Notes

Molecular Orbital Theory: *It says that orbitals of atoms combine to form new orbitals called molecular orbitals. Since orbitals are described by schrodinger's wave functions as described in structure of atom chapter, the combination of these orbitals is simply the superposition of their individual wave functions.*

As waves can be added in same phase or opposite phase, we get two types of molecular orbitals namely ***bonding orbitals*** *(formed by in phase addition of wave functions) and* ***antibonding orbitals*** *(formed by addition in opposite phase of wave functions).*

Conditions for combination of atomic orbitals to form molecular orbitals:

1. *Combining orbitals must have same or nearly equal energy.*
2. *Combining orbitals must have same symmetry about molecular axis.*
3. *Combining orbitals must overlap to the maximum extent.*

∗ By convention, $z-$ axis is taken as molecular axis.

σ *&* ***π orbitals***: *When two atomic orbitals combine if the resultant molecular orbitals are symmetrical about the molecular axis then they are called $\sigma(sigma)$ orbitals. If they are not symmetrical then they are called $\pi(pi)$ orbitals.*

Energy level diagrams: *Orbitals of different atoms are combined and the resultant molecular orbitals are arranged in increasing order of energy and then electrons are filled in accordance with Aufbau's principle, Pauli's exclusion principle, and Hund's rule of maximum multiplicity*

Bond order:

It is calculated as $\boldsymbol{BO = \frac{n_b - n_{ab}}{2}}$ *, where n_b are no. of electrons in bonding molecular orbitals and n_{ab} are no. of electrons in antibonding molecular orbitals*

Bond order represents the strength of a bond.

It is also a measure of bond length, higher the Bond order smaller the bond length and vice $-$ versa, provided the combining atoms are kept same or of nearly same size.