Molecular orbital is the formation of molecular orbitals resulting from the overlap of atomic orbitals. The two new orbitals which are formed from the interaction of two atomic orbitals, are antibonding and bonding orbital. The antibonding orbital is destabilized and has higher energy than stabilized bonding orbital. How do they interact in the molecule orbitals? And what are the factors that affect the orbital interaction?

**Molecular orbitals**

Atomic orbitals are the quantum states of the individual electrons forming the electron cloud and moving around an atom. In the same orbitals, electrons have the same energy and each orbital contains a maximum of two electrons.

Similar to the way electrons occupy the atomic orbitals, electrons occupy the molecular orbitals surrounding the molecule. The formations of molecular orbitals are from the combination of atomic orbitals or more specific, from the wave interaction of atomic orbitals.

**Orbital interaction- general concepts:**

The interaction between two atomic or molecular orbitals will form two new orbitals. One new orbital is antibonding orbital which has the higher energy than the original molecule orbital. The other new orbital is the bonding orbital which is lower in energy than the initial one.

The stabilization of the bonding molecular orbital and destabilization of the antibonding can increase when the overlap of two orbitals increases. (Jean, Yvesand , page 14)

In the molecular interaction, there are the two important orbitals that interact each other. One is the highest energy occupied molecular orbital is called HOMO. The other one is the lowest energy unoccupied molecular orbital (LUMO). When a pair of electrons filled in one of the molecule orbital and no electron occupy in the other orbital, this interaction is very stable and called filled- empty interaction.

**HOMO-LUMO interaction**

HOMO and LUMO orbitals are a pair and they lie very close together in energy of two molecules. Therefore, the interaction between them is very strong.

The picture 1 shows the filled-empty interaction of HOMO-LUMO interaction:
Factors affect the strength of orbital interaction:

There are several factors that contribute to the overlap of two atomic orbitals; as a consequence, they affect the strength of the orbital interaction: the symmetry of the orbitals, the energy difference between them, their orbital sizes, and distance between the orbitals.

First, the orbital interactions are depending on their symmetry. We stated that orbital interactions are allowed if the symmetries of the atomic orbitals are compatible with one another. (Housecroft, page 46) Under the symmetry’s affect, the result of orbital interaction from anti bonding is non bonding. Based on the symmetry, the orbital interactions from bonding result in three different types.

First, the interaction from bonding that possess the rotational symmetry surrounding the axis between the two atomic nuclei forms sigma bonds. Figure 2 shows the region of high electron density that holds the two nuclear centers together to form a sigma bond.

Secondly, the bonding interaction in which a pair of electrons of an atom occupy an orbital with two lobes overlapping the two lopes of other atom’s orbital, is called pi bond. In figure 3, two p-orbitals form a pi bond. In the pi bond interaction, 2 lobes lie perpendicular to the axis between two nuclei. The pi bond is weaker than the sigma bond. In the sigma bond, 2 atomic orbitals overlap strongly on the region that lie between two nuclei whereas the p orbitals in pi bond less overlap each other because of their parallel orientation.
The third interaction in which four lobes of one atom’s orbital overlapping the other four lobes, results in delta bond. Figure 4 shows a delta bond forming from the overlap of two d orbitals. In the delta bond interaction, 4 lobes are perpendicular to the axis lie between 2 atoms. Comparing to the sigma and pi bond interaction, the delta bond has the weakest interaction.
The difference between energies of two atomic orbitals also takes a significant contribution to the strength of orbital interaction. The relative energies of atomic orbitals of X and Y will dictate whether an interaction will lead to efficient overlap or not. (Housecroft, page 47) The more similar in energy of two atomic orbitals will result in the stronger interaction in the formation of new molecular orbital. The homonuclear diatomics such as O$_2$, N$_2$, Cl$_2$… have the same atomic orbital energies, so the orbital interaction between them is very strong. On the other hand, in the heteronuclear diatomic (CO, HF…), the atomic orbitals lie at different energy, the orbital interaction depends on how close their energy difference is.

Orbital size is another factor that affects the strength of orbital interactions due to the overlap region of orbitals. The orbitals with different sizes have weaker interactions than the same size orbitals; the result of a weaker bond can be explained by the weaker overlap between orbitals. This is shown in figure 5.

![figure 5](image)

The last factor that affects the orbital interaction is the distance between orbitals. The sigma bonding interaction and the pi bonding interaction have strong interaction due to their much closed orbitals. The delta bonding interaction will possess the weakest interaction because their orbitals are far from each other. Show in figure 6
The wave interaction of atomic orbitals

Depending on the phase relationship, there are two different ways that the two orbital overlap. The phase of an orbital has the same properties of the wave-like of electrons. Light waves interaction have two different ways: one is in-phase increasing the intensity of the light and other one is out-of-phase decreasing the intensity of the light. Similarly, electron waves interaction has two types: in-phase and out-of-phase. In-phase interaction increases the intensity of negative charge. On the other hand, decreasing the intensity of the negative charge results from the out of phase interaction.

The orbital phase is presented by a plus or minus sign. When the two same sign orbitals overlap to form a molecular orbital, the electron density will occupy at the region between two nuclei. This negative charge intensity of electrons will increase in the in-phase interaction. The increasing negative charge increases attractions between electrons and nuclei. The molecular orbital resulting from in-phase interaction is defined as the bonding orbital which has lower energy than the original atomic orbital.

The out of phase interaction between two atomic orbitals doesn’t result in electron density between the two atomic nuclei. The negative charge intensity of electrons will decrease in the out of phase interaction. The decreasing negative charge decreases attractions between electrons and nuclei. As a consequence, the out of phase interaction forms the anti bonding molecular orbital with the higher energy than the initial atomic orbital.

The diagram 7 shows the bonding and antibonding between two 1s orbitals
The bonding and anti bonding between two p orbitals are showed in diagram 8.

References

1. Jean, Yves and Volatron, François. *An Introduction to Molecular Orbitals*. Oxford University Press. 11.03. 2005

Outside Links

Problems

1. How do molecules orbitals form?

The formation of molecular orbitals is from the overlap of atomic orbitals; or more specific, from the wave interaction of atomic orbitals.

2. What are the factors that affect the orbital interaction?

There are some significant factors that affect the strength of orbital interaction

- Symmetry of the molecule orbital
- The difference between orbitals’ energies
- The orbitals’ sizes
- The distance between orbitals

3. What are HOMO and LUMO? How do they interact in the molecule orbitals?

The highest energy occupied molecular orbital is called HOMO

The lowest energy unoccupied molecular orbital is called LUMO

These orbitals are a pair and they lie very close together in energy of two molecules. Therefore, the interaction between them is very strong.

4. What are the two types of electron waves interaction?

In-phase and out of phase interactions

5. How do the intensity of negative charge of electrons change in each types of electron waves interaction?

The intensity of negative charge of electrons increases in the in-phase interaction and decreases in the out-of-phase interaction.