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.

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.

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

![Diagram 7](image)

The bonding and anti bonding between two p orbitals are showed in diagram 8
References

1. Jean, Yvesand 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.