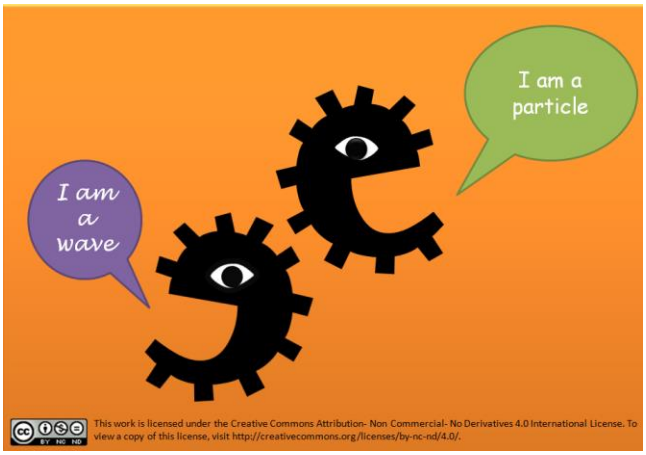
MOLECULAR ORBITAL THEORY: DUAL NATURE OF ELECTRON

The Molecular Orbital Theory is the most advanced theory and developed by Robert S. Mullikan. It is based on the dual nature of electron. You might be surprised to know that electrons also have dual nature, one fake and other real? It is not as simple as that but electrons are going to get you surprised more often than you think.



You have learned that in an atom electrons are found in certain orbits that means electrons are similar to the particles and you can locate them in a space. You have also learned that in an atom electrons are moving around the nucleus that means electrons are like wave that travels continuously in a space. That means electrons are like particle in some ways and like wave in other ways. This dual nature of electron is postulated by De Broglie in 1924.

Have you ever tried to notice the blades of a fan when it is running? You can easily notice them separately when it is at low rpm (rounds per minute) but at higher rpm it becomes so difficult that you can't even judge the number of blades. Similarly

electrons are too small to see and they move so fast that it becomes impossible to measure their velocity and position accurately at the same time. Heisenberg has expressed this uncertainty in mathematical term as:

$$\Delta x . \Delta v \geq \frac{h}{4\pi}$$

Where h = Plank's constant = 6.6262×10^{-34} Js
Δx is uncertainty in position and
Δv is uncertainty in velocity.

That means when we are able to define the position of an electron precisely, we can define its velocity less precisely. It alters the definition of orbit. Until now we have been saying that electrons are following a certain orbit or found in a certain orbital; now we must say that orbit and orbital are the places where there is maximum probability of finding an electron.

So how should we define an electron in this new definition? Schrödinger wave equation provides a satisfactory description of an atom in these terms. Solution to the wave equation is called the wave function and is given by the symbol ψ (psi). We can describe electron either as particle or as wave. That's why electron in an atom may be described as occupying an atomic orbital or by a wave function ψ.

For example last electron of Nitrogen may be described as electron occupying an orbital $2p_z$ or in terms of wave function it can described as ψ_{2pz}.

In VBT we have seen that molecules are made up of atoms. Atomic orbitals of central atom overlap with other atomic orbitals to form bonds. For example, in CH_4 molecule we have seen that sp^3 hybridised orbitals of C overlap with s orbitals of H atoms. And at the end we have mentioned that C has gained 4 electrons from H atoms in CH_4 molecule.

But MOT suggests that in a molecule, atomic orbitals from different atoms get merged and form molecular orbitals that belong to all atoms. In the next post we will see how MOT deals with atomic orbitals.

Source : http://chemistrynotmystery.blogspot.in/2014/08/molecular-orbital-theory-dual-nature-of.html