



Chemistry Lecture Material

Unit-I

Molecular Structures and Theories of bonding

for
B.Tech (CSE,IT,DS,CS) I year – I semester
R18 Regulation



COURSE OBJECTIVES:

1. To impart the basic knowledge of atomic ,molecular and electronic modification which make student to understand the technology based on them.
2. To acquire the knowledge of semiconductors, band structure of solids and crystal field theory of d-orbitals.

. COURSE OUTCOME:

1. The knowledge of atomic, molecular and electronic changes related to conductivity.
2. The required principles of CFT and band structure of solids and their application.
3. The knowledge of pi-molecular orbitals of benzene and butadiene.

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UNIT - I
MOLECULAR STRUCTURE AND THEORIES OF BONDING

SHORT QUESTION AND ANSWERS:

1. Write the difference between atomic and molecular orbital?

Atomic orbital	Molecular orbital
Atomic orbital is the region having the highest probability of finding an electron in an atom	Molecular orbital is the region having the highest probability of finding an electron of a molecule
Atomic orbitals are inherent property of an atom. Formed by the electron cloud around the Atom	Molecular orbitals are formed by combination of atomic orbitals that have nearly the same energy
The shape is determined by the type of atomic orbital(s,p,d or f)	The shape is determined by the shapes of atomic orbitals that make the molecule. They have complex shapes
Monocentric as it is found around a single Reaction	Polycentric as it is found around different nuclei
Schrodinger equation is used	Linear combination of atomic orbitals (LCAO) is used

2. Define bonding and anti bonding molecular orbitals?

Bonding Molecular Orbitals

- When addition of wave function takes place, the type of molecular orbitals formed are called Bonding Molecular orbitals and is represented by $\Psi_{MO} = \Psi_A + \Psi_B$.
- They have lower energy than atomic orbitals involved. It is similar to constructive interference occurring in phase because of which electron probability density increases resulting in formation of bonding orbital.
- Molecular orbital formed by addition of overlapping of two s orbitals . It is represented by s.

Anti-Bonding Molecular Orbitals:

- When molecular orbital is formed by subtraction of wave function, the type of molecular orbitals formed are called Antibonding Molecular Orbitals and is represented by $\Psi_{MO} = \Psi_A - \Psi_B$.
- They have higher energy than atomic orbitals. It is similar to destructive interference occurring out of phase resulting in formation of antibonding orbitals.
- Molecular Orbital formed by subtraction of overlapping of two s orbitals.
- It is represented by s* [(*) is used to represent antibonding molecular orbital) called Sigma Antibonding.

3. Calculate the bond order for molecule N₂, O₂, F₂?

Bond order:

It may be defined as the half of difference between the number of electrons present in the bonding orbitals and the antibonding orbitals that is,

$$\text{Bond order (B.O.)} = (\text{No. of electrons in BMO} - \text{No. of electrons in ABMO}) / 2$$

Bond order of N₂:

$$\text{Bond order} = \frac{1}{2}(10-4) = 3. (\text{N} \equiv \text{N}) \text{ Triple bond is present in the molecule}$$

In N₂ molecule all the electrons are paired therefore it is diamagnetic.

Bond order of O₂:

$$\text{Bond order} = \frac{1}{2}(10-6) = 2. \text{ Double bond is present in the molecule.}$$

Two unpaired electrons are present, so the molecule is paramagnetic.

Bond order of F₂:

$$\text{Bond Order} = \frac{1}{2}(8 - 6) = 1$$

In F-F there are no unpaired electrons, so the molecule is diamagnetic.

4. Write a short notes on molecular orbital theory?

Postulates of MOT are:

- Two atoms come together, interact and forms a bond. All the atomic orbitals on either nuclei mix together to form a new orbital called molecular orbital.
- The molecular orbitals are formed by mixing of the atomic orbital's of same energy level and symmetry.
- After formation of molecular orbital, the atomic orbital's lose their identity.
- Each and every electron in the molecular orbital belongs to all the nuclei of the molecules.
- Atoms have atomic orbitals with one nuclei and Molecules have molecular orbitals with n nuclei. Thus, atoms are monocentric while molecules are polycentric.
- The number of molecular orbitals formed is equal to the atomic orbitals mixing.
- Molecular orbitals can be bonding, anti-bonding, and non-bonding orbitals.
- Bonding molecular orbitals are lower in energy than the corresponding anti-bonding orbitals.

5. Write the salient features of crystal-field theory ?

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 ligands.
2. All types of ligands are regarded as point charges.

- The ionic ligands, like F⁻, Cl⁻, CN⁻, etc., are regarded as point charges, and the neutral ligands, like H₂O, NH₃, etc., are regarded as point dipoles. If the ligand is neutral, the negative end of this ligand dipole is oriented towards the metal atom.
- The interactions between the metal ion and the ligand is purely electrostatic, i.e. the bond 100 percent ionic.
- All the d orbitals on the metal atom have equal energy (degenerate orbitals). As the ligands approach the central metal atom for complex formation, these orbitals lose their degeneracy and split into orbitals of different energies depending upon the direction from which the ligands approach the central metal atom.

6. Write a note on LCAO?

According to LCAO method, the molecular orbital wave function Ψ_{mo} is formed by the linear combination of the wave functions of the individual atomic orbitals Ψ_A and Ψ_B

1. Molecular orbital is formed by the addition of wave function of atomic orbitals. It can be represented as

$$\Psi(mo) = \Psi_A + \Psi_B.$$

This molecular orbital is called Bonding molecular orbital.

2. Molecular orbital is formed by the subtraction of wave function of atomic orbitals. It can be represented as

$$\Psi^*(mo) = \Psi_A - \Psi_B$$

This molecular orbital is called Antibonding molecular orbital.

7. What is doping and dopant?

Doping:

The process by which impurity is added in semiconductor to enhance their conductivity is called doping.

Dopant:

A dopant also called a doping agent is a trace impurity element that is inserted into a substance (in very low concentrations) to increase the electrical properties of the substances.

8. How the materials are classified based on Band theory or Fermi energy gap?

Based on the band theory materials are classified into three types

- Conductors
- Insulators
- Semi-Conductor

The gap between the valence band and conduction band is called Fermi energy gap.

1. In conductor, the valence band and conduction band overlap, so there is no band gap.
2. In insulators there is large band gap between valence band and conduction band.
3. In semiconductor, there is a small band gap between valence band and conduction band. so the electrons can promote from V.B to C.B with rise in temperature or by adding dopants.

9. How to predict the magnetic nature and magnetic momentum of molecules and metal complexes ?

In MOED diagram, if all electrons are paired the molecule is diamagnetic. If single or unpaired electrons are present in the molecule is paramagnetic.

$$\text{Magnetic momentum} = \sqrt{n(n + 2)}$$



LONG QUESTION AND ANSWERS:

1. Explain the molecular orbital energy level diagrams of F₂, N₂ and O₂?

Nitrogen Molecule N₂:

Nitrogen molecule is formed by two nitrogen

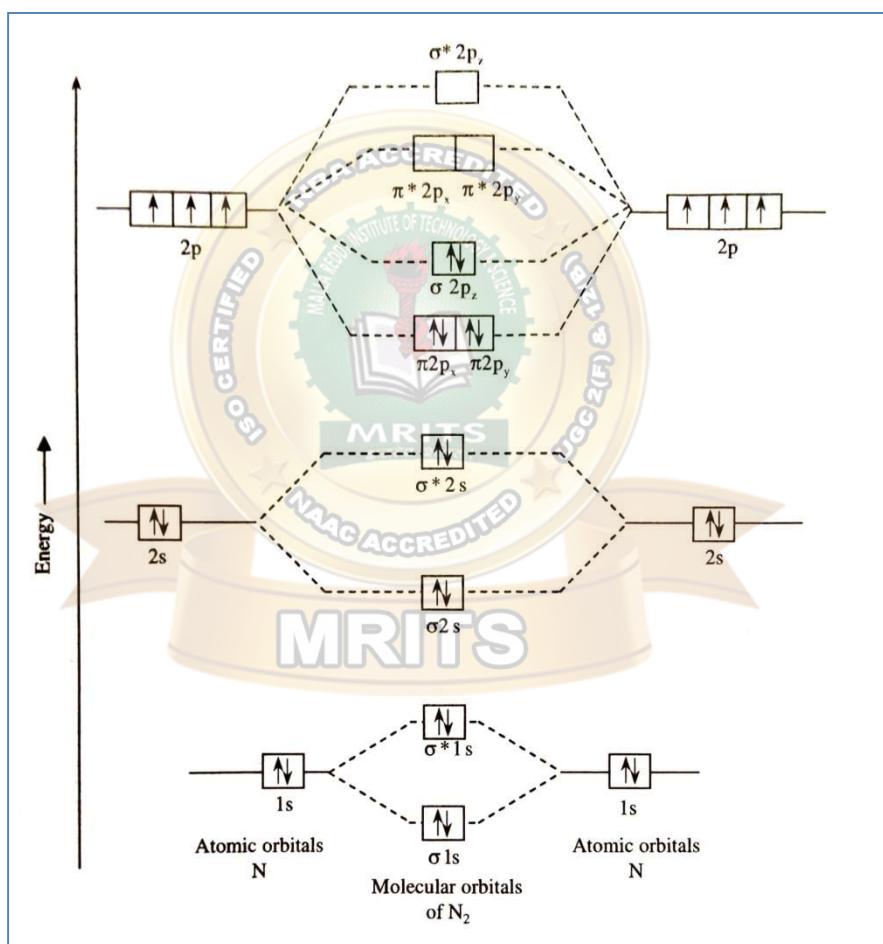
Atomic number of nitrogen is: 7

Electronic configuration of nitrogen is $1s^2 2s^2 2p^3$

In N₂ molecule total electrons are $-7+7=14$

According to molecular orbital approach, the electronic configuration of N₂ is-

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, [\pi 2p_x^2 = \pi 2p_y^2], \sigma 2p_z^2, [\pi^* 2p_x = \pi^* 2p_y], \sigma^* 2p_z$



Bond order of N₂:

Bond order = $\frac{1}{2}(N_b - N_a)$

Bond order = $\frac{1}{2}(10 - 4) = 3$. (N≡N) Triple bond is present in the molecule

In N₂ molecule all the electrons are paired therefore it is diamagnetic.

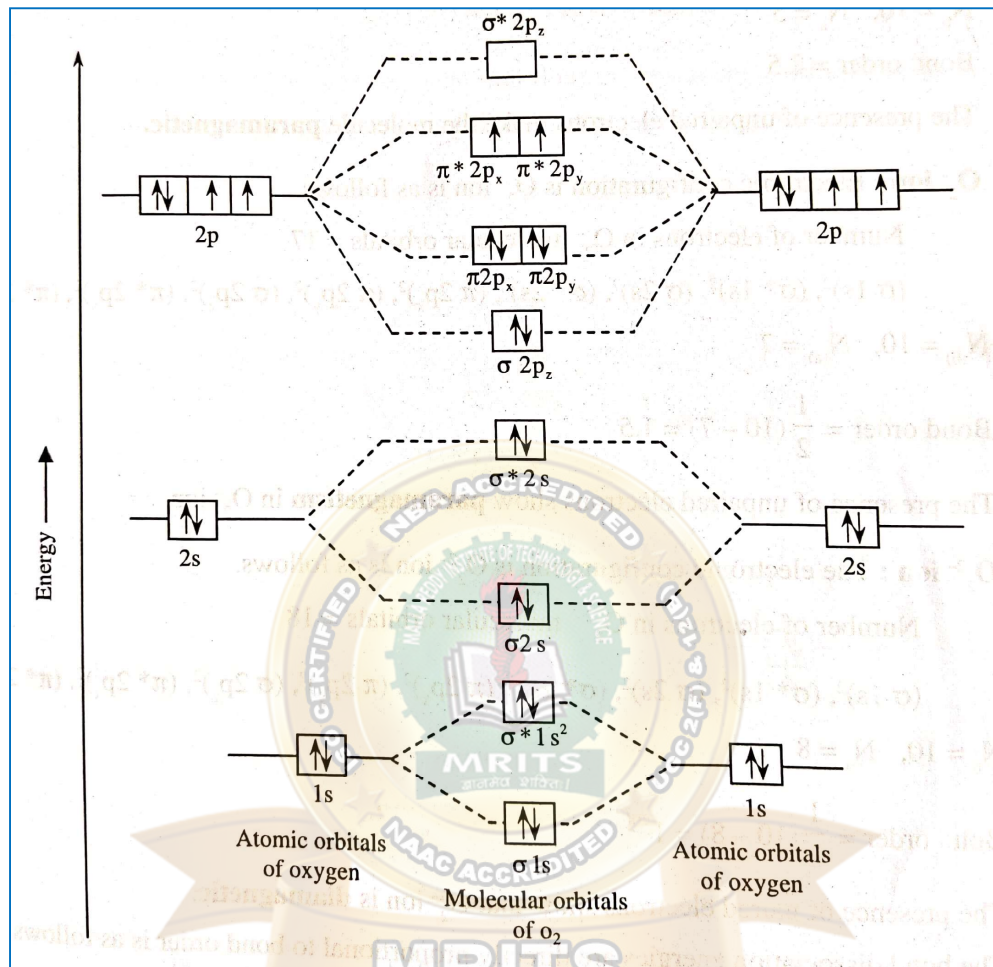
Oxygen Molecule O₂:

The atomic number of oxygen is 8

The electronic configuration of oxygen is $1s^2 2s^2 2p^4$

According to molecular orbital approach, the electronic configuration of O_2 is-

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, [\pi 2p_x^2 = \pi 2p_y^2], [\pi^* 2p_x^1 = \pi^* 2p_y^1], \sigma^* 2p_z$



Bond order of O_2 :

Bond order = $\frac{1}{2}(N_b - N_a)$

Bond order = $\frac{1}{2}(10 - 6) = 2$. Double bond is present in the molecule.

Two unpaired electrons are present, so the molecule is paramagnetic.

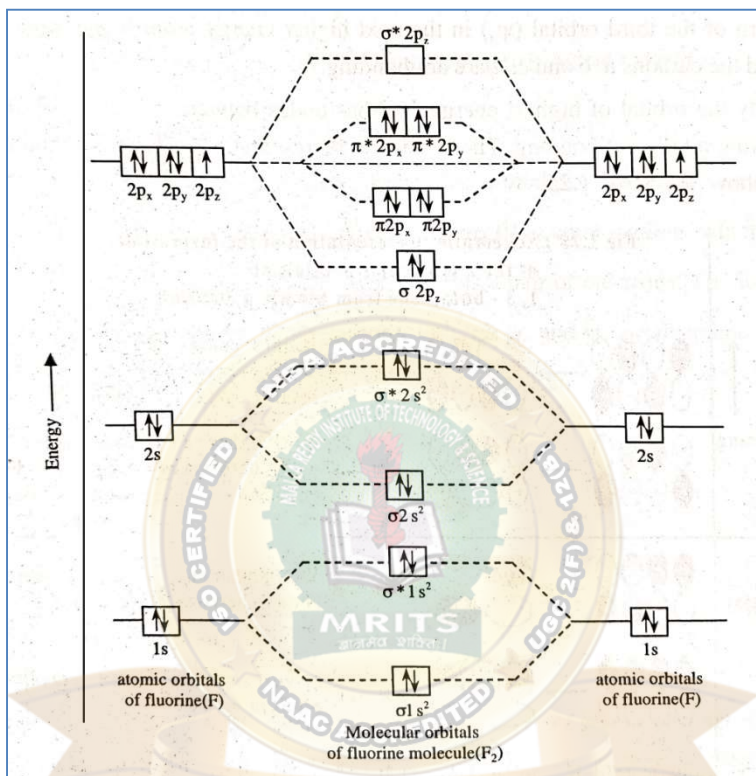
Flourine Molecule F₂:

The atomic number of fluorine is 9

The electronic configuration of fluorine is $1s^2 2s^2 2p^5$

According to molecular orbital approach, the electronic configuration of F₂ is-

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, [\pi 2p_x^2 = \pi 2p_y^2], [\pi^* 2p_x^1 = \pi^* 2p_y^1], \sigma^* 2p_z^1$



Bond order of F₂:

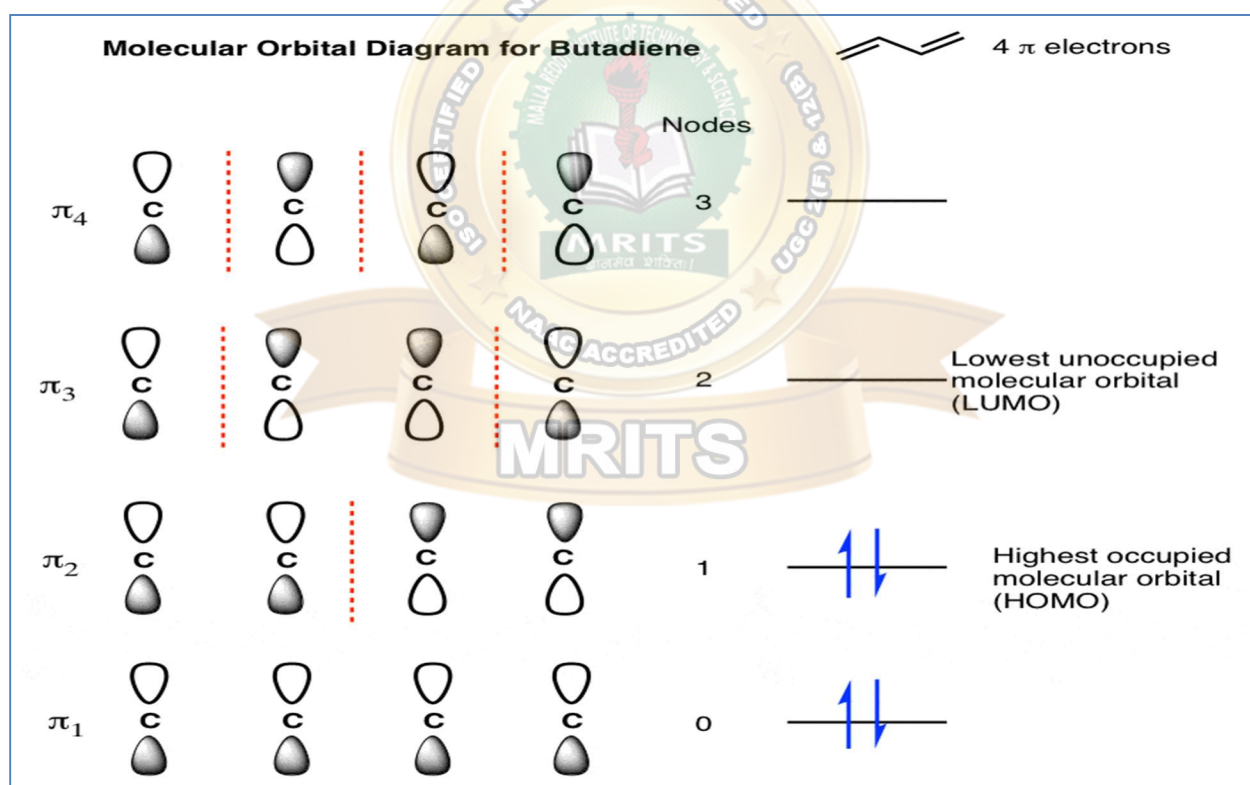
$$\text{Bond Order} = \frac{1}{2}(8 - 6) = 1$$

In F-F there are no unpaired electrons, so the molecule is diamagnetic.

2. Draw and explain the Pi molecular orbitals of Butadiene?

Molecular Orbitals of 1,3-Butadiene

- 1,3-Butadiene contains two double bonds that are conjugated.
- It is "built" from 4 sp^2 hybridised C atoms, each contributing a p atomic orbital containing 1 electron.
- An alternative way to consider "building" the π molecular orbitals is by combining the π molecular orbitals of two ethene molecules.
- This requires that we make an in-phase and an out-of-phase combination for both the π and π^* of ethene.
- Either way, we end up with the same set of 4 π molecular orbitals.
- Notice how the number of nodes and the number of anti-bonding interactions increases as you go up the diagram above.



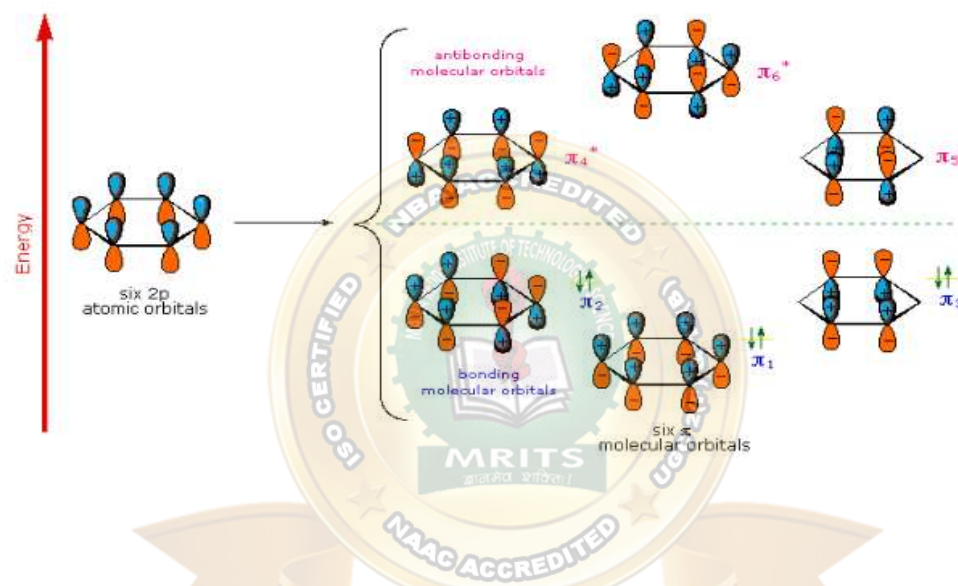
3. Draw and explain the Pi molecular orbitals of Benzene?

Benzene:

Benzene has a planar hexagonal structure in which all the six carbon atoms are sp^2 hybridized. Four valency electrons of each carbon atom, three forms covalent bonds with two carbon atoms and one hydrogen atoms.

The remaining cyclic six p-orbitals(one on each carbon)overlap to generate six molecular orbitals, three bonding and three antibonding.

The Molecular Orbitals of Benzene



The wave equation of benzene is

$$\Psi = \Psi_1 C_1 + \Psi_2 C_2 + \Psi_3 C_3 + \Psi_4 C_4 + \Psi_5 C_5 + \Psi_6 C_6$$

Where Ψ_1 to Ψ_6 are the wave functions of six Pz -orbitals. C_1 to C_6 are their respective coefficients.

4. Explain the crystal field splitting of transition metal ion d-orbitals in octahedral complexes?

Crystal Field Splitting in Octahedral Complexes:

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

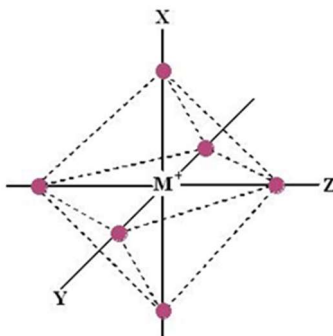
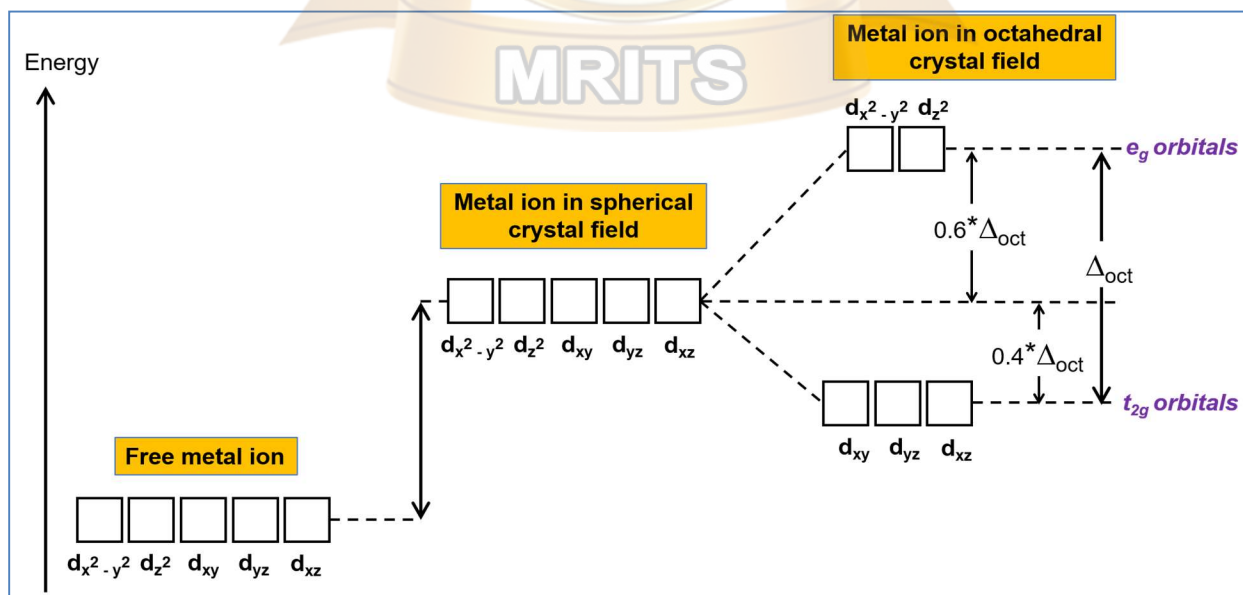


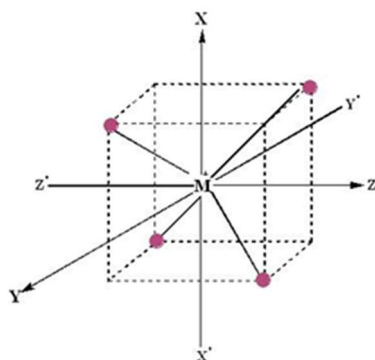
Fig: Splitting of d-orbitals in an octahedral complex

- In octahedral complexes, six ligands approach the central metal atom along the x,y,z axis, as a result the axial orbitals ($d_{x^2-y^2}$, d_{z^2}) show greater repulsion than non axial orbitals (d_{xy} , d_{yz} , d_{zx}).
- The degenerate d-orbitals split into two degenerate sets, one set consists of lower energy and more stable d_{xy} , d_{yz} & d_{zx} orbitals. (t_{2g} orbitals)
- And the other, less stable higher energy d_{z^2} and $d_{x^2-y^2}$ orbitals (e_g orbitals)
- This splitting of degenerate orbitals under the influence of ligands is termed as crystal field splitting and the energy separation between them is denoted by Δ_o .
- The energy of t_{2g} orbitals is decreased by $\frac{2}{5} \Delta_o$ or $0.4 \Delta_o$ or $4 Dq$ and the energy of e_g orbitals rises by $\frac{3}{5} \Delta_o$ or $0.6 \Delta_o$ or $6 Dq$. Above the hypothetical degenerate d- orbitals

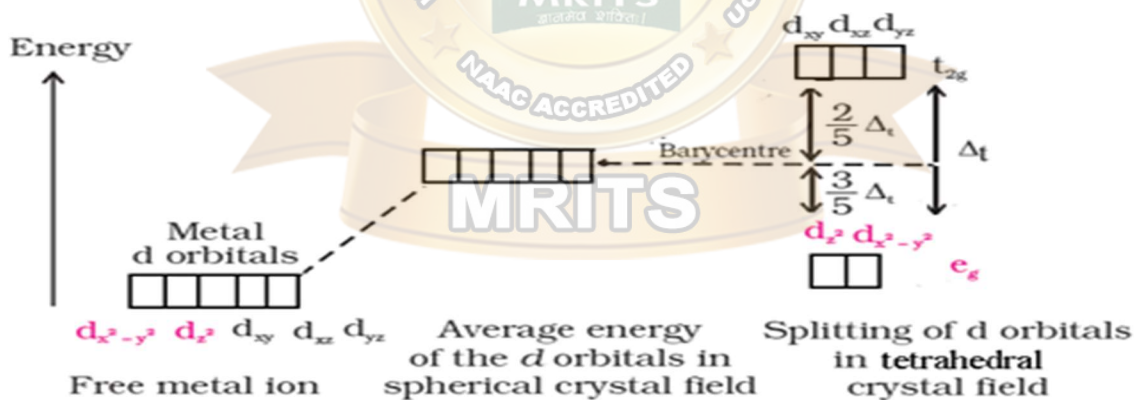


5. Explain the Crystal Field Splitting Tetrahedral Complexes?

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



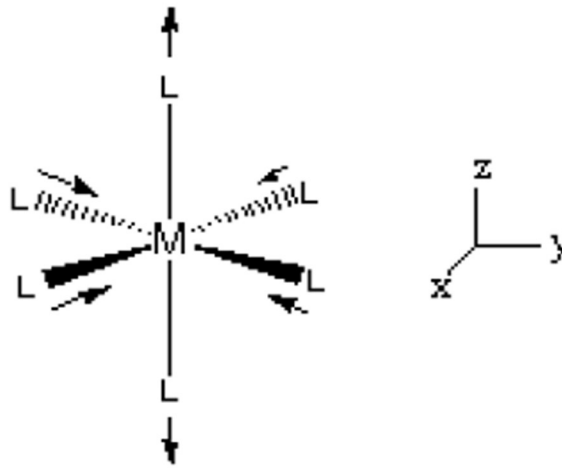
- In tetrahedral complex, the four ligands occupy alternate corners of a cube and the metal ion is placed in the centre.
- Here the d-orbitals are not pointed directly towards the ligands. The non axial orbitals (d_{xy} , d_{yz} & d_{zx}) are closer to ligands than d_{z^2} and $d_{x^2-y^2}$ (axial orbitals).
- Therefore the energy of t_2g orbitals is raised and e_g orbitals is lowered from centre. The crystal field splitting in tetrahedral complex is represented by Δ_t (t = tetrahedral)
- The energy of t_2g orbitals is increased by $\frac{2}{5} \Delta_t$ or $0.4 \Delta_t$ and the energy of e_g orbitals decreased by $\frac{3}{5} \Delta_t$ or $0.6 \Delta_t$.
- $\Delta_t = \frac{4}{9} \Delta_o$ or $\Delta_t = 0.45 \Delta_o$



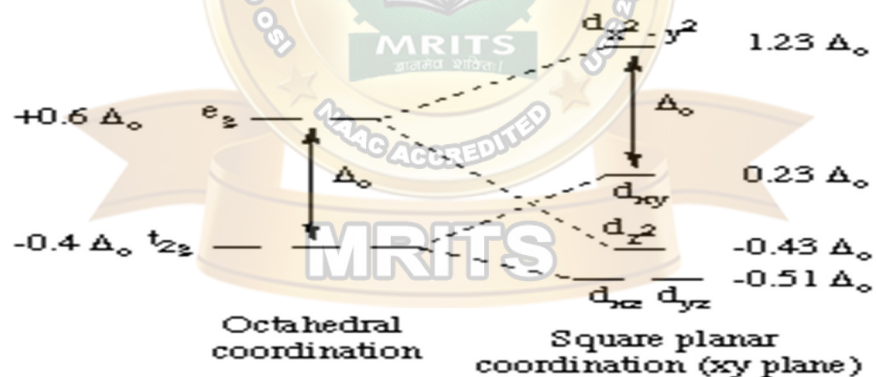
Square Planar Complexes

d-Orbital Splitting in Square Planar Coordination.

- In square planar complex two ligands on the z-axis of an octahedron are removed from the complex, leaving only the ligands in the x-y plane. As the z-ligands move away, the ligands in the square plane move a little closer to the metal.
- The orbital splitting diagram for square planar coordination can thus be derived from the octahedral diagram.



- As ligands move away along the z-axis, d-orbitals with a z-component will fall in energy.
- The d_{z^2} orbital falls the most, as its electrons are concentrated in lobes along the z-axis.
- The d_{xz} and d_{yz} orbitals also drop in energy, but not as much.
- Conversely, the $d_{x^2-y^2}$ and the d_{xy} orbitals increase in energy. The splitting diagram for square planar complexes is more complex than for octahedral and tetrahedral complexes, and is shown below with the relative energies of each orbital.



6. What is the effect of doping on conductance?

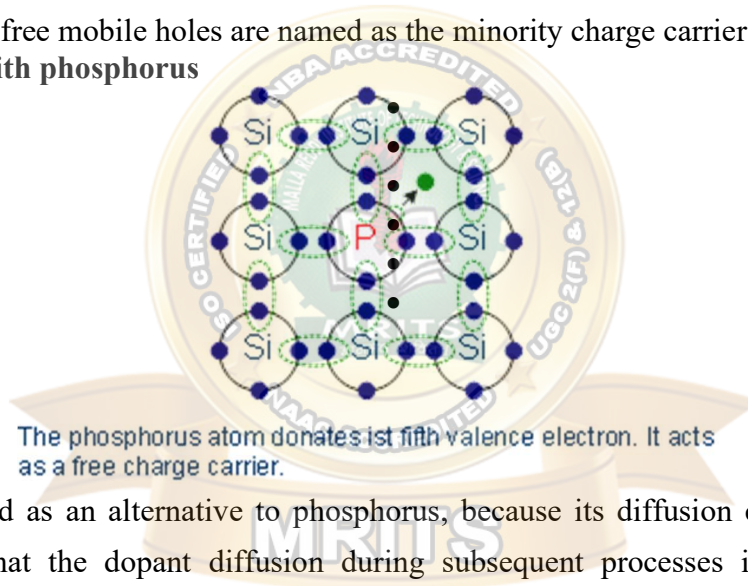
Doping:

- Doping means the introduction of impurities into a semiconductor. Two of the most important materials silicon can be doped with, are boron (3 valence electrons = 3-valent) and phosphorus (5 valence electrons = 5-valent).
- Other materials are aluminium, indium (3-valent) and arsenic, antimony (5-valent).
- The dopant is integrated into the lattice structure of the semiconductor crystal, the number of outer electrons define the type of doping. Elements with 3 valence electrons are used for p-type doping, 5-valued elements for n-doping.

n-doping

- The 5-valent dopant has an outer electron more than the silicon atoms. Four outer electrons combine with every one silicon atom, while the fifth electron is free to move and serves as a charge carrier.
- This free electron requires much less energy to be lifted from the valence band into the conduction band, than the electrons which cause the intrinsic conductivity of silicon. The dopant, which emits an electron, is known as an electron donor (donare, lat. = to give).
- The dopants are positively charged by the loss of negative charge carriers and are built into the lattice, only the negative electrons can move.
- Doped semimetals whose conductivity is based on free (negative) electrons are n-type or n-doped. Due to the higher number of free electrons those are also named as majority charge carriers, while free mobile holes are named as the minority charge carriers.

-doping with phosphorus



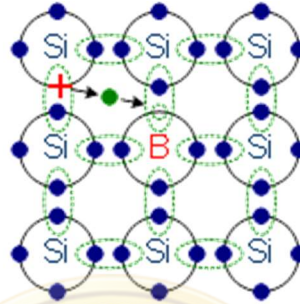
- Arsenic is used as an alternative to phosphorus, because its diffusion coefficient is lower. This means that the dopant diffusion during subsequent processes is less than that of phosphorus and thus the arsenic remains at the position where it was introduced into the lattice originally.

p-doping:

- In contrast to the free electron due to doping with phosphorus, the 3-valent dopant effect is exactly the opposite. The 3-valent dopants can catch an additional outer electron, thus leaving a hole in the valence band of silicon atoms.
- Therefore the electrons in the valence band become mobile. The holes move in the opposite direction to the movement of the electrons. The necessary energy to lift an electron into the energy level of indium as a dopant, is only 1 % of the energy which is needed to raise a valence electron of silicon into the conduction band.

- With the inclusion of an electron, the dopant is negatively charged, such dopants are called acceptors (acceptare, lat. = to add). Again, the dopant is fixed in the crystal lattice, only the positive charges can move.
- Due to positive holes these semiconductors are called p-conductive or p-doped. Analog to n-doped semiconductors, the holes are the majority charge carriers, free electrons are the minority charge carriers.

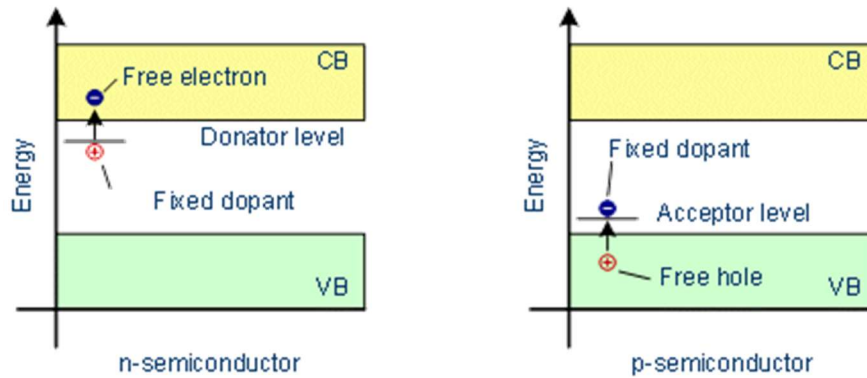
p-doping with boron



The free place on the boron atom is filled with an electron. Therefore a new hole („defect electron“) is generated. This holes move in the opposite direction to the electrons

- Doped semiconductors are electrically neutral. The terms n- and p-type doped do only refer to the majority charge carriers. Each positive or negative charge carrier belongs to a fixed negative or positive charged dopant.
- N- and p-doped semiconductors behave approximately equal in relation to the current flow. With increasing amount of dopants, the number of charge carriers increases in the semiconductor crystal.
- it requires only a very small amount of dopants. Weakly doped silicon crystals contain only 1 impurity per 1,000,000,000 silicon atoms, high doped semiconductors for example contain 1 foreign atom per 1,000 silicon atoms.
- **Electronic band structure in doped semiconductors**
- By the introduction of a dopant with five outer electrons, in n-doped semiconductors there is an electron in the crystal which is not bound and therefore can be moved with relatively little energy into the conduction band.
- Thus in n-doped semiconductors the donator energy level is close to the conduction band edge, the band gap to overcome is very small.
- Analog, through introduction of a 3-valent dopant in a semiconductor, a hole is available, which may be already occupied at low-energy by an electron from the valence band of the silicon. For p-doped semiconductors the acceptor energy level is close the valence band.

- *Band model of doped semiconductors*



p-n junction

7. Explain how the atomic orbitals combine to form bonding and antibonding molecular orbitals? or LCAO

Linear Combination of Atomic Orbitals (LCAO)

- As per this method the formation of orbitals is because of Linear Combination (addition or subtraction) of atomic orbitals which combine to form molecule. Consider two atoms A and B which have atomic orbitals described by the wave functions Ψ_A and Ψ_B .
- If electron cloud of these two atoms overlap, then the wave function for the molecule can be obtained by a linear combination of the atomic orbitals Ψ_A and Ψ_B i.e. by subtraction or addition of wave functions of atomic orbitals

$$\Psi_{MO} = \Psi_A + \Psi_B$$

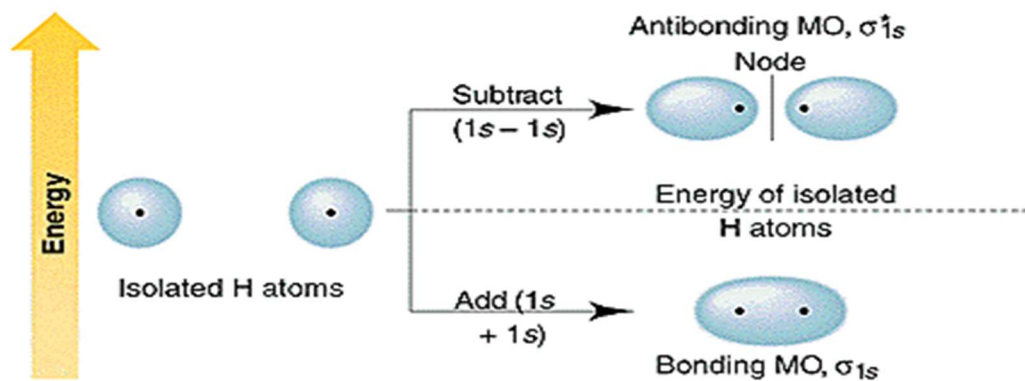
The above equation forms two molecular orbitals

Bonding Molecular Orbitals:

- When addition of wave function takes place, the type of molecular orbitals formed are called Bonding Molecular orbitals and is represented by $\Psi_{MO} = \Psi_A + \Psi_B$.
- They have lower energy than atomic orbitals involved. It is similar to constructive interference occurring in phase because of which electron probability density increases resulting in formation of bonding orbital.
- Molecular orbital formed by addition of overlapping of two s orbitals shown in Figure 1. It is represented by s.

Anti-Bonding Molecular Orbitals

- When molecular orbital is formed by subtraction of wave function, the type of molecular orbitals formed are called Antibonding Molecular Orbitals and is represented by $\Psi_{MO} = \Psi_A - \Psi_B$.
- They have higher energy than atomic orbitals. It is similar to destructive interference occurring out of phase resulting in formation of antibonding orbitals. Molecular Orbital formed by subtraction of overlapping of two s orbitals are shown in figure no. 2.
- It is represented by s^* [(*) is used to represent antibonding molecular orbital) called Sigma Antibonding.



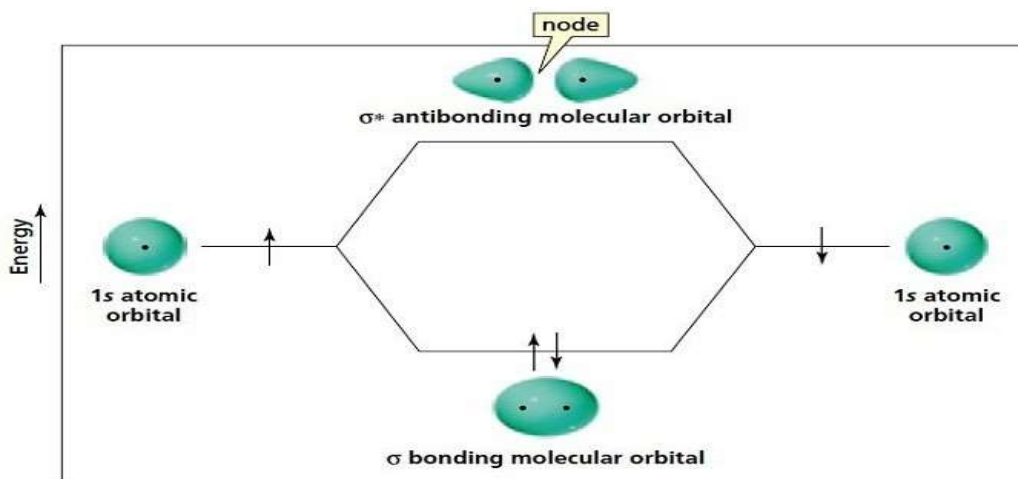
- Therefore, Combination of two atomic orbitals results in formation of two molecular orbitals, bonding molecular orbital (BMO) whereas other is anti-bonding molecular orbital (ABMO). BMO has lower energy and hence greater stability than ABMO.
- First BMO are filled then ABMO starts filling because BMO has lower energy than that of ABMO.
- Formation of molecular orbitals occurs by the combination of atomic orbitals of proportional symmetry and comparable energy. Therefore, a molecular orbital is polycentric and atomic orbital is monocentric. Number of molecular orbitals formed is equal to the number of atomic orbitals.

Relative Energies of Molecular Orbitals

Bonding Molecular Orbitals (BMO) - Energy of Bonding Molecular Orbitals is less than that of Anti Bonding Molecular Orbitals because the attraction of both the nuclei for both the electron (of the combining atom) is increased.

Anti-Bonding Molecular Orbitals (ABMO) - Energy of Anti Bonding Molecular Orbitals is higher than Bonding Molecular Orbitals because the electrons move away from the nuclei and are in repulsive state.

The Energies of Bonding Molecular Orbitals and Anti-Bonding Molecular Orbitals are shown in Fig 2 :



8. Explain the formation of bands in solids?

- According to the MOT molecular orbitals are formed by the combination of atomic orbitals.
- The numbers of molecular orbitals formed are equal to the number of atomic orbitals taking part in molecular orbital formation.

Example: **Formation of crystal of lithium(Li)-metal**

In order to understand the band theory of solids, let us imagine the construction of crystal lithium metal by adding Li atoms like Li_2, Li_3, \dots, Li_n

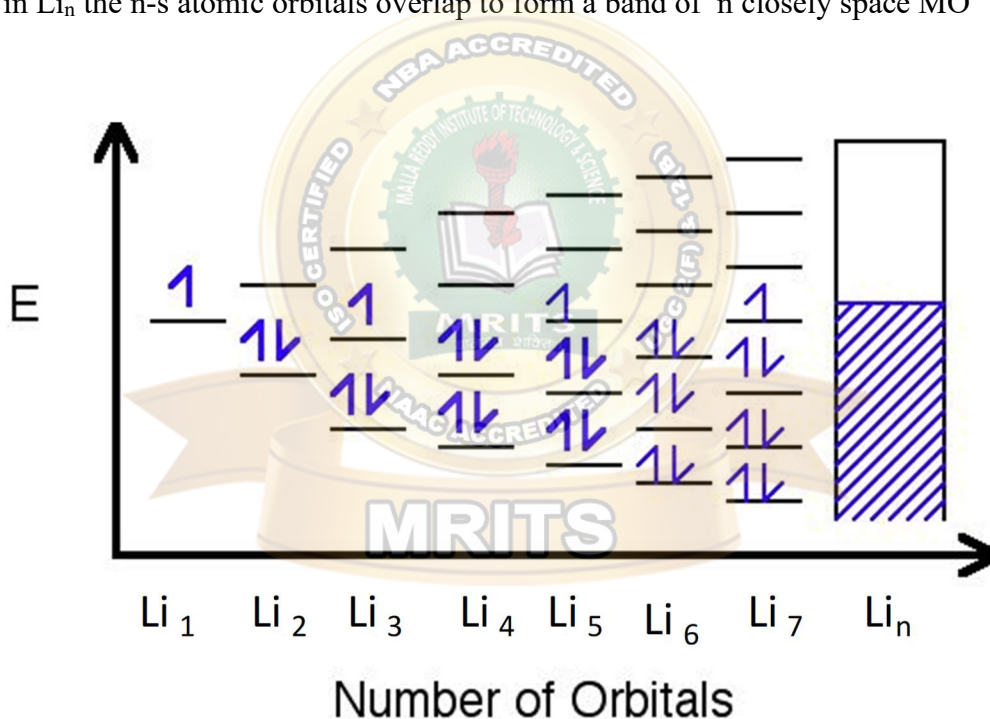
Explanation:

The electronic configuration of Li atom is $1s^2, 2s^1, 2p^0$

The 2s atomic orbital overlap in Li_2 to form two molecular orbitals.

In Li_3 the 3s atomic orbital overlap to form three molecular orbitals.

Similarly in Li_n the n-s atomic orbitals overlap to form a band of n closely space MO



Formation of various bands in solids:

Example:

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

1s Band:

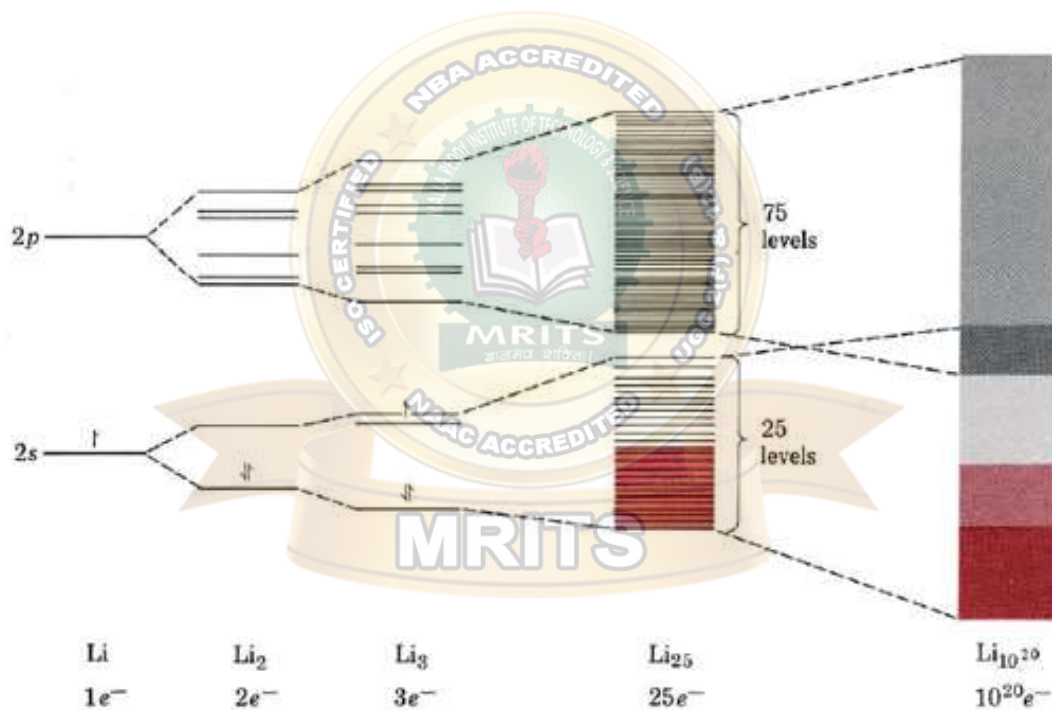
This is called non-conduction band. It is formed by the combination of completely filled orbitals.

2s Band:

This is called valency band as it is half filled. The upper half of the this band is empty, while the lower half is completely filled. Since the energy difference between these two halves is very small, the electrons can move from lower half to lower 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 2s orbitals can move to 2p orbitals. Thus it is also called conduction band.



TUTORIAL QUESTIONS:

1. List out the Differences between Bonding and Anti-Bonding molecular orbitals.
2. Calculate the bond orders of Nitrogen, Fluorine and Oxygen molecules
3. Give the crystal field stabilisation energies of Octahedral, Tetrahedral and Square planar complexes.
4. Why is Oxygen molecule paramagnetic while Nitrogen molecule is diamagnetic?
5. Define Spectrochemical series .
6. Which complexes are spin free complexes?
7. Explain why benzene is Aromatic in nature.
8. Define Huckel's rule.
9. Draw the Pi molecular orbitals of benzene and Butadiene.
10. Write the increasing order of the splitting power of ligands.

ASSIGNMENT QUESTIONS:

- 1) Draw the molecular orbital energy level diagrams of N_2 , O_2 , and F_2 .
- 2) Define bond order, bond length and bond dissociation energy.
- 3) Give few examples of Dopants
- 4) Sketch the shapes of Molecular orbitals formed by the overlap of 2s and 2p orbitals.
- 5) What is the effect of doping on conductance?
- 6) Define Crystal Field Stabilisation energy.
- 7) What is the maximum number of electrons that can occupy a molecular orbital and why?
- 8) Write the Magnetic properties and Bond order of N_2 , O_2 and F_2
- 9) Represent the electronic configuration of molecular orbitals for N_2 , O_2 and F_2
- 10) Draw the shapes of s, p and d orbitals
- 11) Give the differences between p type and n type semi conductors.
- 12) Why is Fluorine molecule very stable.
- 13) How is a Nodal plane produced in molecular orbitals?
- 14) What is the relationship between bond order and Bond length.
- 15) Differentiate the properties of diamagnetic and paramagnetic molecules.
- 16) Define Magnetic moment.
- 17) Give examples of conductors, semiconductors and insulators.
- 18) Sketch the diagrams of square planar, tetrahedral and octahedral complexes

MULTIPLE CHOICE QUESTIONS

01. Schrodinger's wave equation calculates one of the following. (a)

- a) the probability of finding an electron at various points in an atom b) momentum of an electron
c) radius of an electron d) velocity of an electron

02. An atomic orbital contains (a)

- a) pairs of electrons b) single electron
c) three paired electrons d) two pairs of electrons

03. One of the following is a lowest energy bonding molecular orbital (d)

- a) σ^* b) π^*
c) n d) σ

04. The node in the wave function of the molecular orbitals (b)

- a) helps to decrease kinetic energy b) helps to raise kinetic energy
c) helps to keep kinetic energy constant d) no effect on kinetic energy

05. The bond order for oxygen molecules (b)

- a) 3 b) 2
c) 0 d) 1

06. The bond dissociation of oxygen species is in the following order (a)

- a) $O_2^* > O_2 > O_2^{-1} > O_2^{-2}$ b) $O_2 > O_2^* > O_2^{-1} > O_2^{-2}$
c) $O_2^{-2} > O_2 > O_2^* > O_2^{-1}$ d) $O_2^{-1} > O_2^{-2} > O_2^* > O_2$

07. The number of internuclear nodes between ψ_2 energy level of (c)

1,3-butadiene is

- a) 2 b) 3
c) 1 d) zero

08. The two orbitals with equal energy and equal electron density at all six carbons in benzene are (b)

- a) $\psi_2 \psi_4$ b) $\psi_2 \psi_3$
c) $\psi_1 \psi_2$ d) $\psi_1 \psi_3$

09. Based on the strength of metal – ligand bonds, one of the following Property of the complex changes (a)

- a) magnetic property & color b) only color

c) only magnetic property

d) electromagnetic property

10. During the formation of an octahedral complex, the energy of t_{2g} set is directed by (c)

a) $0.6E_o$

b) $1.0E_o$

c) $0.4E_o$

d) $0.656E_o$

11. If there is only one unpaired electron ($n = 1$) in a paramagnetic complex, the magnetic moment is given by (d)

a) 2.83BM

b) 3.87BM

c) 4.9BM

d) 1.73BM

12. The square planar complexes are (c)

a) high spin electron

b) medium spin electron

c) low spin electron

d) no spin electron

13. If the fermi energy gap is more, the material becomes (b)

a) semiconductor

b) Insulator

c) conductor

d) either conductor or semi-conductor

14. By introducing a trivalent impurity into silicon, one of the following type is produced (a)

a) positive hole

b) doping

c) insulator

d) conductor

FILL IN THE BLANKS

01. The bonding between the central metal ion and its ligands arise purely _____.(electrostatic)

02. Paired electrons in a molecule do not exhibit _____.(magnetic properties)

03. _____ is an example of elemental semiconduction.(Si or Ge or Ga)

04. Magnetic quantum number is otherwise known as _____.(orientation quantum number)

05. The stability of benzene ring is due to _____ of electrons.(delocalization)

06. The antibonding molecular orbitals of fluorine remain as _____ in HF molecule(non bonding)

07. The cyclic molecules in which delocalization actually leads to stabilization are just _____.(aromatic)

08. The crystal field stabilization energy (CFSE) is denoted by _____
Type equation here. _____ (Δ_o)

09. If the number of bonding electrons are less than the number of antibonding electrons, the molecule becomes ----- (unstable)

10. In Greek the word atom means ----- (indivisible)

