

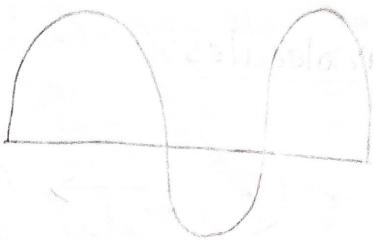
## Molecular Orbital theory

- Hund & Mullikan introduced (MoT) molecular orbital theory.
- To overcome the failures in the V.B.T.
- $2AO \rightarrow 2MO$
- Linear Combination of A.O. to form equivalent M.O. with same energy, same symmetry.

①



$$\psi_A + \psi_B$$



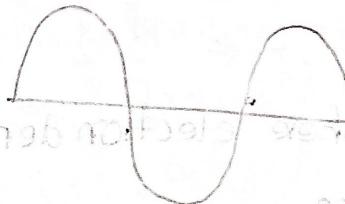
Constructive interference.

Bonding molecular orbital (BMO).

②



$$\psi_A - \psi_B$$



$$\psi_A - \psi_B$$

Destructive interference.

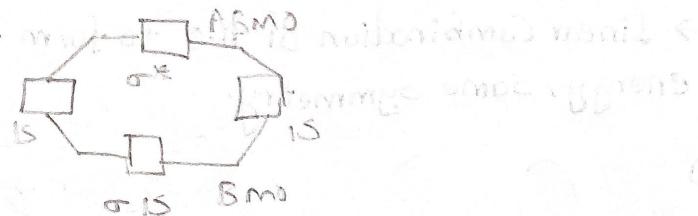
Anti-Bonding molecular orbital (ABMO).

- $AO + AO \rightarrow 2MO$
- BMO has less energy & more stable.
- ABMO has more energy & less stable.
- S-orbitals combine to form σ molecule orbitals.
- $P_z$ -S-orbital combines to form σ MO's.
- $P_x$ -orbital Combines to form  $\pi_x$  MO's.
- $P_y$ -orbital Combines to form  $\pi_y$  MO's.

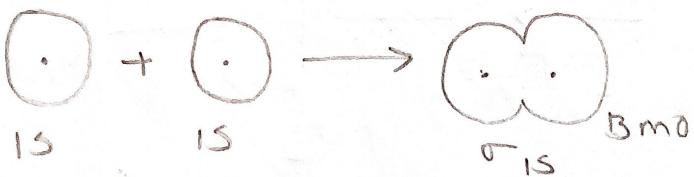
Orbital	MO
S	$\sigma$
P <sub>z</sub>	$\sigma$
P <sub>x</sub>	$\pi$
P <sub>y</sub>	$\pi$

→ Antibonding mo's forms Subtractive effect  $\sigma^*$ ,  $\pi^*$ .

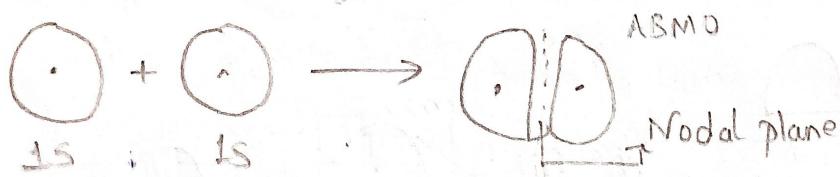
→ Bmo forms Addition effect  $\sigma$ ,  $\pi$ .



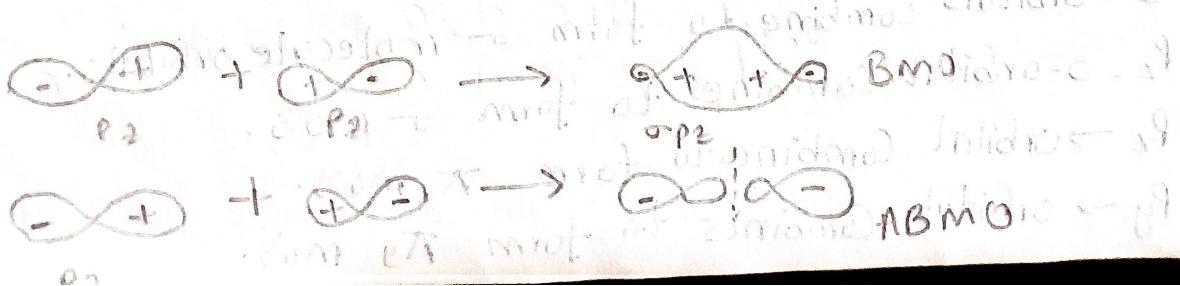
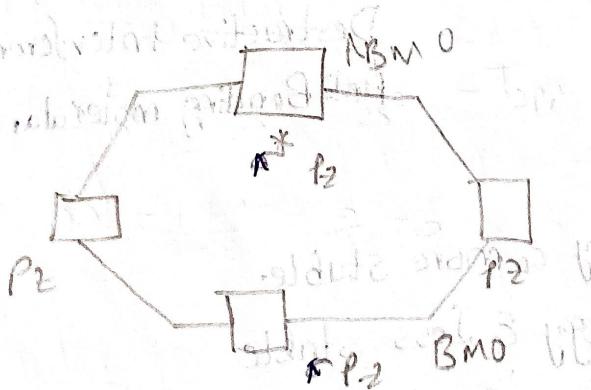
→ Bonding molecules:



→ Anti bonding molecules:



→ Plane where electron density of electron is zero is called Nodal plane.



$$\rightarrow \psi_{AB} = \psi_A + \psi_B$$

$$= \psi_A$$

$$= \psi_B$$

→ e<sup>-</sup> are

1. Affbari

↓  
Lower

→ Electr

Case-1:- N

σ<sub>IS</sub> <

Case-2:-

σ<sub>IS</sub> <

→ B.C

tractive

lone pair

X-

and S.

weak

covalent

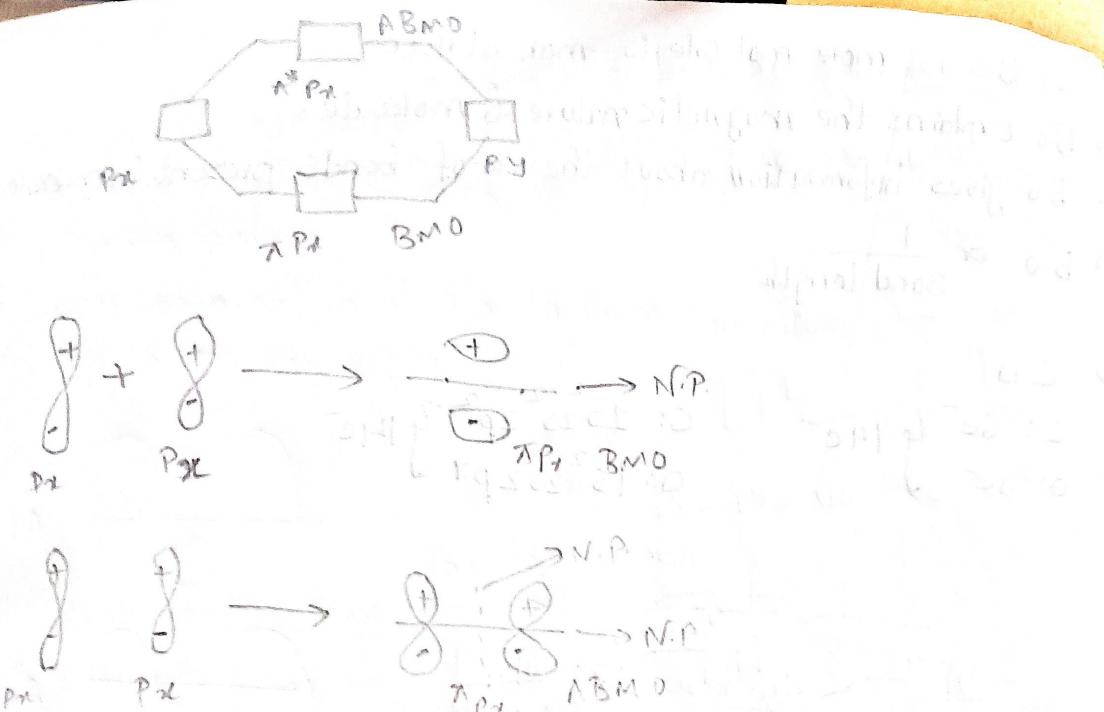
oxygen

water

hydrogen

bond

3D



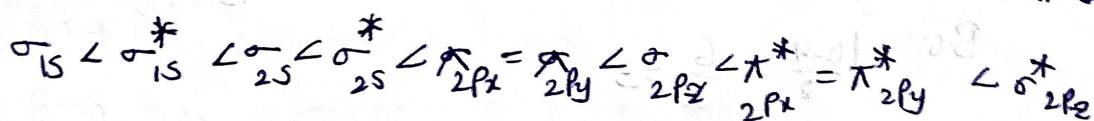
$$\begin{aligned}\psi_{AB} &= \psi_A \pm \psi_B \\ &= \psi_A + \psi_B (\text{BMO}) \\ &= \psi_A - \psi_B (\text{A.B.M.O.})\end{aligned}$$

→ e<sup>-</sup> are filled in the mo by follow three principles they were

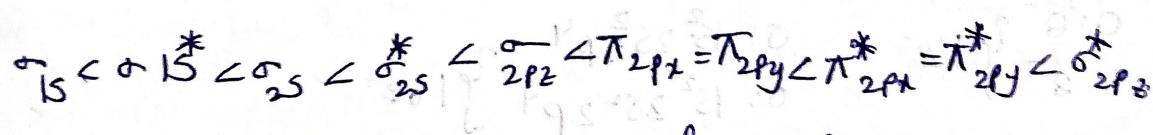
1. Aufbau's
  2. Hund's.
  3. Paulis exclusive.
- ↓      ↓      ↓  
Lower    Later    next

→ Electrons are filled in the mo's as follows.

Case-1: No. of electrons in a molecule are 14 (or) less than 14.



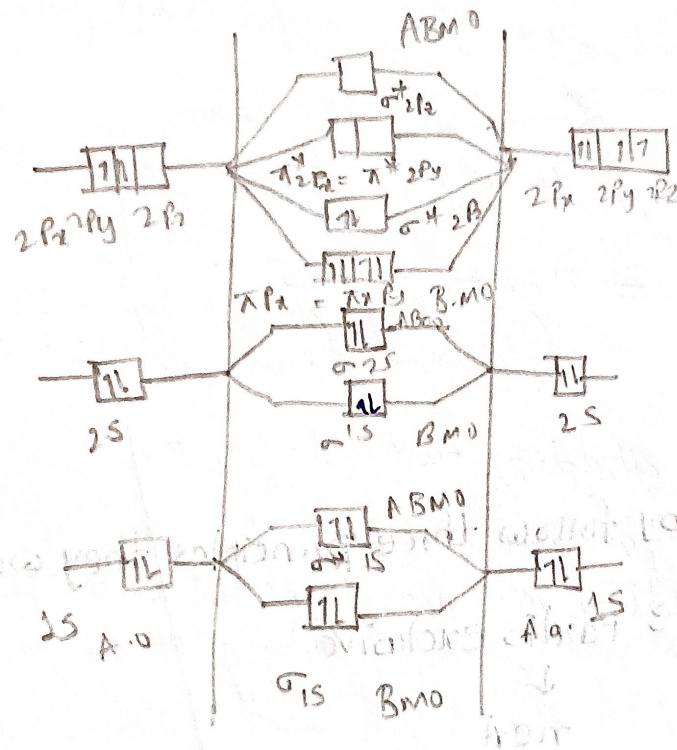
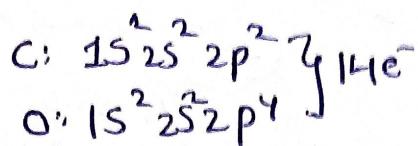
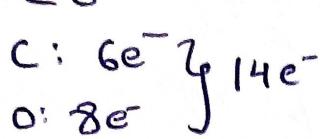
Case-2: No. of electrons in a molecule more than 14.



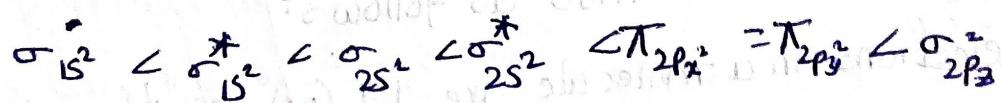
$$\rightarrow \text{B.O.} = \frac{\text{no. of } e^- \text{ in BMO} - \text{no. of } e^- \text{ in A.B.MO}}{2}$$

- If B.O. is more molecule is more stable.
- B.O. explains the magnetic nature of molecule.
- B.O. gives information about the no. of bonds present in molecule.
- $B.O. \propto \frac{1}{\text{Bond length}}$

→ CO

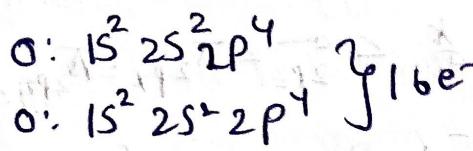
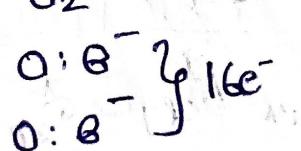


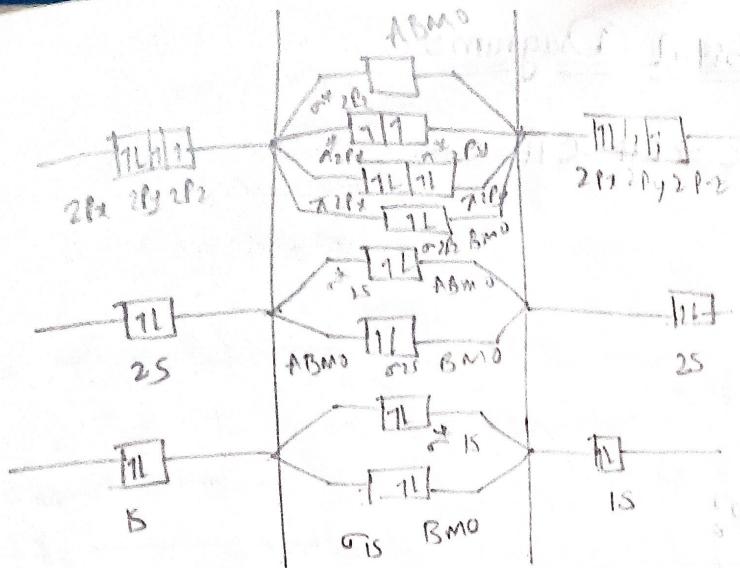
→ Electronic Configuration:



$$B.O. = \frac{10 - 4}{2} = \frac{6}{2} = 3$$

→ O<sub>2</sub>





→ Electronic Configuration:

$$\sigma_{1s}^2 < \sigma_{1s}^{*2} < \sigma_{2s}^2 < \sigma_{2s}^{*2} < \sigma_{2p_z}^2 < \pi_{2p_x}^2 = \pi_{2p_y}^2 < \pi_{2p_z}^{*2} = \pi_{2p_y}^{*2}$$

$$\rightarrow O_2, O_2^+, O_2^-, O_2^{2-}$$

Electron	Bo	Electron	B.O.
14	3	14	3
13	2.5	15	2.5
12	2.0	16	2.0
11	1.5	17	1.5
10	1.0	18	1.0
9	0.5	19	0.5
8	0	20	0

$O_2 \rightarrow 2.0$   
 $O_2^+ \rightarrow 2.5$   
 $O_2^- \rightarrow 1.5$   
 $O_2^{2-} \rightarrow 1.0$

$O_2^+$  is more stable.  
 $O_2^+ > O_2 > O_2^- > O_2^{2-}$

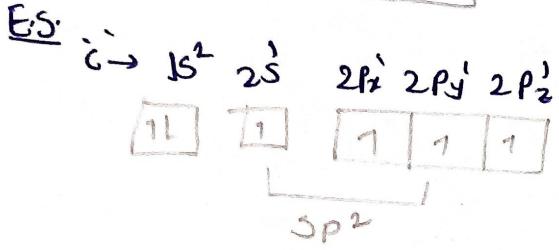
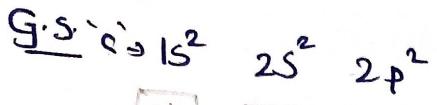
→  $N_2, N_2^+, CN, CN^-$

$$\downarrow \quad \downarrow \quad \downarrow \quad \downarrow \\ 2.5 \quad 3 \quad 2.0 \quad 3$$

$$N_2^+ = CN^- \rightarrow CN = N_2$$

## Molecular Orbital Diagrams

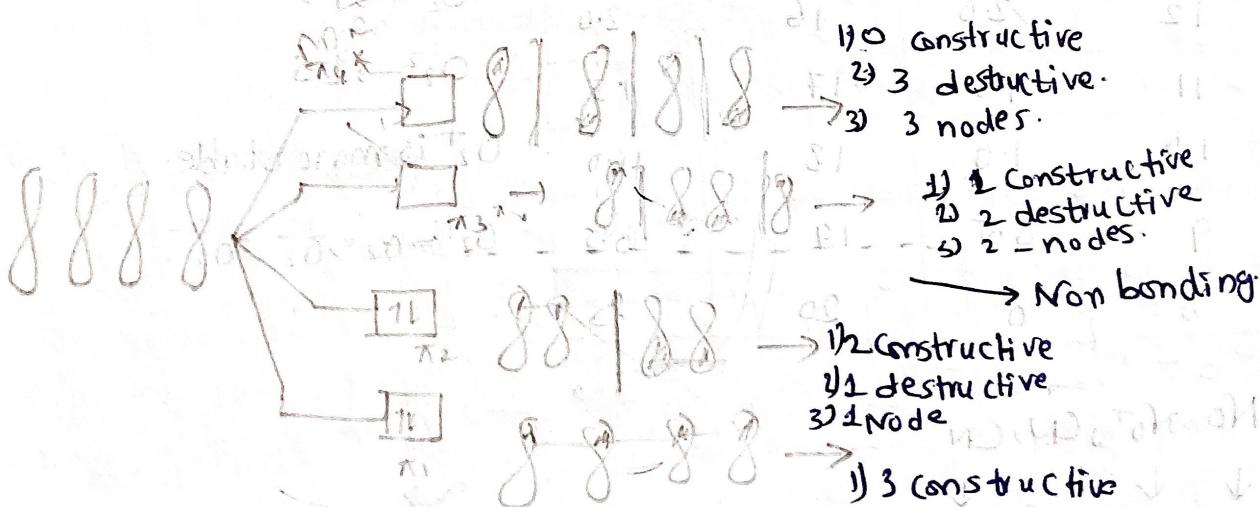
- ① 1,3 butadiene  $\rightarrow \text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CH}_2$
- ② Benzene.



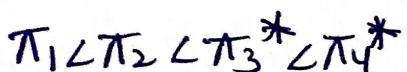
→ Each carbon include in  $sp^2$  hybridisation.

→ Molecule contains 4 hybrid orbitals.

→ molecule Contains 4 molecular orbitals.



→ Energy order:



\* Below the horizontal line B.m.o forms

\* Above the horizontal line A.B.m.o forms

→ Nodal  
D m  
 $\pi$  1

- ① Hetero
- ② don't
- ③ Stab
- ④ It

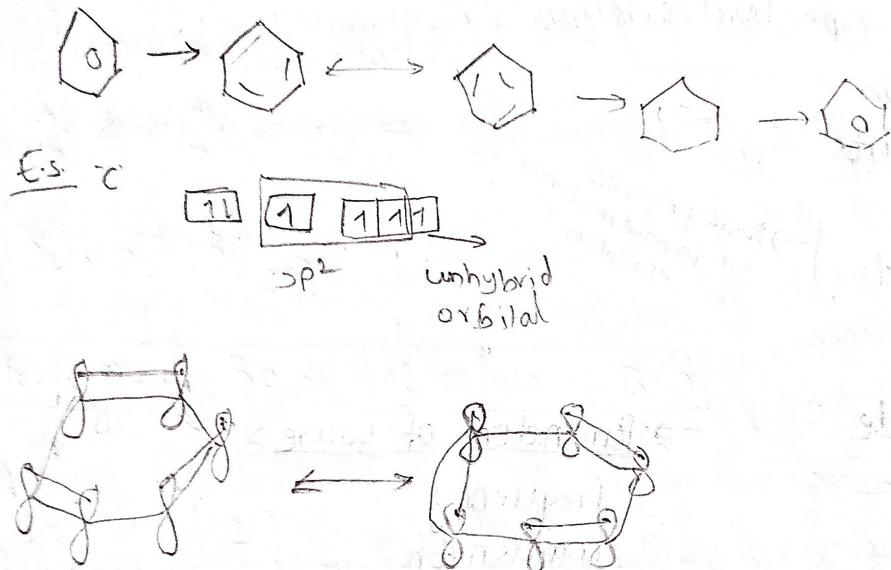
⑤ B

→ Node =  $(n-1)$   
D n = energy level

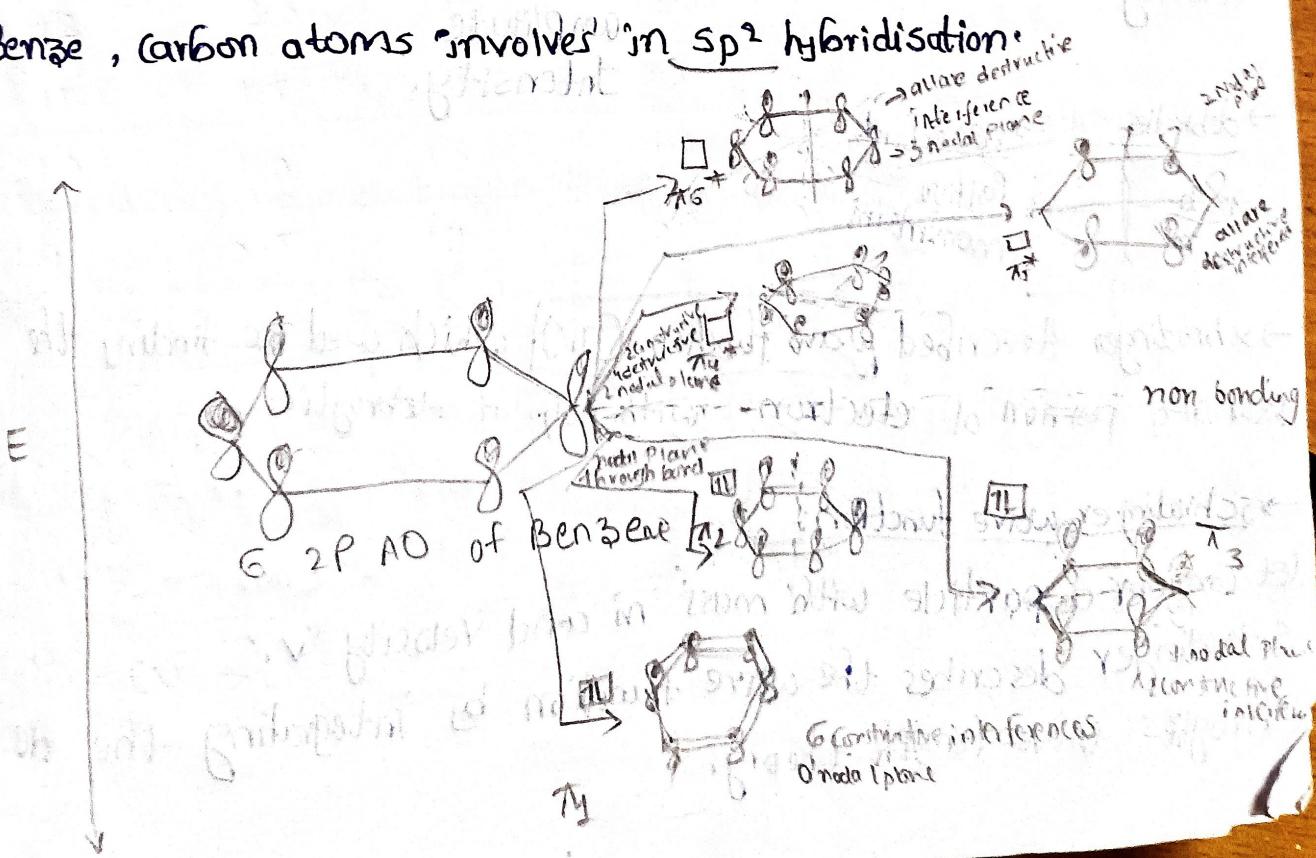
$$\pi_1=0; \pi_2=1, \pi_3=2, \pi_4=3$$

### $\pi$ -molecular orbital diagram of benzene

- ① Hexagonal planar & Cyclic Structure.
- ② Double bonds present in Conjugation.
- ③ Stable compounds due to delocalisation of  $e^-$ .
- ④ It contains 6 unhybridized p-orbitals which are perpendicular to each other.



- ⑤ Benzene, carbon atoms involves in  $sp^2$  hybridisation.



## Quantum mechanics

Classical computers

Super Computers

Quantum Computers.

Industrial revolution

Digital revolution

Quantum technology.

### \* wave-particle duality

It is the branch of physics, where it deals the behaviour of materials and energy at microscope level / subatomic level.

\* Solidity is an illusion.

\* Double slit Experiment.

\* Super position. ✓

\* Quantum Entanglement ✓

\* Spooky action at a distance.

↳ Basic properties  
for quantum mechanics  
applications

### → parameters of particle

mass

energy

velocity

### → parameters of wave

frequency

wavelength

amplitude

Intensity.

### → de Broglie

$$\lambda = \frac{h}{mv}$$

### → Heisenberg

Position  
momentum

→ Schrodinger described wave function, ( $\psi$ ), which used to finding the location & position of electron. with help of de Broglie.

### → Schrodinger wave function:

Let consider a particle with mass 'm' and velocity 'v.'

Schrodinger describes the wave function by integrating the de.

Broglie's wave length theory,

Consider de Broglie  
as  $\psi(x)$  di

$$\Delta^2 \psi =$$

Solution of

$$\psi(x,t)$$

we can

different

$$\frac{\partial^2 \psi}{\partial t^2}$$

$$\frac{\partial^2 \psi}{\partial x^2}$$

Subs

↓

10

incorp

Total

Consider deBroglie wave at a location  $r$  at a time  $t$  can be represented as  $\psi(r,t)$ . differential equation of wave motion in that three dimensions.

$$\nabla^2 \psi = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2}$$

Solution of the above equation.

$$\psi(r,t) = \psi_0 e^{-i\omega t}$$

$\omega$  angular momentum

Differentiating above equation twice

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \psi}{\partial r^2} = -\omega^2 \psi(r,t)$$

Substituting in eqn ①

$$\nabla^2 \psi = \frac{-\omega^2}{v^2} \psi(r,t)$$

$$\nabla^2 \psi = -\frac{\omega^2}{v^2} \psi$$

$$\nabla^2 \psi^2 = -\frac{4\pi^2}{\lambda^2} \psi$$

$$\nabla^2 \psi + \frac{4\pi^2}{\lambda^2} \psi = 0$$

$$\text{Since } \omega = 2\pi\nu$$

$$= 2\pi \frac{v}{\lambda}$$

$$\nu = \frac{v}{\lambda}$$

Incorporating the deBroglie equation  $\lambda = \frac{h}{mv}$

$$\nabla^2 \psi + \frac{4\pi^2 m^2 v^2}{h^2} \times \psi = 0$$

Total energy ( $E$ ) = k.E. + P.E.

$$E = \frac{1}{2} mv^2 + v$$

$$\frac{1}{2} mv^2 = E - v$$

$$mv^2 = 2(E - v)$$

$$m^2 v^2 = 2m(E - v)$$

$$\nabla^2 \psi + \frac{4\pi^2 m(E-V)}{\hbar^2} \psi = 0$$

$$\nabla^2 \psi + \frac{8\pi^2 m}{\hbar^2} (E-V) \psi = 0$$

Since  $\hbar = \frac{h}{2\pi}$

$$\hbar = \frac{h}{2\pi}$$

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E-V) \psi = 0$$

$$\nabla^2 \psi + \frac{2m}{h^2} (E-V) \psi = 0$$

$$\boxed{\nabla^2 \psi + \frac{2m}{\hbar^2} (E-V) \psi = 0}$$

This Schrodinger wave equation and here time is not appear.  
so it is time independent Schrodinger wave equation.

In one dimension it can be written as

$$\boxed{\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E-V) \psi = 0}$$

for time dependent need to eliminate  $E$  from the equation

$$\psi_{(r,t)} = \psi_0(r,t) e^{-i\omega t}$$

differentiation

$$\text{on here } \frac{\partial \psi}{\partial t} = i\omega \psi_0(r,t) e^{-i\omega t}$$

$$\frac{\partial \psi}{\partial t} = -i(2\pi V) \psi$$

$$\frac{\partial \psi}{\partial t} = (-i\frac{2\pi E}{\hbar}) \psi$$

$$\frac{\partial \psi}{\partial t} = -i\frac{2\pi E}{\hbar} \psi \times \frac{i}{i} = -C^{-1} \psi$$

$$\frac{\partial \psi}{\partial t} = \frac{2\pi E \hbar \psi}{ih}$$

$$\text{Since } \hbar = \frac{h}{2\pi} \Rightarrow h = \hbar 2\pi$$

$$\frac{\partial \psi}{\partial t} = \frac{2\pi E}{i(2\pi)^2}$$

$$\frac{\partial \psi}{\partial t} = \frac{E\psi}{i\hbar}$$

$$E\psi = i\hbar \frac{\partial \psi}{\partial t}$$

substituting the values in ~~second~~ Schrodinger wave

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E\psi - V\psi) = 0$$

$$\nabla^2 \psi = -\frac{2m}{\hbar^2} (E\psi - V\psi)$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V\right) \psi = i\hbar \frac{\partial \psi}{\partial t}$$

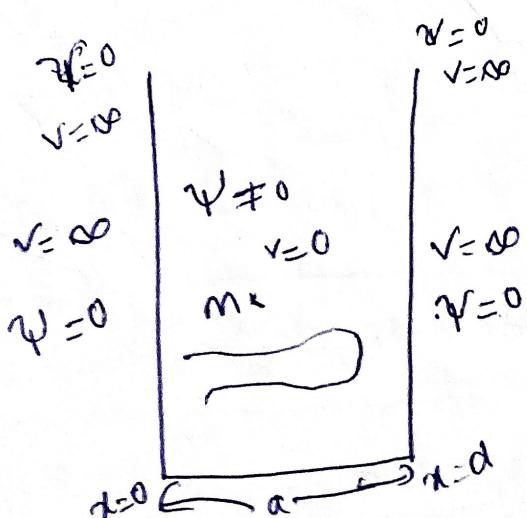
$H = -\frac{\hbar^2}{2m} \nabla^2 + V$  is called Hamiltonian operation.

So,

$$H\psi = i\hbar \frac{\partial \psi}{\partial t}$$

→ Schrodinger wave equation of particle in 1D Box

\* Define potential energy and wavefunction of particle in 1D dimensional box.



②

Solution of Schrödinger wave eqn of particle in 1D box

Schrödinger wave eqn in one 8<sup>th</sup> particle moving 1D Box

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

Schrödinger wave eqn 8<sup>th</sup> particle moving 1D Box

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E \psi = 0 \quad \text{--- (1)}$$

$$\frac{d^2\psi}{dx^2} + k^2 \psi = 0 \quad \text{--- (2)}$$

where

$$k^2 = \frac{8\pi^2 m E}{h^2}$$

$$\psi = A \cos(kx) + B \sin(kx) \quad \text{--- (3)}$$

where A & B are constant

for finding A & B

we apply boundary condition.

$$\psi = 0 \text{ at } x=0 \text{ i.e. } \psi(0) = 0$$

$$\psi = 0 \text{ at } x=a \text{ i.e. } \psi(a) = 0$$

At  $x=0$

$$0 = A \cos(0) + B \sin(0)$$

$$A = 0$$

$$\psi = B \sin kx \quad \text{--- (4)}$$

At  $x=a$

$$0 = B \sin ka$$

$B \neq 0$  (always not equal)

$$\sin k\alpha = 0 \quad \sin \theta [ \theta = 0, 180, 360, 540, 720 ]$$

$$k\alpha = n\pi$$

(where  $n = 0, 1, 2, 3$ )

$$\psi_n = B \sin \frac{n\pi}{a} x \rightarrow (6)$$

Evaluating B,

applying normalization condition

$$\int_0^a |\psi_n|^2 dx = 1$$

$$\int_0^a B^2 \sin^2 \frac{n\pi x}{a} dx = 1$$

$$B^2 \int_0^a \sin^2 \frac{n\pi x}{a} dx = 1$$

$$\sin^2 \theta = \frac{1}{2} [1 - \cos 2\theta]$$

$$B^2 \int_0^a \frac{1}{2} [1 - \cos \frac{2n\pi x}{a}] dx = 1$$

$$\frac{B^2}{2} \int_0^a [1 - \cos \frac{2n\pi x}{a}] dx = 1$$

$$\frac{B^2}{2} \int_0^a dx - \frac{B^2}{2} \int_0^a \cos \frac{2n\pi x}{a} dx = 1$$

$$\frac{B^2}{2} [a - 0] - \frac{B^2}{2} \left[ \sin \frac{2n\pi x}{a} + C \right] = 1$$

$$\frac{B^2}{2} a = 1$$

$$\frac{B^2}{2} = \frac{1}{a} \Rightarrow B = \sqrt{\frac{2}{a}}$$

$$\boxed{\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \quad (n=1, 2, 3)}$$

normalised wave function of particle in 1D box is

$$\boxed{\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}}$$

## Determination of energy of a particle moving 1D Box

$$k^2 = \frac{8\pi^2 m E}{h^2}$$

$$\frac{n^2 k^2}{a^2} = \frac{8\pi^2 m E}{h^2}$$

$$E = \frac{n^2 h^2}{8ma^2}$$

$$E_n = \frac{n^2 h^2}{8ma^2}$$

## Energy difference between two successive energy levels:

$$E_n = \frac{n^2 h^2}{8ma^2}$$

$$\Delta E = \frac{(2n+1)h^2}{8ma^2}$$

$$E_{n+1} = \frac{(n+1)^2 h^2}{8ma^2}$$

$$\Delta E \propto n$$

$$\Delta E \propto \frac{1}{m}$$

$$\Delta E = E_{n+1} - E_n$$

$$= \frac{(n+1)^2 b^2}{8ma^2} - \frac{n^2 b^2}{8ma^2}$$

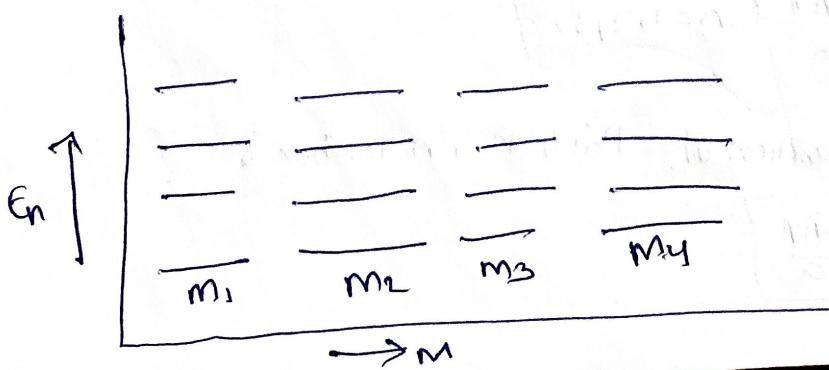
$$= \frac{(n^2 + 2n + 1)h^2}{8ma^2} - \frac{n^2 h^2}{8ma^2}$$

$$= \frac{h^2}{8ma^2} [n^2 + 2n + 1 - n^2]$$

$$\Delta E = \frac{(2n+1)h^2}{8ma^2}$$

$$\Delta E \propto n$$

$$\Delta E \propto \frac{1}{m}$$



$m_1 < m_2 < m_3 < m_4$

$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

for  $n=1$

at  $x=0$

$$\psi_1(0) = \sqrt{\frac{2}{a}} \sin \frac{\pi(0)}{a} = 0$$

at  $x=\frac{a}{4}$

$$\psi_1\left(\frac{a}{4}\right) = \sqrt{\frac{2}{a}} \sin \frac{\pi \cdot \frac{a}{4}}{a} = \sqrt{\frac{2}{a}} \times \frac{1}{\sqrt{2}} = \frac{1}{\sqrt{a}}$$

at  $x=\frac{a}{2}$

$$\psi_1\left(\frac{a}{2}\right) = \sqrt{\frac{2}{a}} \sin \frac{\pi a}{2a} = \sqrt{\frac{2}{a}}$$

at  $x=\frac{3a}{4}$

$$\psi_1\left(\frac{3a}{4}\right) = \sqrt{\frac{2}{a}} \sin \frac{\pi \cdot \frac{3a}{4}}{a} \quad \sin 135^\circ = \frac{1}{\sqrt{2}}$$

$$= \sqrt{\frac{2}{a}} \sin \frac{3\pi}{4}$$

$$\Rightarrow \sqrt{\frac{2}{a}} \times \frac{1}{\sqrt{2}} = \sqrt{\frac{1}{a}}$$

at  $x=a$

$$\psi(a) = \sqrt{\frac{2}{a}} \sin \frac{\pi a}{a} = 0$$

$n=2$

$x=0 \Rightarrow 0$

$x=\frac{a}{4} \Rightarrow \sqrt{\frac{1}{a}}$

$x=\frac{a}{2} \Rightarrow 0$

$x=\frac{3a}{4} \Rightarrow -\sqrt{\frac{1}{a}}$

$x=a \Rightarrow 0$

$n=1$

$x=0 \Rightarrow 0$

$x=\frac{a}{4} = \sqrt{\frac{1}{a}}$

$x=\frac{a}{2} = \sqrt{\frac{1}{a}}$

$x=\frac{3a}{4} = \sqrt{\frac{1}{a}}$

$x=a \Rightarrow 0$

Wave function plots:-

$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

for  $n=2$

$x=0$

$$\psi(0) = \sqrt{\frac{2}{a}} \sin \frac{\pi(0)}{a} = 0$$

$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{2\pi n x}{a} = \sqrt{\frac{2}{a}} \quad \text{for } n=2$$

$$x = \frac{a}{4}$$

For  $n=2$ ;  $x = \frac{a}{2}$

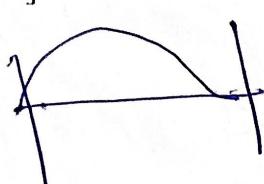
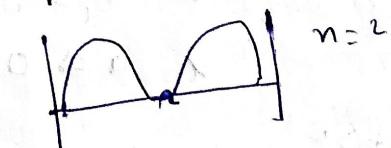
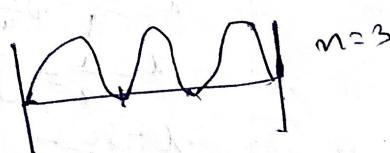
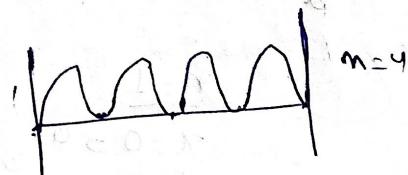
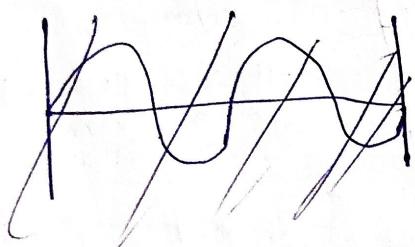
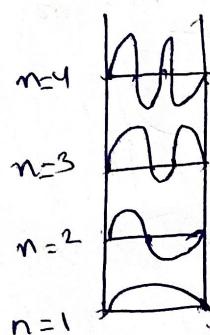
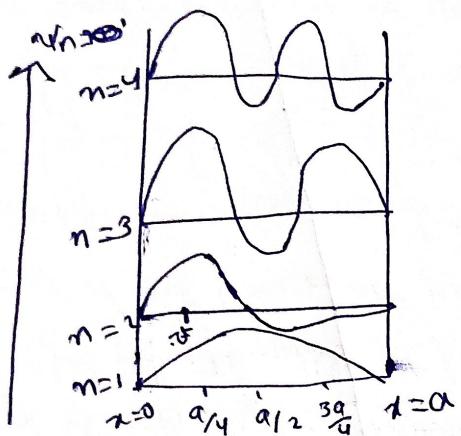
$$\sqrt{\frac{2}{a}} \sin \frac{2\pi \cdot 2 \cdot \frac{a}{2}}{a} = 0$$

for  $n=2$ ;  $x = \frac{3a}{4}$

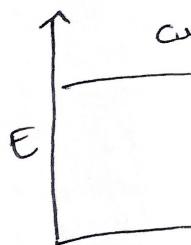
$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{2\pi \cdot 2 \cdot \frac{3a}{4}}{a} = -\sqrt{\frac{2}{a}}$$

for  $n=2$ ;  $x=a$

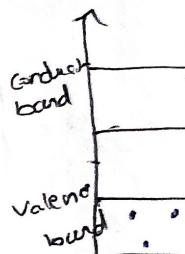
$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{2\pi \cdot 2 \cdot a}{a} = 0$$



\*Conductors



\*Semiconductors



Silicon

Types:

① Intrinsic

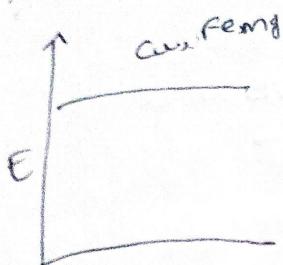
These are

$\text{Si}(Z=14)$

Dopants

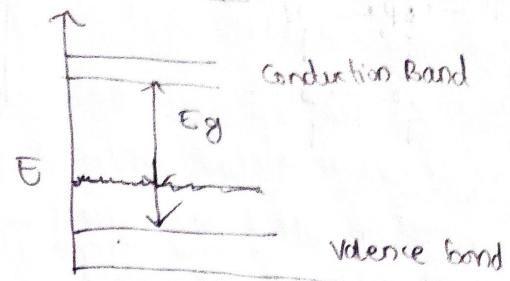
## Semi Conductors

\* Conductors:

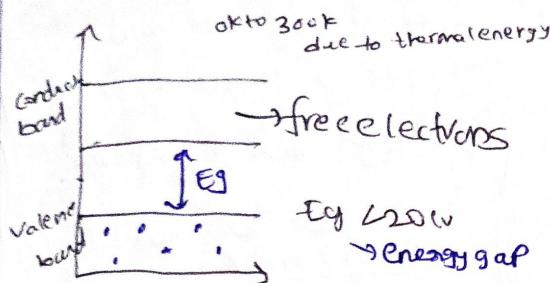


OK

\* Insulator



\* Semi conductor:



silicon Si, Ge

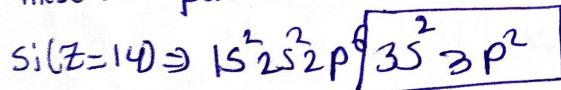
valency band: Highest energy level of element.

wood, diamond

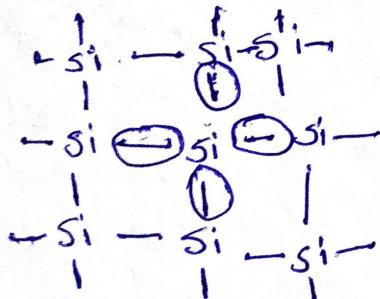
TypeS:

① Intrinsic Semiconductor

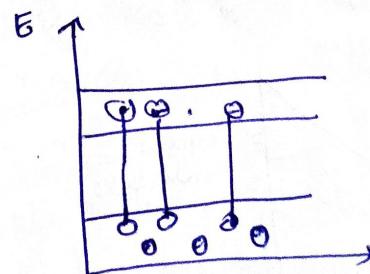
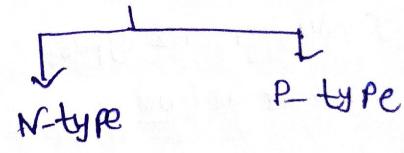
These are pure semiconductors.



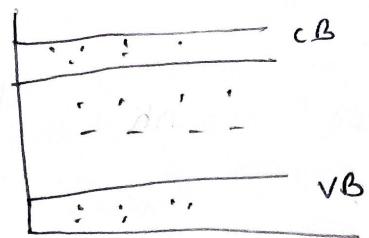
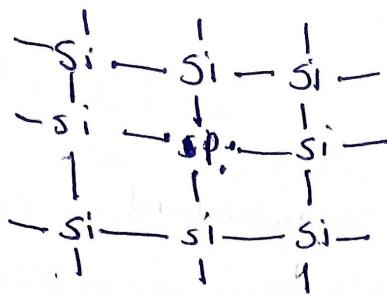
Dopes



② Extrinsic Semiconductor



## N-Type

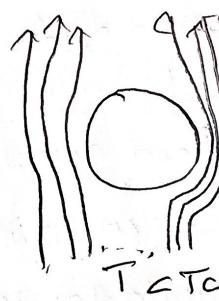


### \*Superconductor:

- \* At zero resistance & low temperature Ex:- mercury(Hg)
- \* It is introduced by Onnes in 1911
- \*  $T_c \rightarrow$  Critical temperature
- \* Below  $T_c \rightarrow$  Superconductor  $\rightarrow$  diamagnetic nature
- \* Above  $T_c \rightarrow$  normal conductor.



$T > T_c$



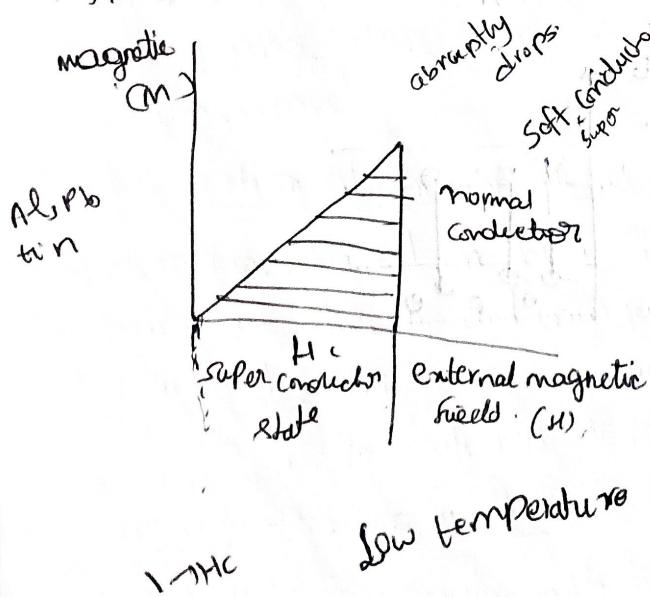
$T < T_c$

meissner effect.

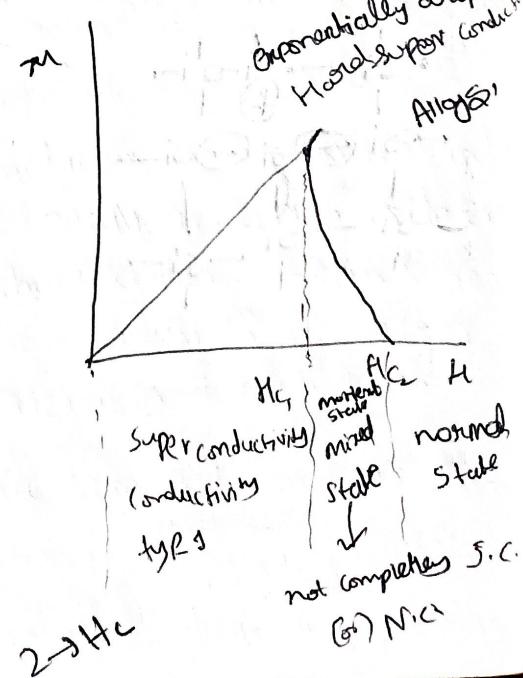
- \*  $H_c$  also same as  $\approx T_c$ .

- \* Semiconductors  $\rightarrow$  2 types.

- \* Type-I semiconductors:



- \* Type-II Semiconductors



Semiconductor properties they play a crucial role in their technology.

\* Semiconductors have unique properties between conductors and insulators.

Conducting energy (superconductors)

Semiconductors

\* In conduction electric current

\* when allowing

Insulating external valence band

\* In the

do not

\* In the flow

charge

① Electrical

electricity like

the electrons

bound to their

Semiconductors: These are a class of materials that have electrical properties that fall between those of conductors & insulators. They play a crucial role in modern electronics and technology because they can be used to control and manipulate electric currents.

\* Semiconductors can act as both conductors and insulators depending on their temperature and the energy of their electrons. Due to this, if have unique energy band structure, which allows them to transition between conducting and insulating states.

→ Conducting state: At higher temperature or when provided with external energy (such as applying a voltage), electrons in the valence band of a semiconductor can gain enough energy to jump into the conduction band.

\* In conductors, the electrons are relatively free to move and can conduct electricity, similar to what happens in conductors like metals.

\* When electrons are in the conduction band, it behaves as a conductor, allowing the flow of electrical current.

→ Insulating state: \* At lower temperatures or in the absence of external energy, most of the electrons in a semiconductor remain in the valence band.

\* In the valence band, electrons are bound to their respective atoms and do not have enough energy to conduct electricity.

\* In this state, the semiconductor behaves as an insulator, resisting the flow of electrical current.

→ Characteristics of Semiconductors:

① Electrical Conductivity: Semiconductors are materials that have intermediate electrical conductivity compared to conductors (like metals) and insulators (like rubber or glass). In conductors, electrons move freely, allowing for the easy flow of electrical current. In insulators, electrons are tightly bound to atoms and do not move freely. Semiconductors fall in b/w their electrons can move, but not as freely as in conductors.

2. Atomic Structure: The electrical properties of semiconductors are primarily determined by their atomic structure. Semiconductors are typically crystalline in nature, with atoms arranged in regular lattice structures. These atoms have valence electrons that are involved in electrical conduction.

3. Energy Bands: The behavior of electrons in semiconductors can be understood through the concept of energy bands. In a semiconductor, there are two main energy bands: the valence band is empty under normal conditions. To conduct electricity, electrons need to move from the valence band to conduction band.

4. Band Gap: The energy difference b/w the valence band and the conduction band is known as the band gap. Semiconductors have a relatively small band gap compared to insulators, which have a large band gap. The band gap is a critical parameter as it determines the energy required to move electrons from the conduction band.

5. Doping: One of the essential characteristics of semiconductors is their ability to be doped, which means intentionally introducing impurities into the crystal lattice. Doping can increase or decrease the electrical conductivity of the semiconductor. There are two main types of doping: n-type (adding electrons) and p-type (adding holes, or positive charge carriers). Doping allows for the creation of semiconductor devices like transistors.

\* Classification of Semiconductors: Semiconductors can be classified into two main types based on their electrical behavior, which is determined by their atomic structure and energy band characteristics: Intrinsic semiconductors and extrinsic semiconductors. These categories are further divided into specific materials. Here's an overview of each type.

① Intrinsic Semiconductors: \* Intrinsic semiconductors are pure semiconductor materials with no intentional impurities. They consist of a single type of semiconductor element - silicon (Si) & germanium.

are the most  
\* These materials

intrinsic properties  
\* Intrinsic semiconductors have holes) that is relatively

2. Extrinsic Semiconductors:

\* Extrinsic semiconductors have intentional

Doping is a characteristic of extrinsic semiconductors.

\* Extrinsic semiconductors are based on the type of dopant used.

a) N-Type:

\* In N-type semiconductors, extra electrons are added.

\* These contribute to negative charge carriers.

\* N-Type: Semiconductors with negative charge carriers.

b) P-Type:

\* In P-type semiconductors, extra holes are added.

\* These contribute to positive charge carriers.

\* P-Type: Semiconductors with positive charge carriers.

\* P-type semiconductors have positive charge carriers.

- \* These materials have their electrical properties determined solely by the intrinsic properties of the Semiconductor crystal lattice.
- \* Intrinsic Semiconductors natural number of charge carriers (electrons & holes) that are generated at room temperature. However, their conductivity is relatively low compared to extrinsic semiconductors.

## 2. Extrinsic Semiconductors:

- \* Extrinsic Semiconductors are doped Semiconductor materials, meaning they have intentional impurities added to modify their electrical properties. Doping is done to increase the conductivity and tailor the material's characteristics for specific applications.
- \* Extrinsic semiconductors are further divided into two types based on the type of doping:

### a) N-Type Semiconductors:

- \* In N-type (negative-type) Semiconductors, impurity atoms with extra electrons are introduced into the crystal lattice of the semiconductor.
- \* These extra electrons become the majority charge carriers, and they contribute to electrical conduction.
- \* N-type semiconductors have an excess of negative charge carriers and are electron dominated.

### b) P-Type Semiconductors:

- \* In P-type (positive-type) Semiconductor, impurity atoms with fewer electrons than the host semiconductor's atoms are added.
- \* These impurities create holes in the crystal lattice which act as Positive charge carriers.
- \* P-type Semiconductors have an excess of positive charge carriers and are hole dominated.

\* Applications: Semiconductors are the foundation of many electronic devices, including transistors, diodes, integrated circuits (ICs), and more. Transistors, for example are essential components in computers and countless other electronic devices, as they can amplify or switch electronic signals.

Semiconductors are used from microelectronics and telecommunications to power electronics industry and enabled the development of smaller, more efficient and more powerful devices.

\* Superconductors: Superconductors are materials that can conduct electrical current with zero resistance at extremely low temps. This unique property makes them valuable for a wide range of applications.

\* Introduction to Superconductors: Superconductor was first discovered in 1911 by dutch physicist Heike Kamerlingh Onnes when he observed that certain materials lose all electrical resistance at low temperatures. This phenomena occurs because of the formation of Cooper pairs, which are pairs of  $e^-$  that couple together and move through the material without scattering, leading to the absence of resistance. The critical temperature ( $T_c$ ) is the temperature below which a material becomes superconducting. Superconductivity is a quantum mechanical phenomena and it has been a subject of extensive research and technological development.

\* Classification of Superconductors: The classification of superconductors into type 1 & type 2 is based on their magnetic behaviour in the presence of external magnetic field. These distinctions are typically visualized through specific graphs that describe their magnetic properties. Let's explain these graphs:

1) Type 1: Shows abrupt transition to their magnetization (M) magnetic field.



\* Diamagnetic: material has a negative susceptibility. The magnetic flux density decreases as the temperature increases.

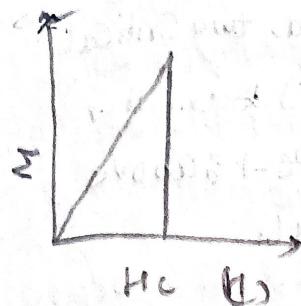
\* Meissner effect: material expels a magnetic field. It has a critical temperature above which it no longer exhibits this transition.

\* Critical magnetic field: from the Meissner effect, the critical magnetic field is the maximum magnetic field that can be applied to the material before it loses its superconducting properties.

\* No magnetic field: where there is no magnetic field, the material remains superconducting.

Pure

1) Type I Superconductors: In type I superconductors there is a sharp & abrupt transition from the normal state (above the critical temperature) to their magnetic properties. The relevant graph depicts the magnetization ( $M$ ) of the material as a function of an applied external magnetic field ( $H$ ).



for a type I superconductor magnetic flux is expelled, producing a magnetization ( $M$ ) that increases with magnetic field ( $H$ ) until a critical field ( $H_c$ ) is reached, at which it falls to zero as with a normal conductor.

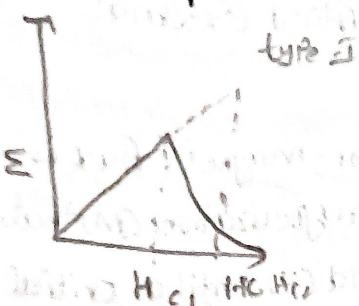
\* Diamagnetic Behaviour: When  $H=0$  (no applied magnetic field), the material becomes perfectly diamagnetic, meaning it expels all magnetic flux. The graph shows a sharp increase in magnetization as soon as the temperature drops below  $T_c$ , indicating the expulsion of the magnetic field.

\* Meissner Effect: As the magnetic field is increased from zero, the material continues to exhibit diamagnetic behaviour until it reaches a critical magnetic field strength ( $H_c$ ). At this point, the superconductor can no longer completely expel the magnetic field, and it transitions back to the normal state, with  $M$  decreasing sharply.

\* Critical Magnetic field ( $H_c$ ): The point where the material transitions from the superconducting state to the normal state is defined as the critical magnetic field ( $H_c$ ). In type-I superconductors,  $H_c$  is relatively low.

\* No Mixed State: Type I superconductors do not have a mixed state where magnetic flux can partially penetrate. They can only exist in a pure superconducting state or a pure normal state.

2. Type-II Superconductors: The graph for type-2 Superconductors differs significantly from that of type-1 Superconductors due to their more complex behaviour in the presence of external magnetic fields. In a type-2 Superconductor, the following are the observed characteristics



A type-2 Superconductor has two critical magnetic fields ( $H_{c1}$  &  $H_{c2}$ ) below  $H_c$ . At  $H_{c1}$ , it becomes a mixed state. Above  $H_{c2}$ , it becomes normal.

\* Mixed state: Below  $T_c$ , the type-2 Superconductor allows partial penetration of magnetic flux, resulting in a mixed state. This means it can exist in regions of superconductivity & normal conductivity.

\* Critical Magnetic field ( $H_{c1}$  &  $H_{c2}$ ): Type-2 Superconductors have two critical magnetic fields,  $H_{c1}$  &  $H_{c2}$ .  $H_{c1}$  is the lower critical field marking the point at which the material starts allowing some magnetic flux to penetrate.  $H_{c2}$  is the upper critical field; indicates the point where the superconductivity state is completely suppressed and the material transitions to normal state.

\* Gradual Transition: The transition from superconducting to normal state in type-2 Superconductors is gradual. As the external magnetic field ( $H$ ) increases beyond  $H_{c1}$  & up to  $H_{c2}$ .

→ Applications of Superconductors: Superconductors have a wide range of applications due to their unique properties, including zero electrical resistance, perfect diamagnetism, and the Meissner effect. Some notable applications include:

1. Magnetic Components  
fields for

2. Particle  
accelerators  
particle

3. Magnets  
used in  
due to

4. Electrical  
and re

5. Energy  
the fo  
more e

6. Quantum  
computing  
for lo

7. Sensors  
app  
and

8. in s

9. Stud  
m

1. Magnetic Resonance Imaging: Superconducting magnets are essential components of MRI machines. They provide strong and stable magnetic fields for high resolution medical imaging.
2. Particle Accelerators: Superconducting magnets are used in large particle accelerators like the Large Hadron Collider (LHC) to guide & focus particle beams.
3. Magnetic Levitation (Maglev) Trains: Superconducting materials are used in the development of maglev trains, which levitate above the track due to magnetic repulsion, resulting in high speed, low friction transportation.
4. Electric Power Transmission: Superconducting materials are used to transmit electricity with minimal losses, improving the efficiency of power distribution and reducing energy waste.
5. Energy Storage: S.C. Energy storage (SMES) systems store energy in the form of a magnetic field and release it when needed, providing a more efficient and compact energy storage solution.
6. Quantum Computing: S.C. qubits are used in the development of quantum computers due to their ability to maintain coherent quantum states for longer durations.
7. Sensors & Detectors: S.C. are employed in sensors & detectors for various applications, including radiation detection, astronomical observations, and materials characterisation.
8. Transportation: S.C. have been explored for electrical Propulsion Systems in ships & aircraft, offering the potential for efficient & clean transportation.
9. Scientific Research: S.C. are used in various scientific experiments such as studying fundamental particle physics & exploring the properties of matter at extremely low temperatures.

Supercapacitors: Supercapacitors, also known as ultracapacitors, are energy storage devices that store and release energy via electrostatic charge separation. Unlike traditional capacitors, supercapacitors store energy electrostatically rather than electrochemically. Supercapacitors have several advantages over traditional batteries, such as high power density (rapid bursts of energy), rapid charge & discharge capabilities, and long cycle life.

Introduction: Supercapacitors consist of two electrodes separated by an electrolyte and a separator. The electrodes are typically made of activated carbon, and the electrolyte can be aqueous or organic-based. When a voltage is applied across the electrodes, ions from the electrolyte are attracted to the surface of the electrodes, creating an electrostatic double layer. This process stores energy as charges accumulate at the electrode-electrolyte interface. The energy stored in supercapacitors is typically measured in farads (F), which is much higher than the capacitance of standard capacitors.

Classification: Supercapacitors can be classified into different types based on their construction, materials, design. The main categories of supercapacitors include:

### 1. Electrochemical Double Layer Capacitors (EDLCs) :-

-Also known as electric double layer capacitors (EDLCs) or supercapacitors.

-Energy storage is based on the formation of a double layer charges at electrode-electrolyte interface.

-High power density, fast charge/discharge, and long cycle life.

### 2. Pseudo-capacitors

- Utilize redox reactions
- Offer higher energy densities
- Lower power densities
- Materials such as transition metals are commonly used.

### 3. Hybrid supercapacitors

- Combine the characteristics of both
- To achieve a balanced performance

- These often use transition metal oxide/hydronium salts as electrolytes

\*Applications:  
-Their unique combination of properties makes them suitable for various applications, including:

#### 1. Energy storage in renewable energy systems

-Upholding power during fluctuations

#### 2. Transportation and traction

-Providing bursts of power for quick acceleration

#### 3. Consumer electronics

-To provide a constant power source

#### 4. Aerospace

-Power backup during emergencies

#### 5. Automotive

-Starting and stopping of vehicles, providing auxiliary energy

## 2. Pseudocapacitors:

- Utilize redox reactions at the electrode surface to store energy.
- Offer higher energy density compared to EDLCs but at the expense of lower power density.
- Materials such as transition metal oxides and conducting polymers are commonly used.

## 3. Hybrid Supercapacitors:

- Combine the characteristics of both EDLCs and Pseudocapacitors to achieve a balance between energy and power density.
- These often use a combination of carbon-based electrodes and metal oxide/hydride materials.

\*Applications: Supercapacitors have a wide range of applications due to their unique combination of high power density, rapid charge/discharge capabilities, and long cycle life. Some common applications are:

1. Energy Storage System (ESS): Used for short-term energy storage in renewable energy systems, grid stabilisation, and uninterruptible power supplies (UPS).

2. Transportation: Supercapacitors are employed in electric buses and trams for regenerative braking, providing quick bursts of power.

3. Consumer Electronics: Some electronic devices use supercapacitors to provide backup power during brief power interruptions.

4. Aerospace and Aviation: Supercapacitors are used for emergency power backup and as part of energy recovery systems in aircraft.

5. Automotive Applications: Supercapacitors are used for cold starting assistance, improving fuel efficiency, hybrid vehicle energy storage.

6. Industrial and manufacturing: Supercapacitors can provide peak power for machinery and equipment, reducing strain on the electrical grid.
7. Medical Devices: Supercapacitors can provide backup power for critical medical equipment in case of power outages.
8. Renewable Energy: They are used to smooth out power fluctuations in solar and wind energy systems.
9. Consumer Electronics: Some electronic devices use supercapacitors to provide backup power during brief power interruptions.

\* Fullerenes: These are a fascinating class of carbon allotropes, which include molecules composed entirely of carbon atoms arranged in closed, cage-like or spherical structures. The most well-known and studied fullerene is C<sub>60</sub>, which consists of 60 carbon atoms arranged in a hollow sphere, resembling a soccer ball. Fullerenes were discovered in 1985 by a team of scientists, including Richard Smalley, R. K. H. Kroto and Robert Curl.

\* Classification of fullerenes: Fullerenes are typically classified based on the number of carbon atoms they contain. The most common fullerene is C<sub>60</sub>, but other fullerenes with different no. of carbon atoms have also been synthesised. Some of the common fullerenes include:

1. C<sub>60</sub> (Buckminsterfullerene): Comprising 60 carbon atoms, it has a soccer ball-like structure.
2. C<sub>70</sub>: Comprising 70 carbon atoms, it's a slightly larger, more elongated sphere.

3. C<sub>84</sub>: with shape than \* properties of Properties than some key pr 1. Hollow Cage with pentagonal stability.

2. Exception despite the 3. Good electrical and their elements.

4. High chemical their exposure with other 5. Bio-compatibility, compactibility.

\* Applications applications

1. Nano materials 2. Medicine and cosmetics

3.  $C_{84}$ : with 84 Carbon atoms, it has a slightly more complex shape than  $C_60$  or  $C_70$ . Similarly,  $C_{76}$ ,  $C_{240}$  &  $C_{540}$  are present.

\*Properties of fullerenes: fullerenes have exhibit a range of unique properties that make them the subject of extensive scientific research. Some key Properties includes

1. Hollow Cage Structure: fullerenes have a hollow cage like structure with pentagonal & hexagonal carbon rings, which contribute to their Stability.

2. Exceptional strength: fullerenes are incredibly strong & resilient despite their relatively low density.

3. Good electrical Conductivity: They have the ability to conduct electricity and their conductivity can be modified by doping with other elements.

4. High chemical Reactivity: fullerenes are highly reactive due to their exposed double bonds. They readily form chemical bonds with other elements and molecules.

5. Bio Compatibility: Some fullerenes have shown potential in biological applications and drug delivery due to their bio-Compatibility.

\*Applications of fullerenes: fullerenes have a wide range of applications across various fields including;

1. Nanotechnology: fullerenes are used as building blocks in nanomaterials and nanodevices.

2. Medicine: They have been explored for drug delivery systems and as antioxidants with potential therapeutic applications.

fullerenes, particularly water soluble fullerene derivatives, have been investigated for their potential use as contrast agents in MRI.

3. Electronics: fullerenes can be used in organic photovoltaics as electron acceptors in solar cells, and in molecular electronics.

4. Catalysis: some metal-containing fullerenes serve as catalysts in chemical reactions.

5. Lubricants & Composites: fullerenes have been used as lubricant additives to enhance lubrication properties and in composite materials to improve mechanical & thermal properties.

6. Energy storage: Research is ongoing on using fullerenes in energy storage devices such as supercapacitors & batteries.