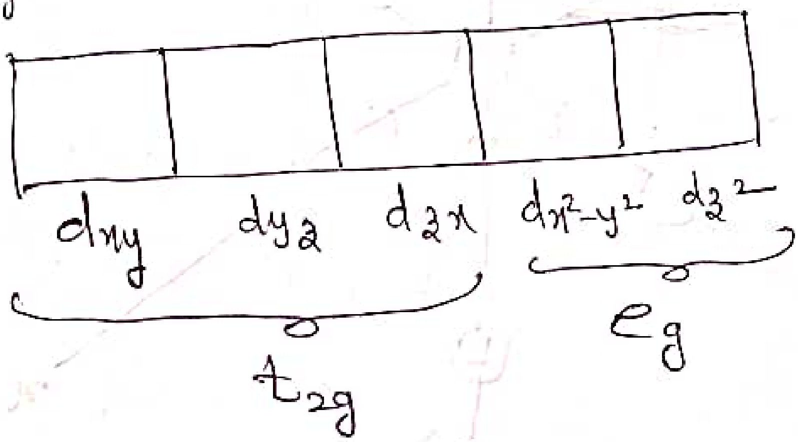
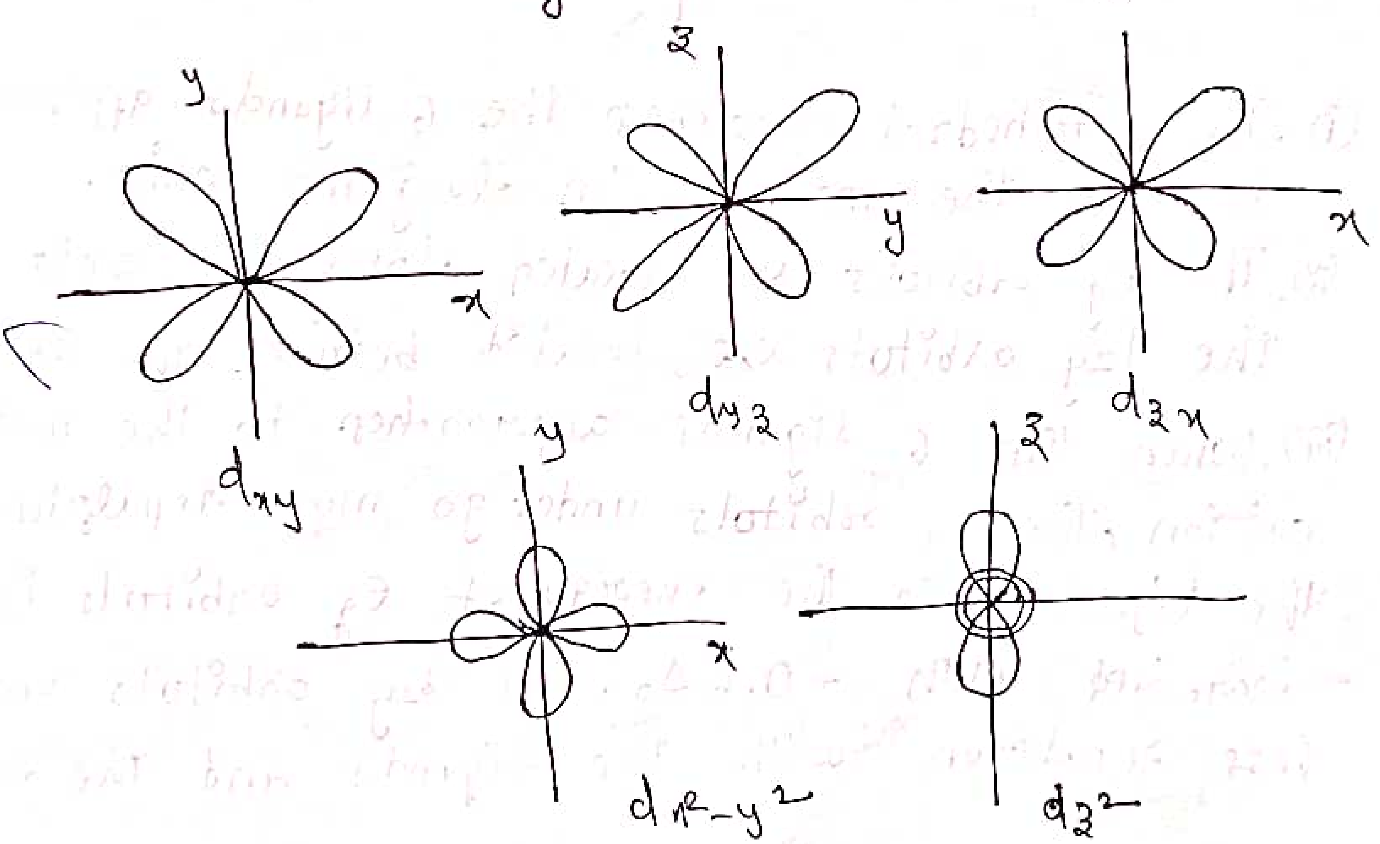
Modern Engineering Materials

1. Write about crystal field theory ?

Sol:- **CFT (Crystal Field Theory):-**

The CFT explains the splitting of d-orbitals which is due to the electrostatic field between metal cation and ligands. In free metal cation all the five d-orbitals posses same energy which is known as degeneracy of d-orbitals. When the ligands approaches to the metal cation undergo splitting of d-orbitals.

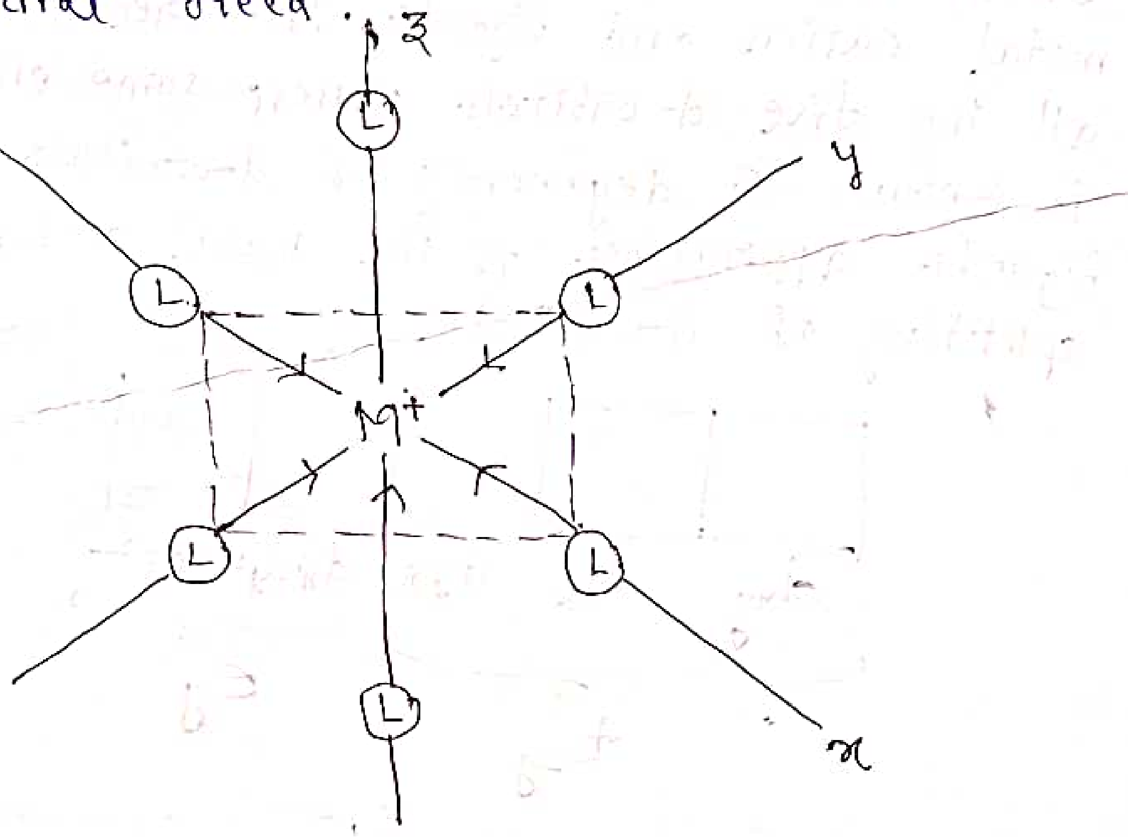




The d_{xy}, d_{yz}, d_{zx} orbitals are called t_{2g} set of d-orbitals which are located between the axis. $d_{x^2-y^2}, d_{z^2}$ orbitals are called e_g set of d-orbitals. which are located along the axis.

Q. Explain the splitting of d-orbitals in octahedral field.

Sol:



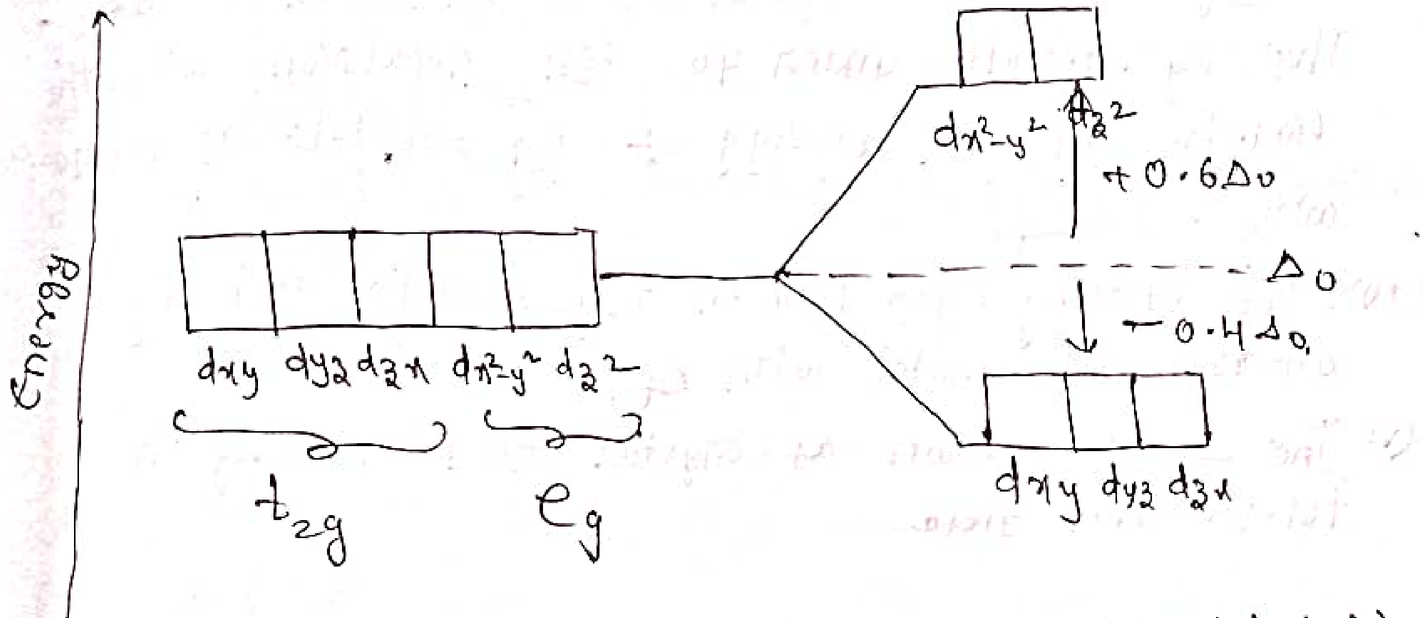
(i). In octahedral complexes the 6 ligands approaches towards the metal cation along the axis.

(ii). The e_g orbitals are located along the axis and the t_{2g} orbitals are located between the axis.

(iii). When the 6 ligands approaches to the metal cation, the e_g orbitals under go more repulsion with the ligands and the energy of e_g orbitals is increased with $+0.6\Delta_0$. The t_{2g} orbitals under go less repulsion with the ligands and the energy of t_{2g} orbitals is decreased with $-0.4\Delta_0$.

(iv). The energy gap between e_g orbitals and t_{2g} orbitals is denoted with Δ_0.

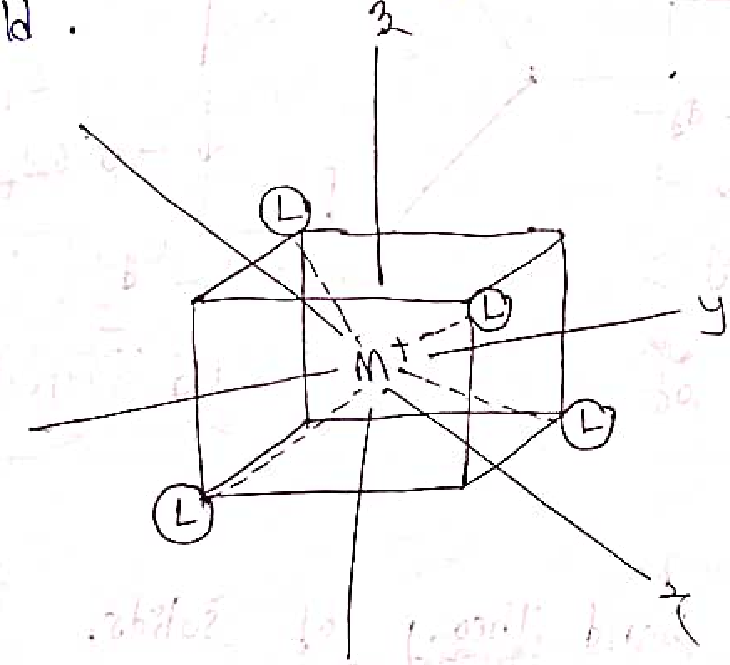
(v). The Δ_0 is known as crystal field splitting in octahedral field.



Splitting of d-orbitals in OH. (Octahedral).

Q. Explain the splitting of d-orbitals in tetrahedral field.

Sol:-



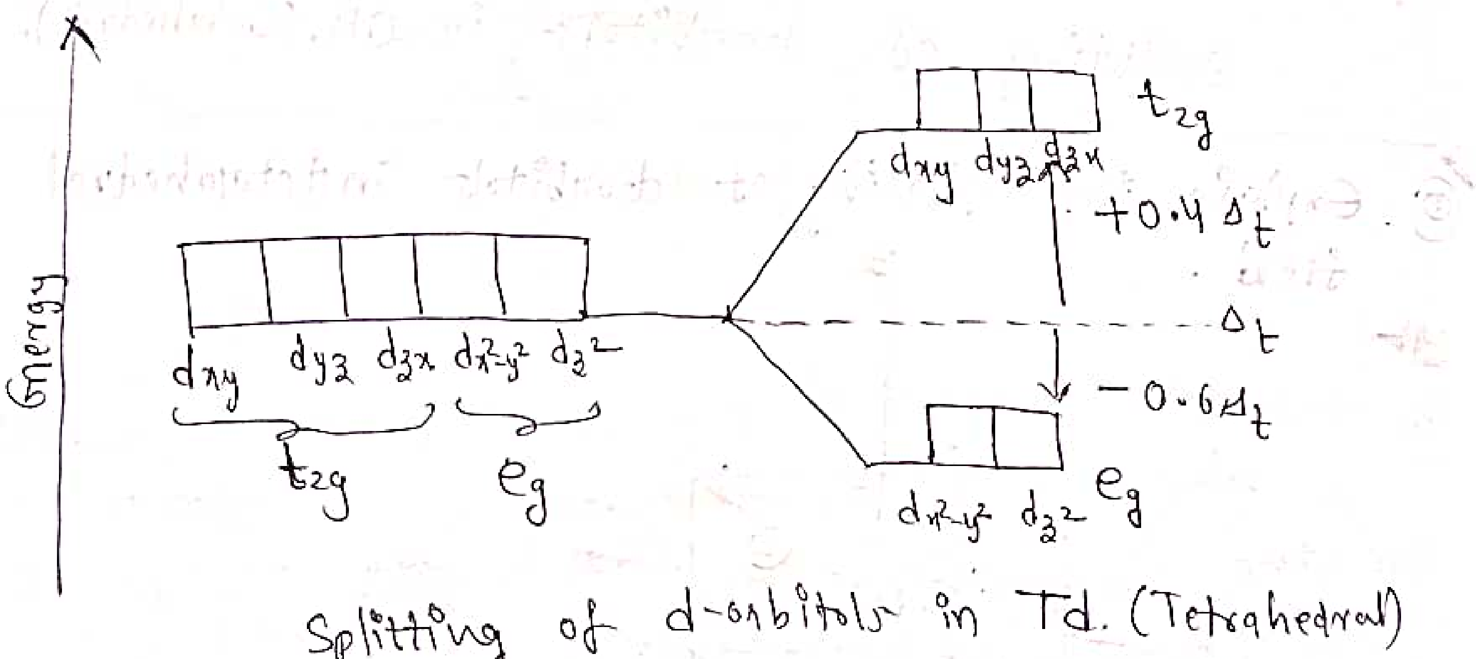
(i) In tetrahedral complexes the four ligands approaches towards the metal cation between the axis.

(ii) The e_g orbitols are located along the axis and the t_{2g} orbitols are located b/w the axis.

(iii) When the four ligands ~~are located b/w the~~ approaches to the metal cation the t_{2g} orbitols under go more repulsion with the ligands and the energy of t_{2g} orbitols is increased with $+0.4\Delta_t$. The e_g orbitols under go less repulsion with the ligands and the energy of e_g orbitols is decreased with $-0.6\Delta_t$.

(iv). The energy gap between t_{2g} orbitols and e_g orbitols is denoted with Δ_t.

(v) The Δ_t is known as crystal field splitting in tetrahedral field.



Splitting of d-orbitols in Td. (Tetrahedral)

Semi Conductors :-

Q. Write a note on Band Theory of Solids.

Sol: In solid crystal lattice, the 'n' number of atoms are combined together as the atomic orbitols to form molecular orbitols. Which are

onsidered as energy levels.
The 'n' number of energy levels interact to form energy band. Thus energy band is a group of energy levels in a solid.
The energy band is classified in to two types.
i) Valency Band (ii) Conduction Band.

Valency Band :-

Valency band is a outermost band. which is filled with electrons.

Conduction Band :-

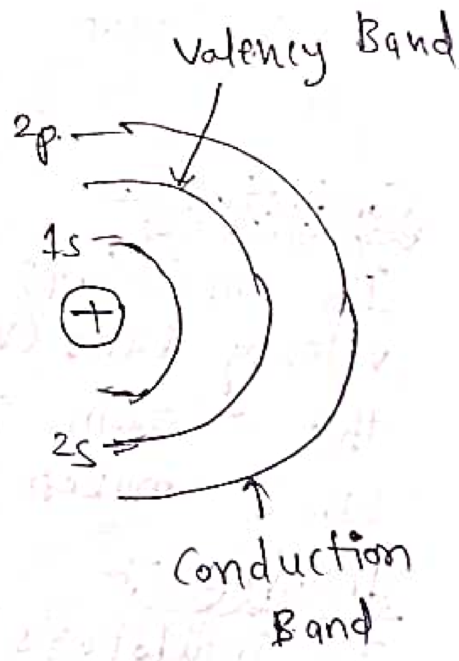
Conduction band is present above the valency band which is empty band.

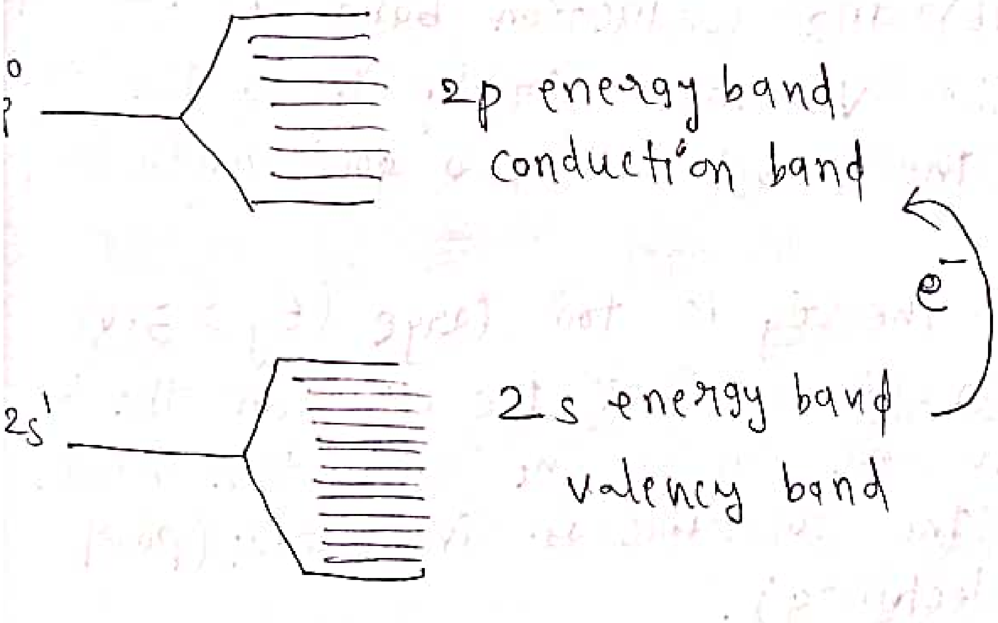
Forbidden Gap (E_g) :-

The energy gap between valency band and conduction band is known as forbidden gap.

Example :- Lithium crystal lattice.

$$EC = 1s^2 2s^1 2p^0$$



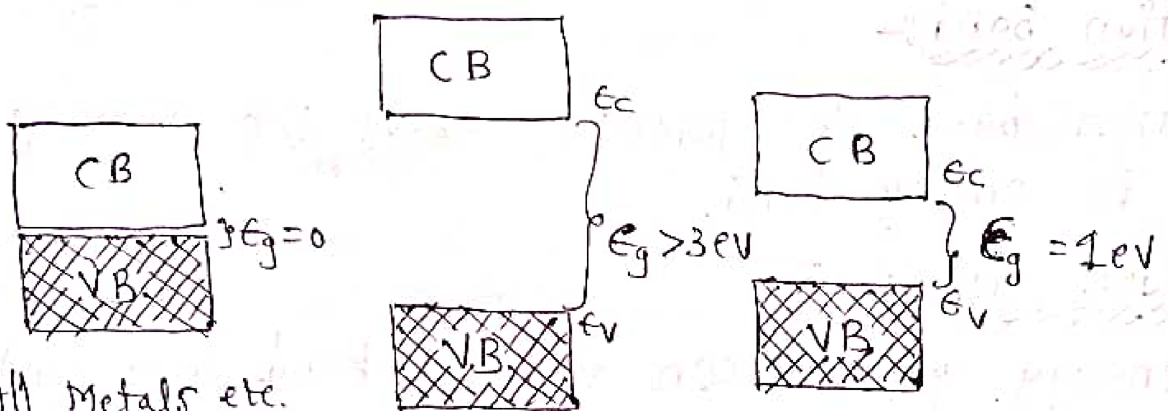


In lithium crystal lattice the e^- from valency band moves in to the conduction band which makes the substance as good conductor.

Q. Write the band diagram of conductors, insulators, semi conductors?

Sol:- The solid substances are classified into Three types, based on the energy gap between valency band and conduction band.

(i) Conductors, (ii) Insulators, (iii) semi Conductors.



ex: All Metals etc.

Conductors

ex:- Wood, Ceramic, etc.

Insulators

ex:- Si, Ge, -- etc.

Semi Conductors

Conductors:-

In conductors the energy gap is zero between valency band (VB) and conduction band (CB). So that the e^- from the VB move freely in to The CB. Which makes the substance as a good conductor.

Insulators:-

In insulators, the E_g is too large ($E_g > 3eV$) between VB and CB. So that the e^- from the VB are not able to move in to the conduction band. Which makes the substance as insulator (poor conductors of electricity).

Semi Conductors:-

In semi conductors the E_g is small ($E_g = 1eV$) between VB and CB. The semi conductors behaves as both insulators and conductors. At absolute zero temparature ($0^\circ K$) the semi conductors behaves as insulators. At room temparature the semi conductors behaves as conductors because at this temparature the e^- can break the covalent bond and come out as a free e^- which are enter into the CB.

Q. Write the effect of doping on semi conductors.

(or)

Explain the p-type and n-type semi conductors.

Sol:- The semi conductors are two types.

(i) Instrinsic Semi Conductors.

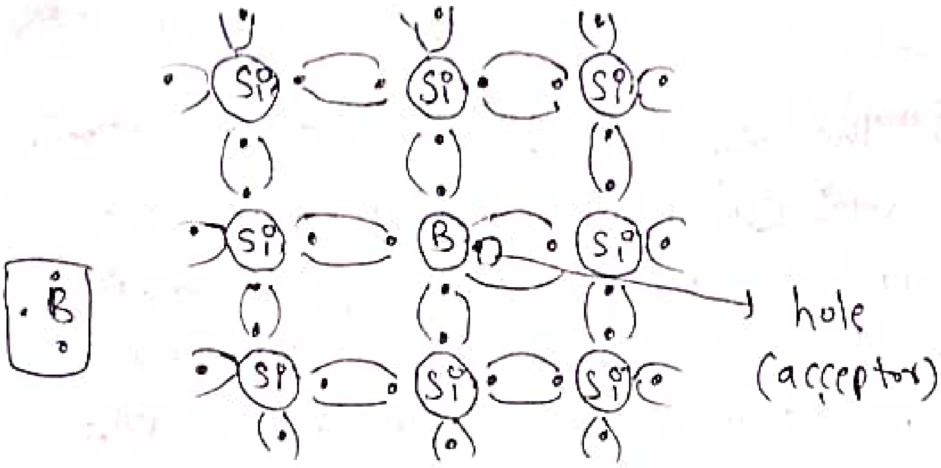
(ii) Extrinsic Semi Conductors.

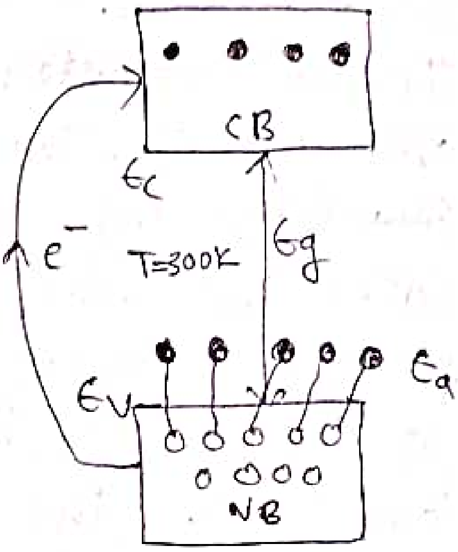
The pure form of semi conductors are known as instrinsic semi conductor. The process of adding of impurities to the instrinsic semi conductor is known as doping, the doped SC's are called extrinsic semi conductors. The extrinsic SC are two types. based on the addition of type of impurities to the instrinsic SC.

(i) P-type SC (ii) N-type SC.

P-type SC:-

The addition of tri-valent impurities like B, Al, Ga to the instrinsic SC is called p-type SC.





E_v = Energy of valency band

E_c = Energy of conduction band

E_a = accepting energy

In Si crystal lattice each si atom forms four covalent bonds with sorrounding si atoms. When the addition of 'B' impurities to the si crystal, the si atom is replaced by boron (B) atom.

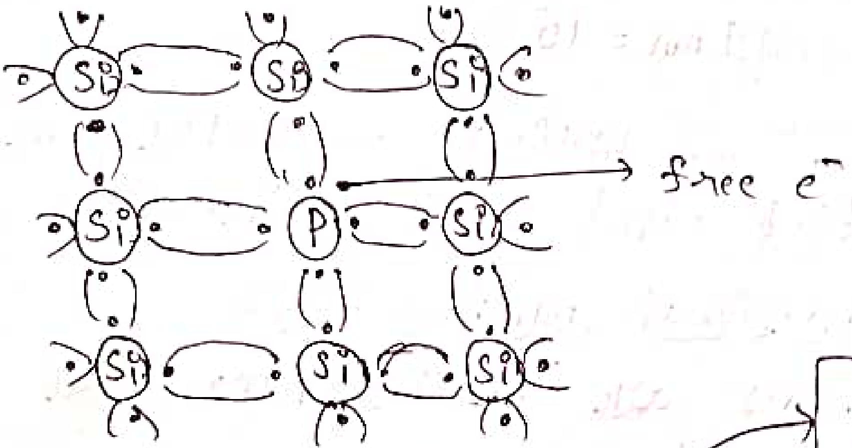
The B forms three covalent bonds with sorrounding si atoms and the 4^{th} bond is incomplete with the deficiency of e^-. which creats a hole. The boran is in the position to accept an e^-; the position ~~to accept an e^-~~, holes are called acceptors. the acceptor energy level (E_a) is closer to the VB.

At T > 0°K, the acceptors (holes) are accepting the e^-, from the sorrounding si atoms and creating new holes in the VB.

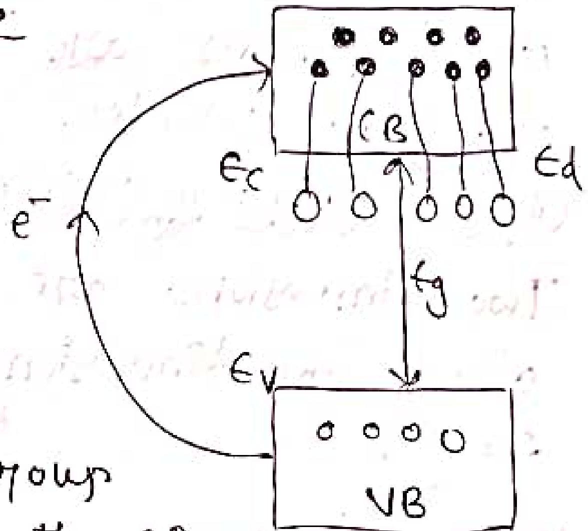
At T = 300k, due to breakage of covalent bonds e^- move in to the CB leaving holes in the VB. In p-type semi conductor the magarity of charge carriers are holes and the minority of charge carriers are electrons.

N-type Semi conductor:-

The addition of pentavalent impurities like P, As, Antimony to the instrinsic SC is known as n-type SC.



E_d = donar energy
E_c = Energy of CB
E_v = Energy of VB



When the addition of phosphorous impurities to the Si crystal, the Si atom is replaced by phosphorous atom. The 'P' has 5 valency e⁻ which forms 4 covalent bonds with surrounding Si atoms. and the 5^{th} e⁻ on the 'P' is left as free e⁻. The P is in the position to donate the e⁻. The donar energy level is closer to the CB.

At T > 0°K, the free electrons enter in to the CB.

At T = 300°K, due to the breakage of covalent bonds e⁻ move in the CB leaving holes in the VB.

In n-type SC the majority of charge carriers are e⁻ and the minority of charge carriers are holes.

Nanomaterials:-

The nano materials are defined as, the study of structures in the nano scale range. The nano scale range is 1nm to 100 nm.

$$\boxed{1\,nm = 10^{-9}\,m}$$

1nm is a one billianth of metre. The nanomaterials are classified based on the dimensions.

(i) 'O' - dimensional nanomaterials:-

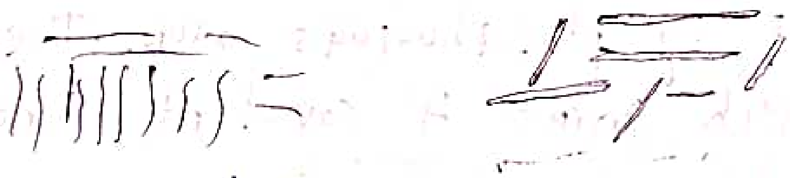
All dimensions are in the nano scale range.

ex:- Nano particles.

(ii) 1-D, nano materials:-

Two dimensions are in the nano scale range other one dimension is not in the nano scale range.

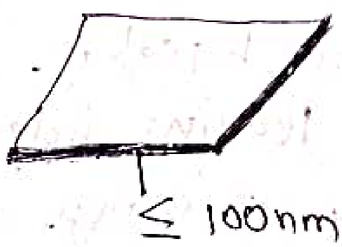
ex:- Nano wires, nano tubes.



(iii) 2-D, nanomaterials:-

One dimension is in the nanoscale range the other two dimensions are not in the nanosale range.

ex:- Nanofilms, nano coating.

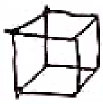


$\leq$ 100nm.

(iv) 3-D nanomaterials:-

No dimensions (x, y, z) in the nano scale range.

eg:- Nano crystals.



Q) Write a note on Graphene.

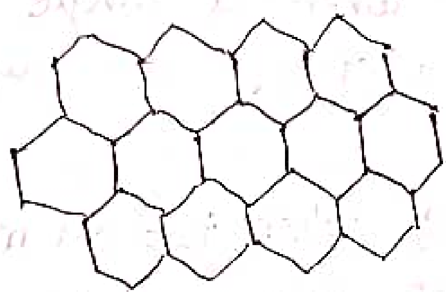
Sol:- (i) Graphene is one of the allotrophies of carbon.

(ii) A single layer of graphite is known as graphene.

(iii) In graphene each carbon atom is bounded with other three carbon atoms by strong covalent bonds.

(iv) In graphene all the carbon atoms are sp^2 hybridized.

(v) Graphene has 2-Dimensional hexagonal structure.



Graphene sheet.

Properties:-

(i) Graphene is the strongest, thinnest, flexible and light weight material.

(ii) Graphene is a excellent conductor.

Applications:-

(i) Graphene is used in high storage batteries and super charge batteries.

(ii) It is used in foldable display's of mobiles and laptops.

(iii) It is used in concrete in construction.
(iv) It is used as water filters.
(v) It is used as anti corrosive agents for metals.

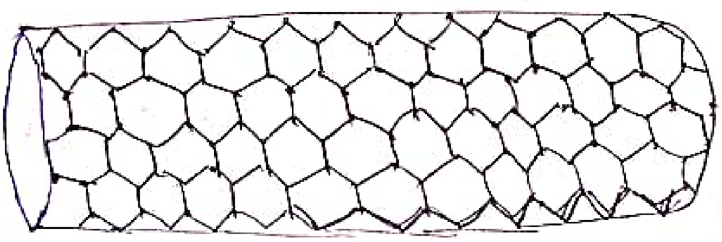
Q. Write the properties and applications of carbon nano tubes (CNT's)?

Sol:- Carbon nano tubes are the allotropies of carbon. CNT are formed when graphene sheets are rolled up into a tube. CNT's are sp^2 hybridized CNT's has cylindrical structure. CNT's are classified into two types.

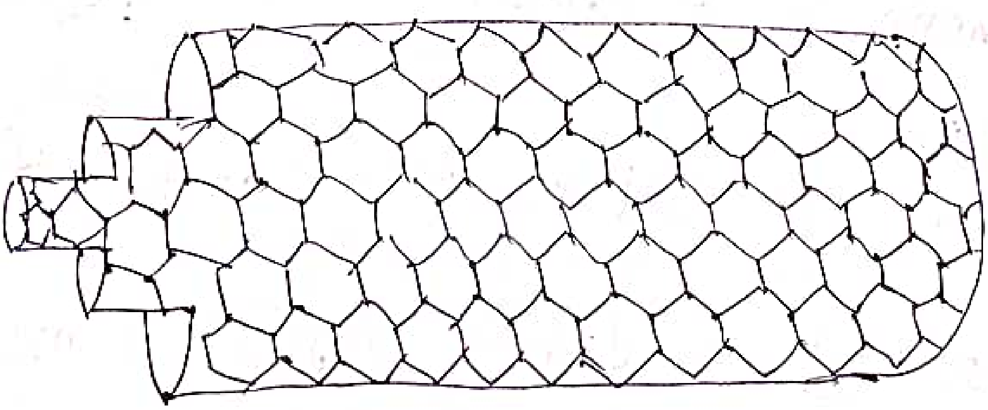
(i) Single walled CNT's
(ii) multi walled CNT's

Single walled CNT's:-
SWCNT's are formed when a single graphene sheets are rolled up into a tube.

Multi walled CNT's:-
MWCNT's are formed when two (or) more graphene sheets are rolled up into a tube.



SWCNT's



MWCNT's

Properties:-

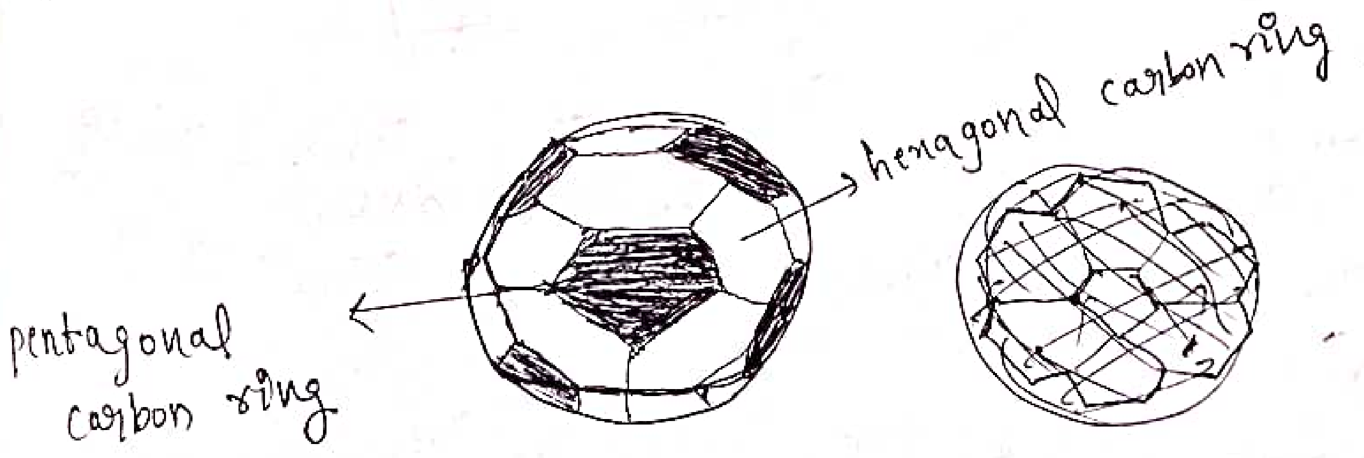
(i) CNT's are the strongest and stiffest materials.
(ii) CNT's have high electrical conductivity.
(iii) CNT's have high thermal conductivity.
(iv) CNT's have high flexibility.
(v) CNT's have low thermal expansion.

Applications:-

(i) CNT's are used in field emission transistors.
(ii) CNT's are used in field emission light devices.
(iii) CNT's are used in bio-sensors.
(iv) CNT's are used in cancer therapy and drug delevary.
(v) CNT's are used in energy storage batteries.

Q. Write the properties and applications of Fullerene.

Sol:- Fullerene are the allotrophes of carbon. It has hallow sphericle structure. It was discovered by R. Buckminister Fuller, So that it is called Buckminster fullerene and it is short named as fullerene (or) Bucky ball. The 'c' atoms are arranged in pentagonal and hexagonal manner.



C_{60} Fullerene

Properties:-

(i) Fullerenes acts as oxidizing agents.

(ii) Fullerenes are unstable at higher temparature.

(iii) C_{60} Fullerene is a very poor conductor of electricity but when reacts with alkalene it acts as super conductor.

(iv) Heat of sublimation increases with increasing the size of fullerene.

Applications:-

(i) Fullerenes are used in micro electronic devices.

(ii) Fullerenes are used in micro electrical devices.

(iii) Fullerenes are used in soft ferro-magnetic materials.

(iv) Fullerenes are used in non-linear optical devices.

(v) Fullerenes are used as super conductors.