# Chemistry Study Materials for Class 11 (NCERT Based Notes of Chapter- 04)

Ganesh Kumar Date:- 13/10/2020

## CHEMICAL BONDING AND MOLECULAR STRUCTURE

### Molecular Orbital Theory

*An approach to bonding in which orbitals encompass the entire molecule, rather than* being localized between atoms.

*Molecular Orbital (MO) theory predicts the actual properties of molecules better than VB theory depicting electron transitions because of the differences in the energy levels of orbitals in the molecule.*

Molecular orbitals are formed when the atomic orbitals of two (or more) different atoms are joined together. The orbitals are then spread across all of the atoms that contributed the atomic orbitals.

The same numbers of molecular orbitals are formed as there were atomic orbitals joined together, and their net energy is the same.

- ***Bonding molecular orbitals***

*-have electron density between the atom*

*-are lower in energy than the original atomic orbitals*

*-when these orbitals are occupied by electrons, it holds the atoms together, forming a bond*

- ***Nonbonding molecular orbitals***

*-may occur when three or more atomic orbitals are combined*

*-have the same energy as the original atomic orbitals*

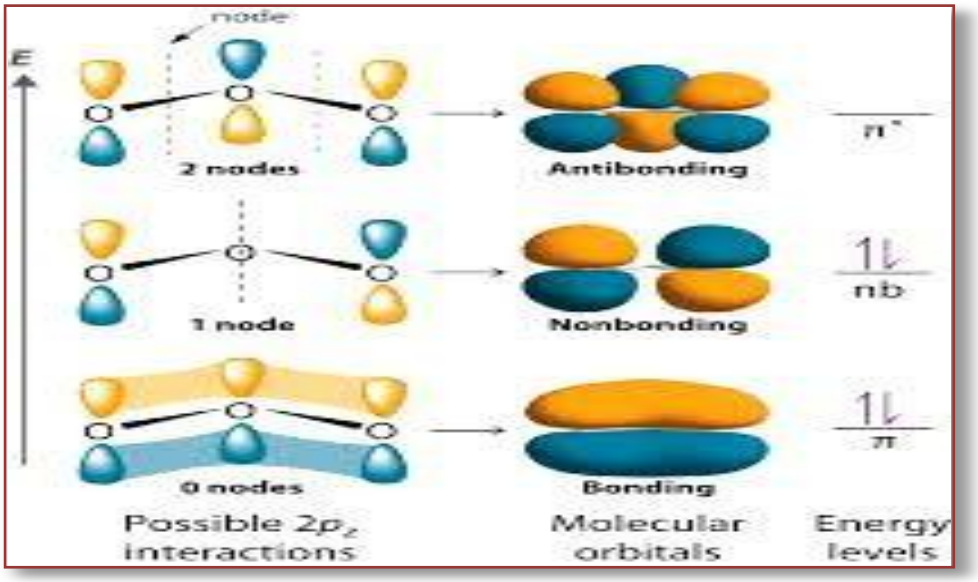
*-electrons occupying these orbitals do not stabilize or destabilize the molecule*

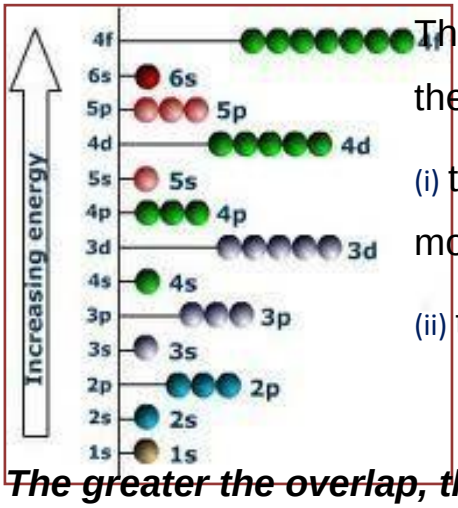
- ***Antibonding molecular orbitals***

*-have electron density which is not between the atoms (there is a node between the atoms)*

*-are higher in energy than the original atomic orbitals*

*-if these orbitals are occupied by electrons, it pulls the atoms away from each other and weakens or prevents bonding.*




The relative energies of molecular orbitals depend upon the following two factors:

(i) the energies of the atomic orbitals combining to form molecular orbitals.

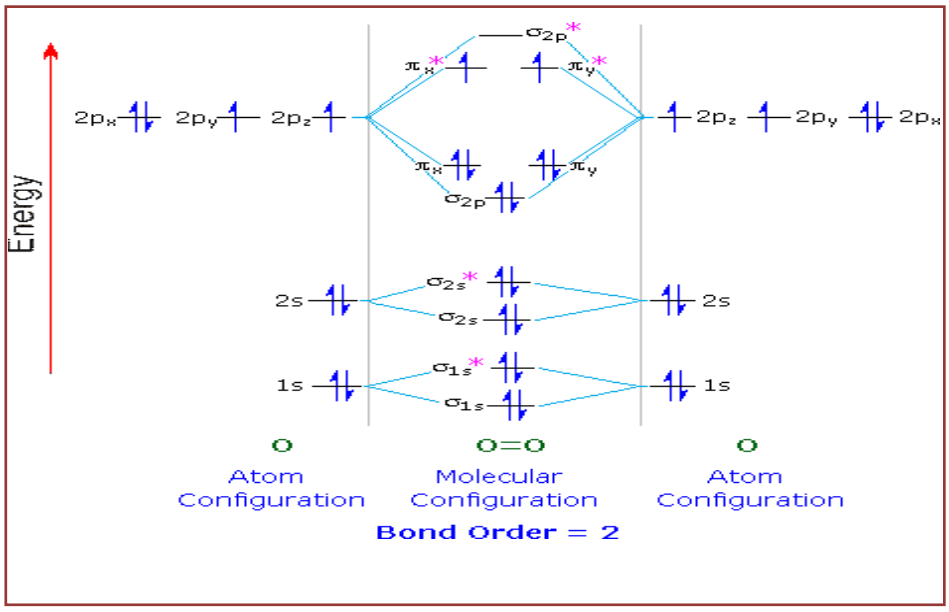
(ii) the extent of overlapping between the a tomic orbitals.

***The greater the overlap, the more the bonding orbital is lowered and the antibonding orbital is raised in energy relative to atomic orbitals.***

*Energy order of various Molecular Orbitals*

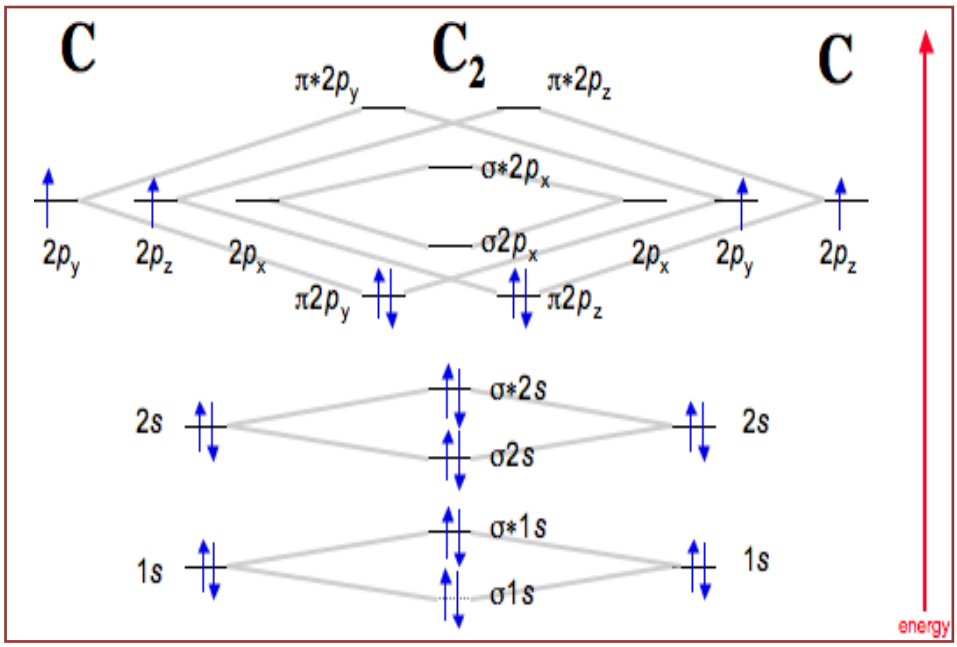
The increasing order of energies of various molecular orbitals for $O_2$ and $F_2$ is given below :

**σ1s < σ*1s < σ2s < σ*2s <σ2pz<(π 2px = π 2py) < (π *2px= π *2py)<σ*2pz**




However, this sequence of energy levels of molecular orbitals is not correct for the remaining molecules $Li_2$, $Be_2$, $B_2$, $C_2$, $N_2$. For instance, it has been observed experimentally that for molecules such as $B_2$, $C_2$, $N_2$ etc. the increasing order of energies of various molecular orbitals is

**σ1s < σ*1s < σ2s < σ*2s < (π 2px = π 2py) <σ2pz < (π *2px= π *2py) < σ*2pz**




**The important characteristic feature of this order is that the energy of σ2pz molecular orbital is higher than that of π 2px and π 2py molecular orbitals.**

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