less dense than the liquid water.

## **Atomic Mass Unit**

An atomic mass unit (symbolized AMU or amu) is defined as precisely 1/12 the mass of an atom of carbon-12. The carbon-12 (C-12) atom has six protons and six neutrons in its nucleus. In imprecise terms, one AMU is the average of the proton rest mass and the neutron rest mass.

## **Specific Heat**

The specific heat is the amount of heat per unit mass required to raise the temperature by one degree Celsius.