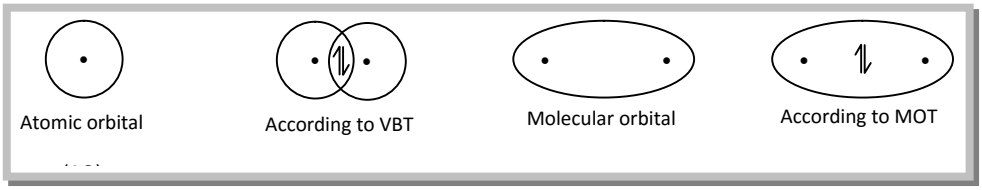
Molecular orbital theory.

Molecular orbital theory was given by Hund and Mulliken in 1932. When two or more constituent atomic orbital merge together, they form a bigger orbital called molecular orbital (MO). In atomic orbital, the electron is influenced by only one nucleus whereas in case of molecular orbital, the electron is influenced by two or more constituent nuclei. Thus, atomic orbital is monocentric and molecular orbital is polycentric. Molecular orbitals follow Pauli's exclusion principle, Hund's rule, Aufbau's principle strictly.



The main ideas of this theory are : (i) When two atomic orbitals combine or overlap, they lose their identity and form new orbitals. The new orbitals thus formed are called molecular orbitals. (ii) Molecular orbitals are the energy states of a molecule in which the electrons of the molecule are filled just as atomic orbitals are the energy states of an atom in which the electrons of the atom are filled. (iii) In terms of probability distribution, a molecular orbital gives the electron probability distribution around a group of nuclei just as an atomic orbital gives the electron probability distribution around the single nucleus. (iv) Only those atomic orbitals can combine to form molecular orbitals which have comparable energies and proper orientation. (v) The number of molecular orbitals formed is equal to the number of combining atomic orbitals. (vi) When two atomic orbitals combine, they form two new orbitals called bonding molecular orbital and antibonding molecular orbital. (vii) The bonding molecular orbital has lower energy and hence greater stability than the corresponding antibonding molecular orbital. (viii) The bonding molecular orbitals are represented by σ, π etc, whereas the corresponding antibonding molecular orbitals are represented by σ^*, π^* etc. (ix) The shapes of the molecular orbitals formed depend upon the type of combining atomic orbitals.