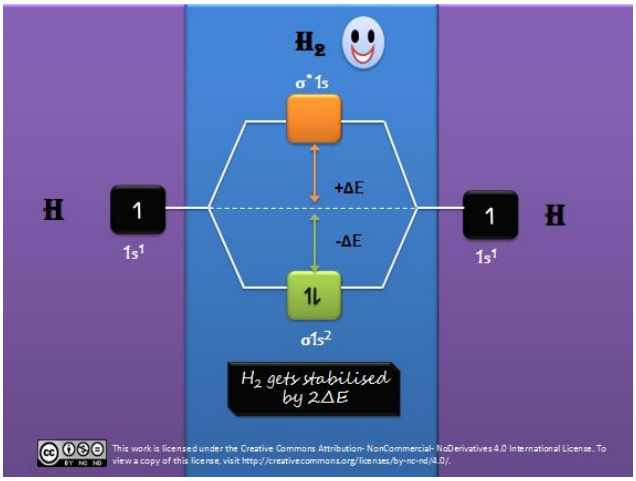
APPLICATIONS OF MOT

MOT helps us to solve a number of mysteries about molecules. We will explore its applications one by one. Now you must be able to interpret the nature of element and predict the type of bond which it would prefer to form. You are familiar with Hydrogen and Oxygen, we have studied a number of molecules which contains H and O. Both of them exist in diatomic state which means Hydrogen exists as H_2 molecule and Oxygen exists as O_2 molecule. Do you know the first element of 18^{th}group is Helium? It is a noble gas. Does Helium exist as He_2 molecule like H_2 and O_2 or not?

MOT can prove that Hydrogen exists as H_2 molecule and Oxygen exists as O_2 molecule and also can solve the question about He_2 molecule. Let's see how MOT solves these mysteries.

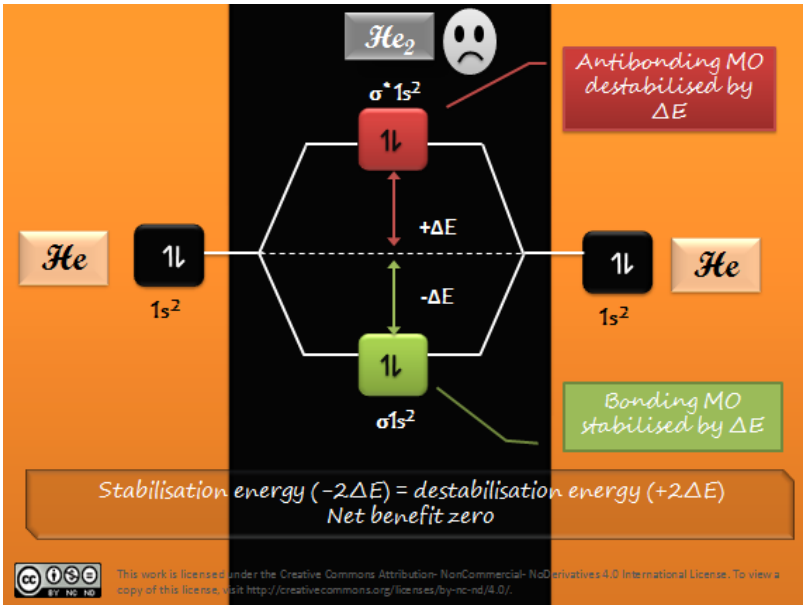
Let's take an example of H_2 molecule. Its electronic configuration is $1s^1$. How do two atoms of H combine to form H_2molecule? 1s orbitals of both H atoms get overlapped and form one bonding MO (σ1s) and one antibonding MO (σ^*1s). Now we have to fill electrons in these MOs. Filling of electron in MO is just similar to filling electrons in atomic orbitals. H_2 molecule gets one electron from each H atom, thus it has 2 electrons. Bonding MO (σ1s) has lower energy so it has to be filled first.



In the last post we have seen that bonding MO is more stable because it has lesser energy than parent AO. In H_2 molecule both electrons are filled in the bonding MO. If stabilization energy for one electron is ΔE, then it will be 2ΔE for two electrons. That means H_2 molecule is stabilised by 2ΔE as compared to the H atom.

Do you know the Darwin's theory of evolution? "Survival of the fittest"; similar concept is applicable in the world of chemistry. Only those molecules exist which have lowest energy. That's why H prefers to form H_2 molecule for stable existence.

Let's examine Helium in the light of MOT. Its electronic configuration is $1s^2$. In order to form He_2 molecule, 1s atomic orbitals of both Helium atoms will have to overlap and form one bonding MO (σ1s) and one antibonding MO (σ^*1s). If this happens, the resulting He_2 molecule will get two electrons from each Helium atom, thus it will have 4 electrons. Bonding MO (σ1s) has lower energy so it has to be filled first. 2 of the 4 electrons will be filled in σ1s and remaining 2 will be filled in σ^*1s.



As a result, the stabilization energy gained by 2 electrons will be cancelled by destabilization of 2 electrons of σ^*1s. As we can see that Helium atom is not benefited by formation of He_2 molecule and prefers to stay alone as Helium atom. That's why He_2molecule doesn't exist.

In the next post we will discuss the formation of O_2 molecule and see how MOT helps us to find the number of bonds formed by O atoms in O_2 molecule.

Source : http://chemistrynotmystery.blogspot.in/2014/09/applications-of-mot.html