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Engineering Chemistry
Unit-I : Atomic & Molecular Structure

Lesson-4

Molecular orbital Energy diagrams

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RECAP……

Key points:

- Atomic orbitals combine to produce the same number of molecular orbitals.
- Atomic orbitals must have the proper symmetry and energy to interact and form molecular orbitals.
- As the overlap between two atomic orbitals increases, the difference in energy between the resulting bonding and antibonding molecular orbitals increases.
- When two atomic orbitals combine to form a pair of molecular orbitals, the bonding molecular orbital is stabilized about as much as the antibonding molecular orbital is destabilized.
- The interaction between atomic orbitals is greatest when they have the same energy.
- LCAO-MO Theory is a simple method for predicting the approximate electronic structure of molecules.

Filling of electrons in molecular orbitals

MO are arranged in the increasing order of their energy.

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

Electrons are filled in the same order based on

- Aufbau principle which states orbitals are filled with electrons in increasing order of their energy.
- Pauli's exclusion principle which states no two electrons in the same orbital will have the same quantum numbers.
- Hund's rule of maximum multiplicity which states that pairing of electrons in the degenerate orbitals occurs only after they are half-filled.

Molecular energy level diagram of homo nuclear diatomic molecules

The relative energies of MOs is in the increasing order.

- For H_2 to N_2

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

- For O_2 to Ne_2

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

- As 2s AO are of higher energy σ 2s and σ *2s posses higher energies than σ1s and σ *1s which are formed from lower energy 1s AO.
- Within the same pair of MO , the ABMO has higher energy than the BMO.
- The MO **$\pi 2p_x = \pi 2p_y$** and **$\pi^* 2p_x = \pi^* 2p_y$** are degenerate.

The order of energy levels **σ 2p_z , π 2p_x = π 2p_y** is reversed in case of O_2, F_2, Ne_2

- In elements of lower effective nuclear charge H_2 to N_2 , the energy difference between the 2s & 2p is least.
- There are repulsive interactions between σ 2s, σ 2p and between σ *2s and σ*2p.
- This leads to stabilization of σ 2s and σ *2s & destabilization of

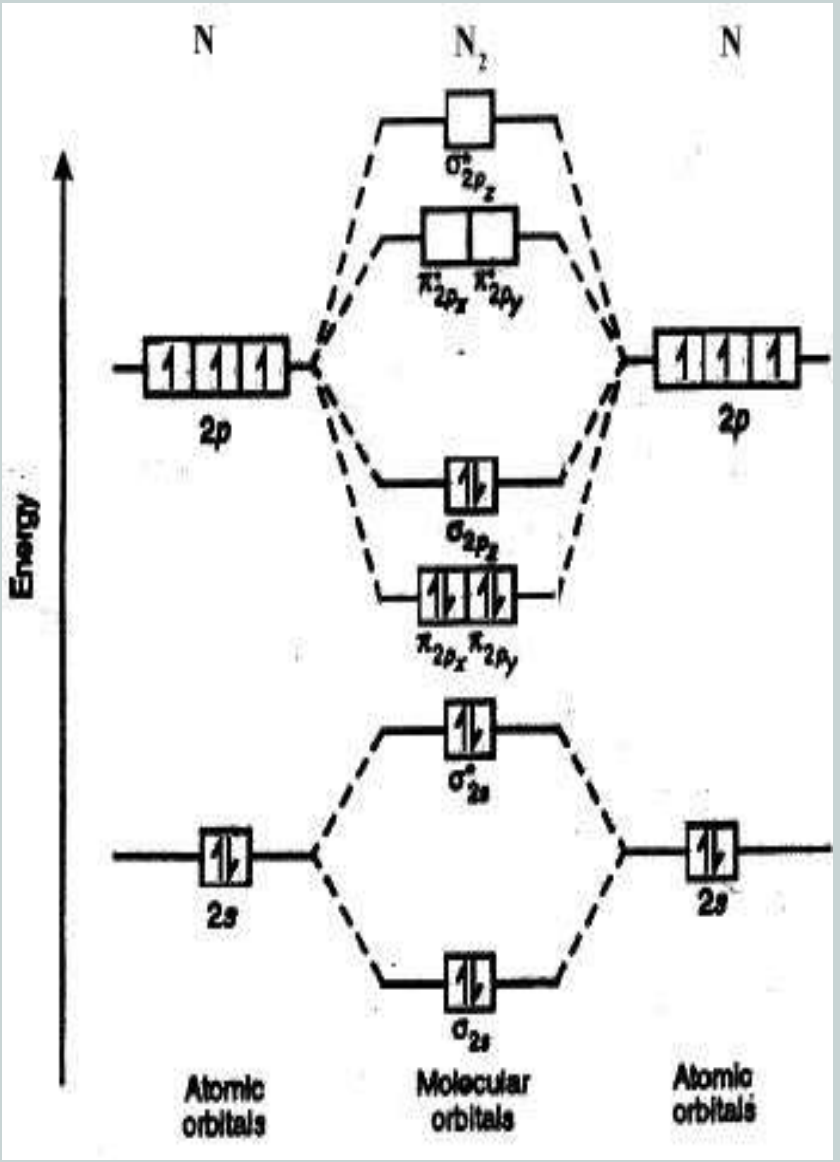
σ 2pand σ*2p

MO energy level diagram of N_2

- The Electronic Configuration of Nitrogen is $1s^2 2s^2 2p^3$
- Nitrogen molecule has 14 electrons.
- The ground electronic configuration of Nitrogen molecule is

  $(\sigma 1s)^2 (\sigma 1s^*)^2 (\sigma 2s)^2 (\sigma 2s^*)^2 (\pi 2px)^2 (\pi 2py)^2 (\sigma 2pz)^2$
- As there are no unpaired electrons , nitrogen is diamagnetic.
- Nb=10, Na=4,

Bond order= ½(10-4)=3, which justifies the presence of triple bond in Nitrogen molecule



MO energy level diagram of O_2

- The Electronic Configuration of Oxygen atom is $1s^2 2s^2 2p^4$
- oxygen molecule has 16 electrons.
- The ground electronic configuration of Oxygen molecule is

  $(\sigma 1s)^2 (\sigma 1s^*)^2 (\sigma 2s)^2 (\sigma 2s^*)^2 (\sigma 2pz)^2 (\pi 2px)^2 (\pi 2py)^2 (\pi 2px^*)^1 (\pi 2py^*)^1$
- As there are two unpaired electrons , oxygen is paramagnetic.
- Nb=10, Na=6,

Bond order= ½(10-6)=2, which justifies the presence of double bond in Oxygen molecule