

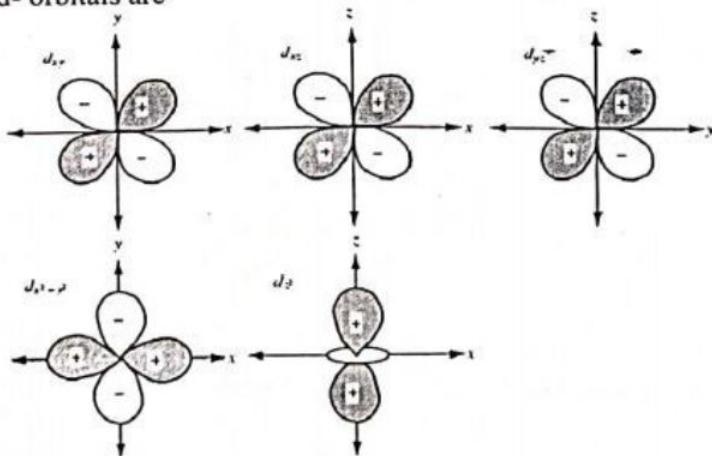
## Unit 2: Modern Engineering materials

### Crystal Field Theory:

Crystal field theory is very much different from valence bond theory. According to valence bond theory, bonding between the metal ion and the ligands is purely covalent, while according to crystal field theory, the interaction between the metal ion and ligands, is purely electrostatic, i.e metal-ligand bonds are 100% ionic.

### Salient features of crystal-field theory are:

1. The transition metal ion is surrounded by the ligands with lone pairs of electrons and the complex is a combination of central ion surrounded by other ions or molecules or dipoles i.e. ligands.
2. All types of ligands are regarded as point charges.
3. The ionic ligands, like  $F^-$ ,  $Cl^-$ ,  $CN^-$ , etc., are regarded as negative point charges, or point charges and the neutral ligands, like  $H_2O$ ,  $NH_3$ , etc., are regarded as point dipoles or just dipoles. (CFT regards neutral ligands as dipolar) If the ligand is neutral, the negative end of this ligand dipole is oriented towards the metal atom.
4. The interactions between the metal ion and the negative ends of anion (or ion dipoles) are purely electrostatic, i.e. the bond between the metal and ligand is considered 100 percent ionic.
5. The ligands surrounding the metal ion produce electrical field and this electrical field influences the energies of the orbitals of central metal ion, particularly d-orbitals.
6. In the case of free metal ion, all the five d-orbitals have the same energy. Such orbitals having the same energies are called degenerate orbitals.
7. The shapes of d- orbitals are



### Crystal field splitting of d orbitals:

In a free transition metal or ion, there are five d-orbitals which are  $dx^2$ ,  $dyz$ ,  $dzx$ ,  $dz^2$  and  $d(x^2-y^2)$ . These are divided into 2 sets based on their orientation in space:

➤  $t_{2g}$  : The 3d-orbitals ( $dx^2$ ,  $dyz$  and  $dzx$ ) which orient in the regions between the coordinate axes . These are non-axial orbitals .  $t_{2g}$  are three fold degenerate.

->  $e_g$  : the other two orbitals ( $d_{z^2}$  and  $d(x^2 - y^2)$ ) which orient along the axis. These are twofold degenerate and also known as axial orbitals.

In an isolated gaseous atom, all the five d orbital are degenerate. (They have same energy). On the approach of the ligands in a complex, the electrons in the d orbital of the central ion are repelled by the lone pairs of the ligands. This repulsion will raise the energy level of the d orbitals. All the ligands approaching the energy of each orbital will increase by the same amount.

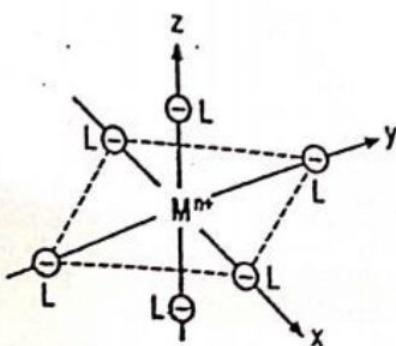
In other words, they will remain degenerate. Since d-orbitals differ in their orientation, those orbitals lying in the direction of the ligands is raised to a larger extent than the others. So, five degenerate d-orbitals will split into two sets, having different amount of energies. This splitting of five degenerate d-orbitals of the metal ion under the influence of approaching ligands, into two sets of orbitals having different energies is called as Crystal-field splitting.

#### Crystal Field splitting is affected by the following factors:

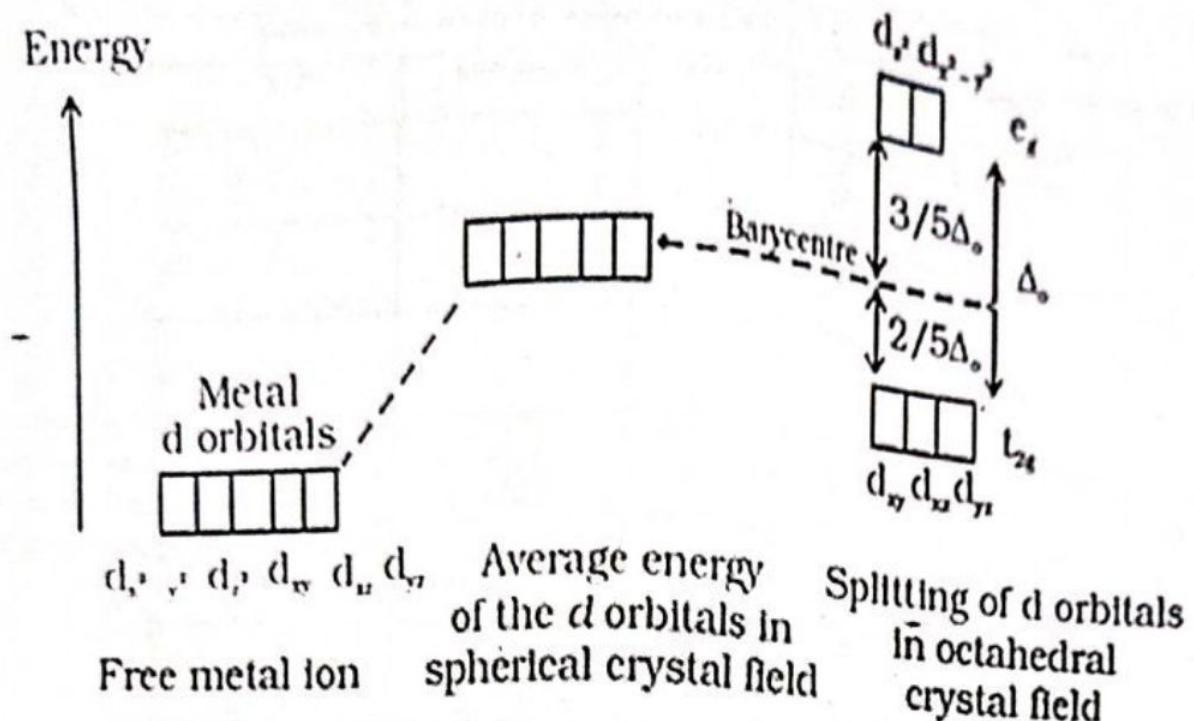
1. Nature of the ligands. The stronger the ligand, the greater is the splitting.
2. Oxidation state of the central metal ion. A higher oxidation state leads to larger splitting.
3. Size of d orbitals (i.e., transition series).
4. Geometry of the complex.
5. Nature of the metal ion
6. Arrangement of the ligands around the metal ion.

#### Crystal Field Splitting in Octahedral Complexes

The octahedral arrangement of six ligands surrounding the central metal ion is as shown in the figure.



In an octahedral complex, the metal ion is at the centre and the ligands are at the six corners. The lobes of the  $e_g$  orbitals ( $d_{z^2}$  and  $d(x^2 - y^2)$ ) point along the x, y and z axis while the lobes of the  $t_{2g}$  orbitals ( $d_{xy}$ ,  $d_{zx}$  and  $d_{yz}$ ) point in between the axes. As a result, the approach of six ligands along the x, y and z directions will increase the energy of  $d_{z^2}$  and  $d(x^2 - y^2)$  orbitals (which point towards the ligands) much more than that it increases the energy of  $d_{xy}$ ,  $d_{zx}$  and  $d_{yz}$  orbitals (which point in between the metal-ligand bond axis).



The approach of the ligands is considered as a two step process. In the first step, it is assumed that the ligands approach the metal ion spherically, i.e. at an equal distance from each of the d-orbitals. At this stage all the d- orbitals are raised in energy by the same amount (The five d-orbitals remain degenerate).

In the second step the spherical field changes to octahedral field leading to splitting of orbitals.

The energy difference between  $t_{2g}$  and  $e_g$  orbitals is known as crystal field splitting and it is denoted by the symbol  $\Delta_o$  or  $10Dq$

This splitting of degenerate level in the presence of ligand is known as crystal field splitting. The difference between energy of  $t_{2g}$  and  $e_g$  level is denoted by " $\Delta_o$ " (subscript o stands for octahedral). Some ligands tend to produce strong fields thereby causing large crystal field splitting whereas some ligands tend to produce weak fields thereby causing small crystal field splitting. Thus, the crystal field splitting depends on upon the field produced by the ligand and the charge on the metal ion. An experimentally determined series based on absorption of light by coordination compound with different ligands known as spectrochemical series has been proposed. Spectrochemical series arranges ligands in order of their field strength as:

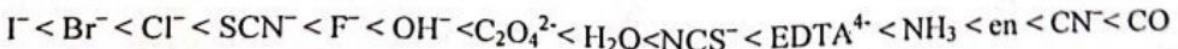
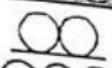
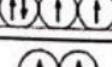
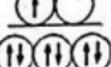
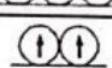
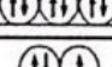


Table Crystal field stabilization energies for metal ions having different numbers of  $d$ -electrons in octahedral complexes.  
(Values for weak and strong fields are given separately where applicable)

Number of electrons	Weak field	CFSE	Strong field	CFSE
$d^1$		$-4 Dq$ or $-0.4 \Delta_0$		
$d^2$		$-8 Dq$ or $-0.8 \Delta_0$		
$d^3$		$-12 Dq$ or $-1.2 \Delta_0$		
$d^4$		$-6 Dq$ or $-0.6 \Delta_0$		$-16 Dq + P$ or $-1.6 \Delta_0 + P$
$d^5$		$0$		$-20 Dq + 2P$ or $-2.0 \Delta_0 + 2P$
$d^6$		$-4 Dq$ or $-0.4 \Delta_0$		$-24 Dq + 2P$ or $-2.4 \Delta_0 + 2P$
$d^7$		$-8 Dq$ or $-0.8 \Delta_0$		$-18 Dq + P$ or $-1.8 \Delta_0 + P$
$d^8$		$-12 Dq$ or $-1.2 \Delta_0$		$-12 Dq$ or $-1.2 \Delta_0$
$d^9$		$-6 Dq$ or $-0.6 \Delta_0$		
$d^{10}$		$0$		

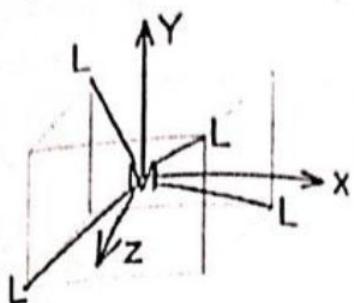
Filling of d-orbitals takes place in the following manner; the first three electrons are arranged in  $t_{2g}$  level as per the Hund's rule. The fourth electron can either enter into  $t_{2g}$  level giving a configuration of  $t_{2g}^4 e_g^0$  or can enter the  $e_g$  orbital giving a configuration of  $t_{2g}^3 e_g^1$ . This depends on two parameters magnitude of crystal field splitting,  $\Delta_0$  and pairing energy, P. The possibilities of two cases can better be explained as:

- $\Delta_0 > P$  – Electron enters in the  $t_{2g}$  level giving a configuration of  $t_{2g}^4 e_g^0$ . Ligands producing this configuration are known as strong field ligands and form low spin complexes.
- $\Delta_0 < P$  – Electron enters in the  $e_g$  level giving a configuration of  $t_{2g}^3 e_g^1$ . Ligands producing this configuration are known as weak field ligands and form high spin complexes.

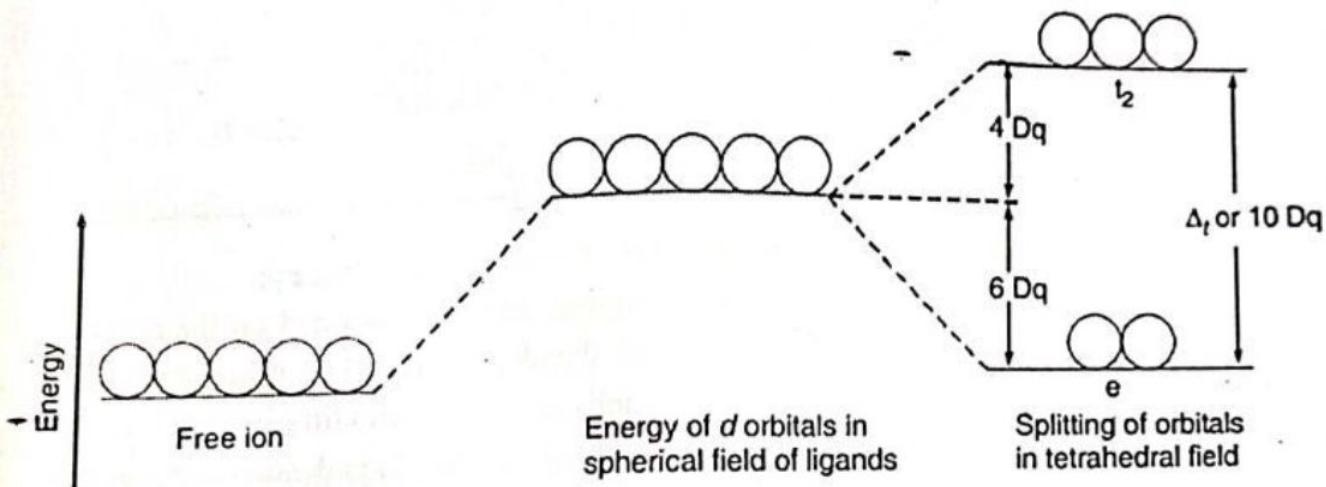
Filling of d-orbitals of remaining electrons are shown table above.

### Crystal Field Splitting in Tetrahedral Complexes:

The tetrahedral arrangement of four ligands surrounding the metal ions is as shown in the figure.



A regular tetrahedron is a cube. One atom is at the centre of the cube and four of the eight corners of the cube are occupied by ligands. The directions x, y and z point to the face centres. The  $d_{z^2}$  and  $d(x^2 - y^2)$  orbitals point along the x, y and z directions and  $d_{xy}$ ,  $d_{zx}$  and  $d_{yz}$  orbitals point in between x, y and z directions.



The direction of approach of ligands does not coincide exactly with either the  $e_g$  or  $t_{2g}$  orbitals. The  $t_{2g}$  orbitals are pointing close to the direction in which the  $e_g$  orbitals are lying in between the ligands. As a result, the energy of  $t_{2g}$  orbitals increases compared to the energy of  $e_g$  orbitals. Thus, d orbitals again split into two sets- triply degenerate  $t_{2g}$  of higher energy and doubly degenerate  $e_g$  orbitals of lower energy. That is,  $t_{2g}$  orbitals are raised by  $0.4 \Delta_t$  in energy and the  $e_g$  orbitals are stabilized by  $0.6 \Delta_t$  in energy.

The energy difference between the two sets of orbitals ( $\Delta_t$ ) will be about half the magnitude of that in an octahedral complex ( $\Delta_o$ ).

There is an interesting point to be noted in splitting in tetrahedral field. The magnitude of crystalfield splitting in tetrahedral field is quite small and is always less than the pairing energy. Therefore, we do not expect the pairing of electrons to take place. Thus, all the tetrahedral complexes are high spin complexes. Filling of d-orbitals electrons takes place in the following table.

Table Crystal field stabilization energies for tetrahedral complexes with metal ions for different $d^n$ .	
$d^1$	 CFSE = - 6Dq
$d^2$	 CFSE = - 12Dq
$d^3$	 CFSE = - 8Dq
$d^4$	 CFSE = - 4Dq
$d^5$	 CFSE = 0
$d^6$	 CFSE = - 6Dq
$d^7$	 CFSE = - 12Dq
$d^8$	 CFSE = - 8Dq
$d^9$	 CFSE = - 4Dq
$d^{10}$	 CFSE = 0

### Colour of Transition Metal Complexes on the basis of crystals field theory:

The cause of the colour of the transition metal compounds can be explained on the basis of crystal field theory. In this theory, the splitting of the d-orbitals takes place under the influence of surrounding ligands. The d-orbitals are split by the surrounding ligands into the upper  $e_g$  and lower  $t_{2g}$  levels. The energy gap between these two levels is denoted by  $\Delta$  and is comparatively small between the non-degenerate d-orbitals ( $e_g$  and  $t_{2g}$ ) in a transition metal complex. Consequently the excitation of an electron from a lower to a higher-level can be achieved by absorption of visible light. This causes the complex to appear coloured.

### Magnetic Properties of Transition metal Complexes

When the transition metal ions or their complexes are placed in a magnetic field, they show different behaviour. On the basis of this behaviour these substances have been classified as paramagnetic substances and diamagnetic substances.

The transition metal complexes whose central atom/ion contains **one or more unpaired electrons** are **paramagnetic** while those with **no unpaired electrons** behave as **diamagnetic substances**. The paramagnetic character increases with the increase in the number of unpaired electrons. The paramagnetism of a substance is expressed in terms of its magnetic moment ( $\mu$ ). Larger the number of unpaired electrons in the central atom/ion greater is its paramagnetic character and hence larger is the value of the magnetic moment. The magnetic moment is expressed in Bohr Magnets (B.M.). Paramagnetic substances have some definite value of magnetic moment while diamagnetic substances have zero value.

**Magnetic Moment ( $\mu$ )** =  $\sqrt{n(n+2)}BM$   
Where n= the number of unpaired electrons in the complex ion

## BAND THEORY OF SOLIDS

According to the molecular orbital theory, molecular orbitals are formed by the combination of atomic orbitals. The number of molecular orbitals formed is equal to the number of atomic orbitals taking part in molecular orbital formation.

**Example:** Formation of crystal of Li metal.

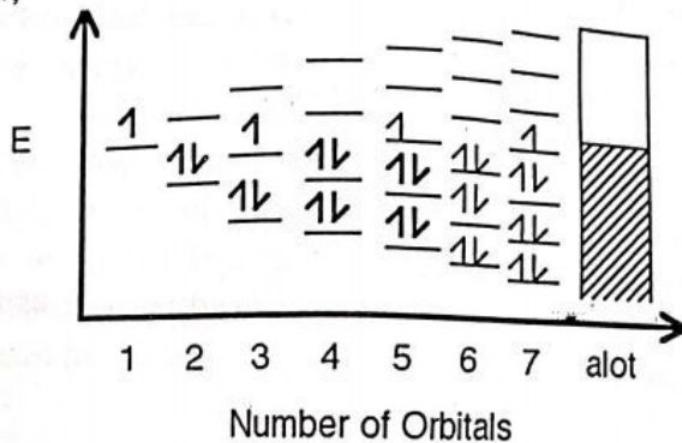
In order to understand the band theory of solids, let us imagine the construction of a crystal lithium metal by adding Li-atoms like  $\text{Li}_2$ ,  $\text{Li}_3$ , and  $\text{Li}_4 \dots \text{Li}_N$ .

### Explanation

The electronic configuration of each Li-atom is  $1s^2, 2s^1, 2p^0$ . The  $2s$ -atomic orbitals overlap in  $\text{Li}_2$  to form two molecular orbitals.

In  $\text{Li}_3$  the  $3s$ -atomic orbitals overlap to form 3 molecular orbitals.

Similarly in  $\text{Li}_N$  the  $Ns$ -atomic orbitals overlap to form a band of  $N$  closely spaced MO as shown in figure below,



## Formation of Various Bands in Solids

### Example-I

Formation of various bands can be explained with the example of lithium crystal.

#### 1s band

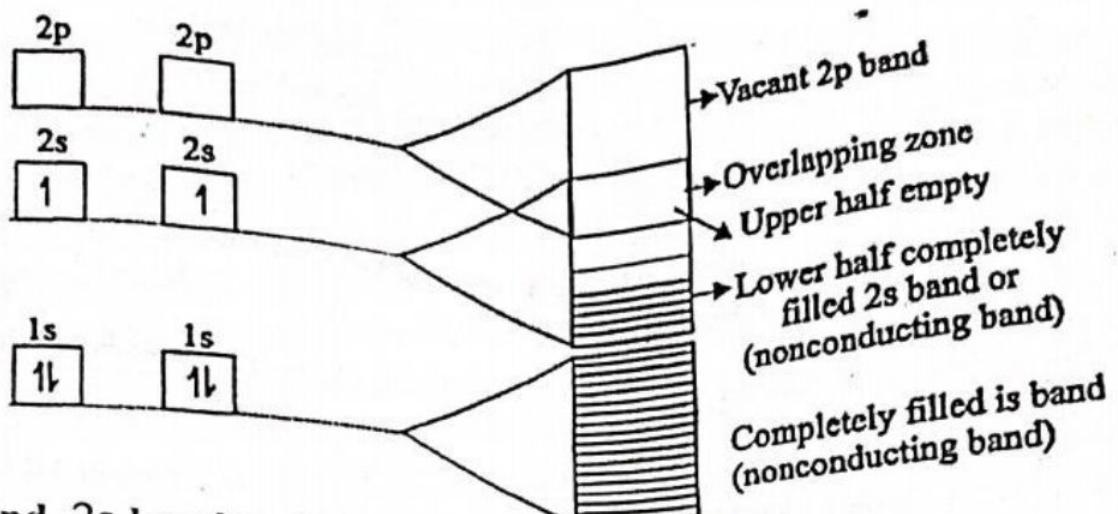
This is called non conduction band. It is formed by the combination of completely filled orbitals.

#### 2s band

This is called valence band as it is half filled. The upper half of this band is empty, while the lower half is completely filled. Since the energy difference between these bands is very small, the electrons can move from lower half to upper half.

#### 2p band

This is called vacant band (or) overlapping band. Since  $2s$  and  $2p$  energy levels are close to each other. These two orbitals can overlap, so that the electrons from  $2s$  orbitals can move to  $2p$  orbitals. Thus it is also called Conduction band.



### 1s band, 2s band and 2p bands in Li crystal

Thus, a band that is either partially filled (or) completely vacant is called Conduction band. When an electric field is applied across a lithium crystal, the electrons start moving in one direction and so lithium is a good conductor of electricity. From the above diagram it is clear that when the number of Li-atoms increase, the spacing between the MO decreases.

### Classification of materials (solids) based on band gap:

The materials are classified into the following categories depending upon the energy gap between the valence and conduction bands.

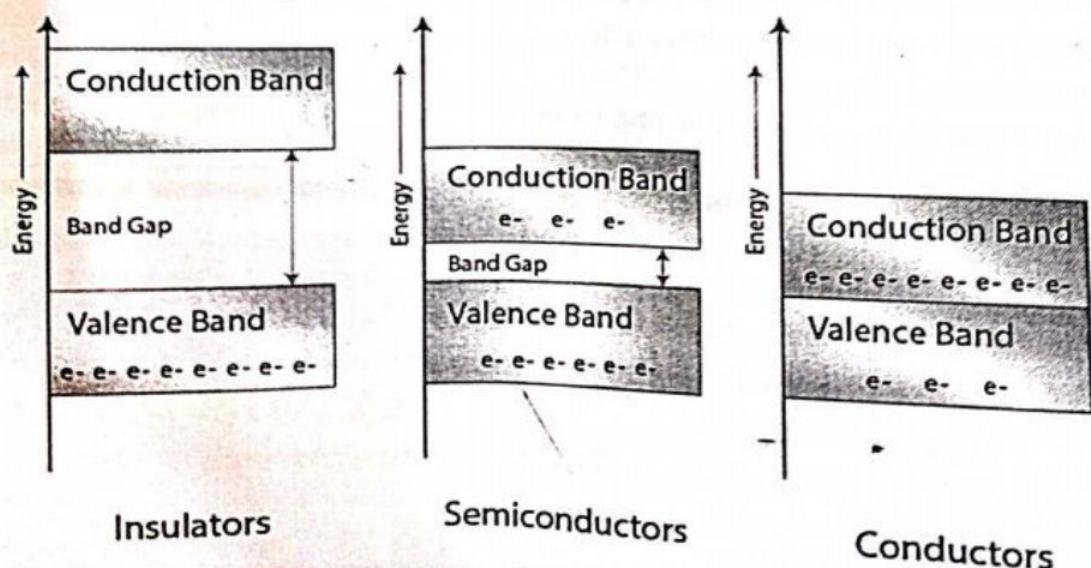
1. Insulators
2. Conductors
3. Semiconductors

### Insulators

In insulators (non-metals) there is a large band gap between the filled valence bands and empty conduction. Therefore electrons cannot be promoted from the V.B to C.B. where they cannot move freely.

### Conductors

In conductors (metals), the valence bands and conduction bands overlap, so there is no band gap. Therefore electrons can freely move.



## Semiconductors

In semiconductors, there is a small band gap between the filled V.B and empty C.B. Therefore electrons can be promoted from V.B to C.B with rise in temperature (or) by adding dopants.

### Effect of Doping On Conductance

The conductivity of semiconductors is very low at room temperature. Therefore, their conductivity is increased by adding an appropriate amount of suitable impurity. This process is known as doping.

### Doping

The process by which impurity is introduced in semiconductors to enhance their conductivity is called doping. It can done with an impurity which is electron rich (or) electron deficient. Such impurities introduce electronic defects in them.

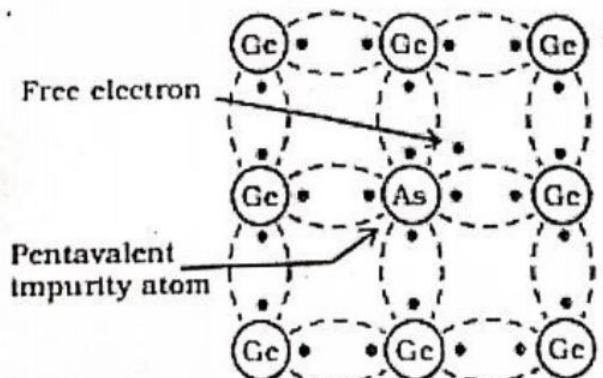
### Types of Doping

On the basis of impurities, added for doping, semiconductors are of two types. They are

1. N-type semiconductor
2. P-type semiconductor

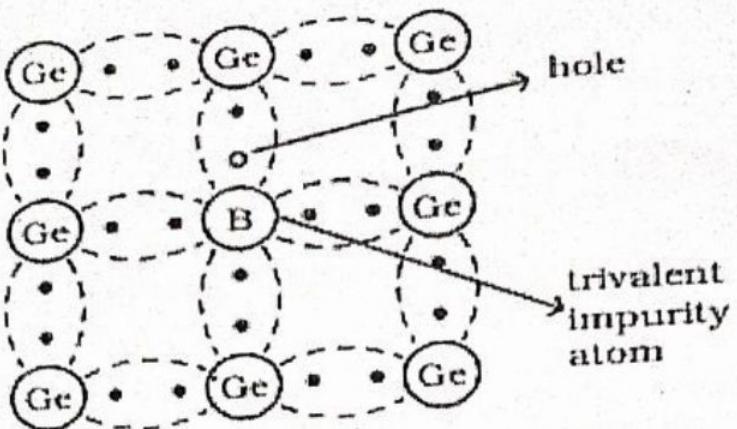
#### N-type semiconductor:

They are obtained by adding a pentavalent impurity such as phosphorus, arsenic or antimony to pure semiconductor (such as silicon, germanium, tellurium, etc.). The four electrons of the dopant form bond with Si or Ge and the fifth electron is the 'excess electron' that is loosely bound and can easily be excited from the valence band to the conduction band. Hence, conduction in n-type semiconductor is because of the presence of excess electrons and hence the name n-type (n is used for negatively charged electrons).



#### P-type semiconductor:

These are obtained by doping a trivalent impurity such as boron or aluminium (both of them have three valence electrons) to pure semiconductor (such as silicon, germanium, tellurium, etc.). The three valence electrons of boron or aluminium form three covalent bonds with three germanium atoms and the fourth germanium atom is linked to boron atom by an incomplete bond containing only one electron from germanium. Thus, the crystal lattice has an electron deficiency called a hole. In the electric field, an electron from an adjacent atom moves into a hole, which is in turn replaced by an electron from another atom. Thus, the condition is brought about because of the migration of holes and hence the name p-type (p is used for positive holes).



## NANOMATERIALS:

The materials that have dimensions from 1 to 100 nm are called Nanoparticles. The chemistry of nanomaterials is known as nanochemistry.

The nanomaterials exhibit totally different properties when compared to bulk materials.

**A "nanometre" (nm) is equal to one billionth of a metre.**

Note that  $1 \text{ nm} = 10^{-3} \text{ pm} = 10^{-6} \text{ mm} = 10^{-9} \text{ m}$

One of the main reasons for the nanomaterials to exhibit interesting properties is the availability of larger surface area.

The following examples provide information about the sizes of the nanomaterials.

- (i) One human hair is approximately 80,000 nm thick.
- (ii) If we keep 10 hydrogen atoms side by side, then it would be equal to 1 nm.
- (iii) Proteins and nucleic acids are the examples of natural nanoparticles.
- (iv) A DNA molecule is about 2.5 nm wide.
- (v) The diameter of a red blood cell is about 5,000 nm.

Nanotechnology is an interdisciplinary field, which involves subjects like chemistry, physics, biology, engineering, computer science, etc. The field of nanotechnology is expanding very rapidly.

## Classification of Nanomaterials:

Nanomaterials are classified into 3 types based on atoms/molecules array:

### 1. Materials with one dimension in the nano scale.

For example, Thin films, surface coatings

### 2. Materials that have two dimensions in nano scale.

For example, Nanowires, nano-tubes, Biopolymers, inorganic nano tubes

### 3. Materials in three dimensions in nano scale are quantum dots

For example, Tiny particles of semiconductors materials such as nanometre sized grains, fullerenes, nano particles, dendrimers.

## **Properties of Nanomaterials:**

This is mainly due to the nanometer size of the materials which make them: (i) large surface area (ii) high surface energy, which do not exist in the corresponding bulk materials.

### **Size:**

- Chemical sensors from nanoparticles and nanowires enhanced the sensitivity and sensor selectivity.
- The nanometer feature sizes of nanomaterials also have spatial confinement effect on the materials, which bring the quantum effects.

### **Catalytic Activity:**

- Metallic nanoparticles can be used as very active catalysts. For example, reaction rate at nano-aluminum can go so high, that it is utilized as a solid-fuel in rocket propulsion, whereas the bulk aluminum is widely used in utensils.

### **Optical properties**

- One of the most fascinating and useful aspects of nanomaterials is their optical properties. Applications based on optical properties of nanomaterials include optical detector, laser, sensor, imaging, phosphor, display, solar cell, photocatalysis, photoelectrochemistry and biomedicine.

### **Magnetic properties**

- Bulk gold and Pt are non-magnetic, but at the nano size they are magnetic. Surface atoms are not only different to bulk atoms, but they can also be modified by interaction with other chemicalspecies, that is, by capping the nanoparticles.

### **Electrical Properties**

- "Electrical Properties of Nanoparticles" discuss about fundamentals of electrical conductivity in nanotubes and nanorods, carbon nanotubes, photoconductivity of nanorods, electrical conductivity of nanocomposites.

### **Application of Nanomaterials:**

Nanomaterials having wide range of applications in the field of electronics, fuel cells, batteries, agriculture, food industry, and medicines, etc

### **Fuel cells:**

- The microbial fuel cell is thus a device that converts the chemical energy present in water-soluble waste into electrical energy by the catalytic reaction of microorganisms.

### **Nano rods of nano wires**

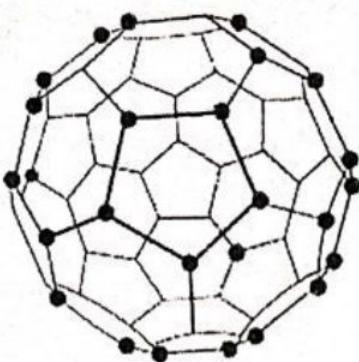
- Silicon nano wires shows photoluminescence.
- Zinc oxide nanowires exhibit ultraviolet laser at room temperature.
- Semiconductor nanowires used in making of field effect transistor.

### **Other applications of nanomaterials and their uses**

- Sunscreens, cosmetics, coating on surfaces, hard cutting tools.
- Fuel cells, displays, batteries, catalysts.
- Magnetic materials, lubricants, machinable ceramics, military bottle suits.

## Fullerenes:

The discovery of C<sub>60</sub> has a long and very interesting history. It is a new form of carbon called fullerene. The structure of fullerene was Cage and Richard Smalley succeeded in building it. They named C<sub>60</sub> as Buckminster fullerene because of similarity of the structure to be geodesic structures widely credited to R. Buckminster fuller. The fullerenes are even number of Sp<sup>2</sup> hybrid carbon atoms over the surface of a closed hollow cage. The structure of C<sub>60</sub> as shown in below,



## Properties of fullerenes:

Unlike graphite and diamond fullerenes are closed-cage carbon molecules consisting of a number of five membered rings and six membered rings. The structure of C<sub>60</sub> is truncated icosahedron which looks like a soccer ball with 12 pentagons and 20 hexagons. The bonds in C<sub>60</sub> have two kinds. The bond length in a pentagon is 1.45 Å and that between pentagons is 1.40 Å. At room temperature the solubility of C<sub>60</sub> is 2.8 mg/ml in toluene. As the size increases, the heat of sublimation of fullerene increases. Fullerenes are ready to reduce and hence it acts as good oxidising agent. It is unstable at higher temperature. C<sub>60</sub> is a very poor conductor of electricity but when react with reducing agent (alkali) the resulting compound has high electrical conductivity and even become super conducting.

## Preparation of fullerenes:

Fullerenes can be prepared in simple processes. Graphite rods are vapourised in an inert atmosphere (Helium), by passing a high electric current through them. This produces a light condensate called fullerene soot which contain variety of different fullerenes. The fullerenes can be extracted through toluene. Separation and purification can be achieved by column chromatography.

## Applications:

Because of wide range of magnetic and conducting properties, fullerene has the following applications.

1. Microelectric devices, 2. Non-linear optical devices
3. Soft ferromagnetic materials, and
4. Superconductors.

### **Carbon Nano Tubes (CNT):**

- Carbon nanotubes (CNTs) are allotropes of carbon with a cylindrical nanostructure.
- Carbon nanotubes was discovered by Sumio Lijima in 1991
- Nanotubes are members of the fullerene structural family which includes the spherical bucky balls.
- Their name is derived from their size, since the diameter of a nanotube is on the order of a few nanometers (approximately 1/50,000 times smaller than the width of a human hair)
- Nanotubes are categorized as single-walled nanotubes (SWNTs) and multi-walled nanotubes (MWNTs).
- The chemical bonding of nanotubes is composed entirely of  $sp^2$  bonds, similar to those of graphite.
- These bonds, which are stronger than the  $sp^3$  bonds found in alkanes and diamond, provide nano tubes with their unique strength.
- Nanotubes naturally align themselves into "ropes" held together by Vander Waals forces.

### **PROPERTIES:**

1. CNTS posses' high tensile strength up to 100giga Pascal's.
2. These are very hard and can withstand a pressure up to 25 gpa without deformation.
3. Multi walled CNTS exhibit striking telescopic properties.
4. CNT is semi conducting and involves quantum effects.
5. CNTS show optical properties due to the absorption of photo luminal scene.
6. CNTS are very good thermal conductors and posses a thermal conductivity of  $3500\text{wm}^{-1}\text{k}^{-1}$ .
7. CNTS are toxic and can induce harmful effects and can cause cell death.

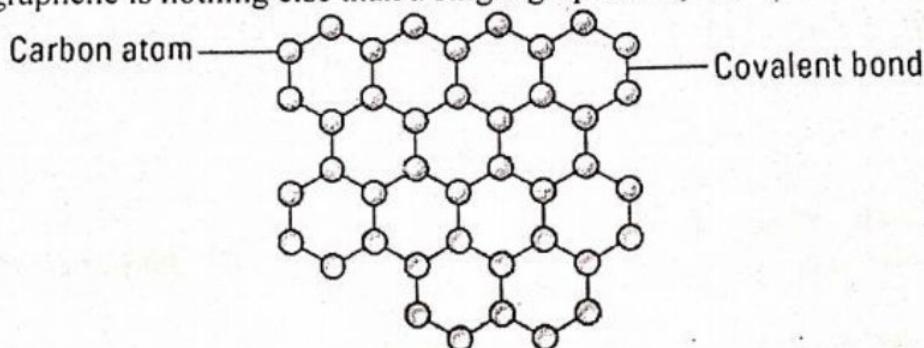
### **GRAPHENE**

- Graphene can be described as a one- atom thick layer of graphite. It is the basic structural element of other allotropes, including graphite, charcoal, carbon nanotubes and fullerenes.
- Graphene is the strongest, thinnest material known to exist. Graphene is an atomic-scale honeycomb lattice made of carbon atoms.

- Graphene is a 2D crystal of carbon atoms, arranged in a honeycomb lattice. Each carbon atom is sp<sup>2</sup> hybridized and it is bound to its three neighbors.

## STRUCTURE

- Graphene is a 2-dimensional network of carbon atoms.
- These carbon atoms are bound within the plane by strong bonds into a honeycomb array comprised of six-membered rings.
- By stacking of these layers on top of each other, the well known 3-dimensional graphite crystal is formed.
- It is a basic building block for graphitic materials of all other dimensionalities. □ It can be wrapped up into 0D fullerenes, rolled into 1D nanotubes or stacked into 3D graphite.
- Thus, graphene is nothing else than a single graphite layer.



## Properties of Graphene:

### Chemical Properties

- Graphene is chemically the most reactive form of carbon. Only form of carbon (and generally all solid materials) in which each single atom is in exposure for chemical reaction from two sides (due to the 2D structure). Carbon atoms at the edge of graphene sheets have special chemical reactivity. Graphene burns at very low temperature (e.g., 350 °C). Graphene has the highest ratio of edgy carbons (in comparison with similar materials such as carbon nanotubes). Graphene is commonly modified with oxygen- and nitrogen- containing functional groups

### Electronic Properties

- It is a zero-overlap semimetal (with both holes and electrons as charge carriers) with very high electrical conductivity. Electrons are able to flow through graphene more easily than through even copper. The electrons travel through the graphene sheet as if they carry no mass, as fast as just one hundredth that of the speed of light.

### Mechanical Properties

- It was found that graphene is harder than diamond and about 300 times harder than steel. The tensile strength of graphene exceeds 1 TPa. It is stretchable up to 20% of its initial length.

## **Thermal Properties**

- Graphene is a perfect thermal conductor. Its thermal conductivity is much higher than all the other carbon structures as carbon nanotubes, graphite and diamond

## **Optical Properties**

- Graphene, despite it is only 1 atom thick, is still visible to the naked eye. Due to its unique electronic properties, it absorbs a high 2.3% of light that passes through it.
- Photograph of graphene in transmitted light. This one-atom-thick crystal can be seen with the naked eye.

## **Applications of Graphene:**

### **Optical Electronics**

- Graphene's high electrical conductivity and high optical transparency make it a candidate for transparent conducting electrodes

### **Filters Desalination:**

- By very precise control over the size of the holes in the graphene sheet, graphene oxide filters could outperform other techniques of desalination by a significant margin.

### **Solar cells**

- Graphene turned to be a promising material for photoelectrochemical energy conversion in dye sensitized solar cells.

### **Energy Storage Devices**

- Due to the extremely high surface area to mass ratio of graphene, one potential application is in the conductive plates of Supercapacitors. It is believed that graphene could be used to produce Supercapacitors with a greater energy storage density than is currently available.

### **Anti- Bacterial**

- In 2010, the Chinese Academy of Sciences has found that sheets of graphene oxide are highly effective at killing bacteria such as Escherichia coli. This means graphene could be useful in applications such as hygiene products or packaging that will help keep food fresh for longer periods of time.

## **SUPERCAPACITORS**

Supercapacitor is an electronic device that store large amount of electric charge. These capacitors are also known as ultracapacitors or electric double layer capacitors.

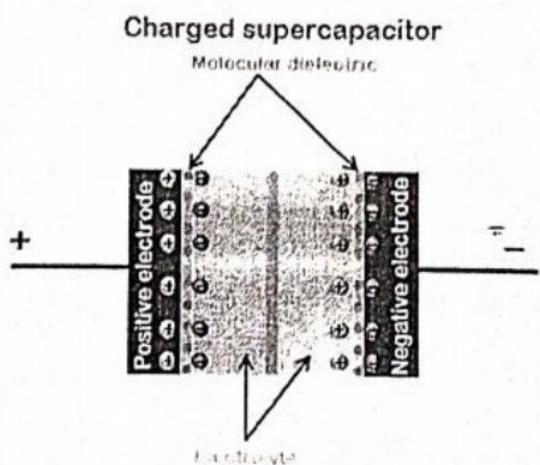
A supercapacitor consists of two electrodes, an electrolyte, and a separator which isolates the two electrodes electrically. Electrode material is the most important component of a supercapacitor.

Based on the energy storage mechanism supercapacitors are classified into three classes. They are 1) Electrochemical double-layer capacitors (EDLC), 2) Pseudocapacitors, 3) Hybrid supercapacitors

### ELECTROCHEMICAL DOUBLE LAYER CAPACITORS:

Electrochemical double layer capacitor consists of two electrodes, separator, and electrolyte. The electrolyte is the mixture of positive ions and negative ions dissolved in water. The two electrodes are separated by a separator.

The principle of energy storage used by EDLCs is the electrochemical double layer. When voltage is applied, there is an accumulation of charge on electrode surfaces, due to the difference in potential there is an attraction of opposite charges, these results to ions in electrolyte diffusing over the separator and onto pores of the opposite charged electrode. To avoid recombination of ions at electrodes a double layer of charge is formed. The double layer, combined with the increase in specific surface area and distances between electrodes decreased, allows EDLCs to attain higher energy density



The most commonly used electrode materials for electrochemical double layer capacitors are activated carbon, carbon aerogel, carbon fibre-cloth and carbon nanotubes.

### PSEUDOCAPACITORS:

The pseudo-capacitors store electrical energy by electron charge transfer between electrode and electrolyte (electrons from electrolyte to cathode or from cathode to electrolyte). This can be done by Redox reaction (reduction-oxidation reaction).

When voltage is applied to the pseudo-capacitor, the charged atoms or ions in the electrolyte move towards the oppositely charged electrode. In between the surface of the electrode and adjacent electrolyte, two electric layers or electric double layers are formed. These two electric layers are separated by electrolyte molecules.

The charged atoms in the electrolyte within the double layer act as electron donors and transfers electrons to the atoms of electrode. As a result, the atoms in electrode become charged. Thus, charge is stored at electric double layers.

The pseudo-capacitors use conductive polymers or metal oxide as electrodes. The amount of electric charge stored in a pseudo-capacitor is directly proportional to the applied voltage. The pseudo-capacitance is measured in farads.

### **HYBRID CAPACITORS:**

The hybrid capacitors are developed by using the techniques of double layer capacitors and pseudo-capacitors. In hybrid capacitors, both double layer capacitance and pseudo capacitance is achieved.

### **ADVANTAGES OF SUPERCAPACITORS:**

- Stores large amount of charge compared to the conventional capacitors (High capacitance).
- Delivers energy or charge very quickly (high power density)
- Long lifetime
- Low cost
- Supercapacitors do not explode like batteries even if it is overcharged.

### **APPLICATIONS OF SUPERCAPACITORS:**

- Flash light applications
- Solar power applications
- Supercapacitors are used in electronic devices such as laptop computers, portable media players, hand held devices, and photovoltaic systems to stabilize the power supply.
- Supercapacitors are used as temporary energy storage devices for energy harvesting systems.
- Supercapacitors are used in defibrillators (an instrument that controls irregular heart beat by supplying electric current to the chest wall).