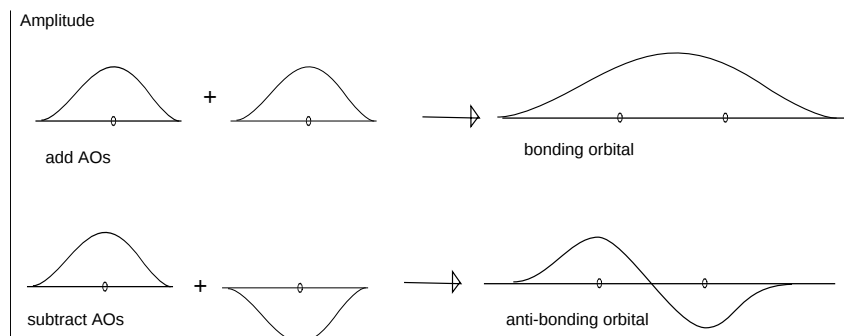![LibreTexts logo]

MO Theory: Simplest Examples
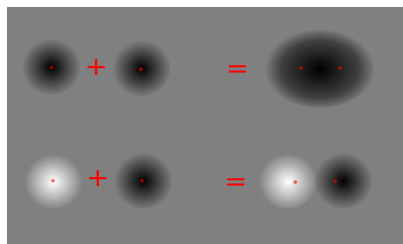
Skills to Develop

- Construct MO diagrams for H_2 and He_2
- Define bond order in theory and calculation

MO Theory for H_2

Let's find the MO description of H_2. We are going to use one electron on each H atom, each in a 1s orbital. When we bring the 2 atoms next to each other, we can make 2 MOs out of the 2 1s AOs. As always, we will do a + combination and a — combination. These combinations are illustrated in the figure below.
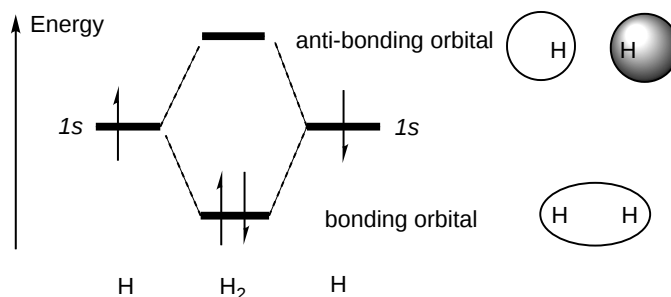

The formation of MOs from 1s orbitals, illustrated with approximate 1D waves, showing Ψ vs radius. The small circles show the positions of the nuclei. We add the 2 waves on the left to get the total wave on the right.

The formation of MOs from 1s orbitals, illustrated with approximate 2D drawings. The small pink dots show the position of the nuclei. Positive amplitude of Ψ is shown with black, negative amplitude of Ψ is shown with white, on a gray background. Where positive and negative amplitude waves overlap, the sum approaches zero (gray background).

Notice that the + combination produces an MO with more electron density between the nuclei, because the waves interfere constructively. The — combination produces an MO with a node between the nuclei, and not much electron density there, because the waves interfere destructively. If you think about the Coulomb's law forces, and imagine putting 2 electrons in the + MO, they will usually be between the nuclei, and the attractions between the electrons and nuclei will hold the nuclei together, making the molecule. For this reason, the + MO is called a **bonding MO**. On the other hand, if we imagine putting 2 electrons in the — MO, they will usually be on the outside of the nuclei, so the repulsion between the nuclei will push them apart, and no molecule will form. For this reason, the — MO is called an **anti-bonding MO**.
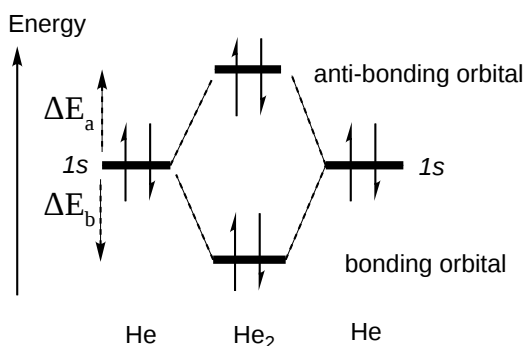
You've seen before that more nodes means higher energy. (For instance, if you try to swing a jump rope so it has a standing wave with 2 nodes, that is much harder than making a standing wave with no nodes.) So it makes sense that the bonding MO (no nodes) is lower in energy than the anti-bonding MO (1 node). Thus, in H_2, both electrons will go in the bonding MO, and the molecule is stable. In fact, the bonding orbital will be lower in energy than the AOs it was made from, because of the increased Coulomb attractions. The anti-bonding orbital will be higher in energy than the AOs because of the increased Coulomb repulsions. We can represent this with an MO diagram, shown in the figure.

MO energy level diagram for H_2. The vertical axis represents energy and the thick bars represent orbitals. The outside bars (labeled 1s) represent the H AOs. The middle bars represent the bonding and anti-bonding MOs. Because the bonding MO is lower in energy, both electrons ($\uparrow$ and $\downarrow$) go there.

MO Theory for He_2

Now let's think about He_2. We still have a combination of 2 AOs, both 1s. The bonding and anti-bonding orbitals will look very similar. But now we have 4 electrons, so we will have to put 2 electrons in each MO. Because the molecule He_2 does not exist, we can conclude that the anti-bonding orbital increases in energy more than the bonding orbital decreases in energy, so that He_2 is higher energy than 2 He.

MO energy level diagram for He_2. Because He_2 doesn't exist, we can conclude that $\Delta E_a + \Delta E_b > 0$.

Bond Order in MO Theory

One great thing about MO theory is that it makes it really simple to think about partial bonds and weird molecules, like radicals. The table shows some data for a few examples.

Molecule	Bond Length (Å)	Bond energy (kcal/mol)
He_2	*	*
H_2^+	1.06	61
He_2^+	1.08	55
H_2	0.74	103

Now try drawing the MO diagram for each molecule. What do you notice? If we calculate

net bonding electrons = (number of bonding electrons) — (number of anti-bonding electrons)

we get:

Molecule	Bonding Electrons	Anti-Bonding Electrons	Net Bonding Electrons	Bond Length (Å)	Bond energy (kcal/mol)
He_2	2	2	0	*	*
H_2^+	1	0	1	1.06	61

Molecule	Bonding Electrons	Anti-Bonding Electrons	Net Bonding Electrons	Bond Length (Å)	Bond energy (kcal/mol)
He_2^+	2	1	1	1.08	55
H_2	2	0	2	0.74	103

The number of net bonding electrons predicts the length and strength of the bond! Since we normally think of a chemical bond as a 2-electron bond, we can define the bond order like this:

$$Bond\ Order = \frac{(bonding\ e^-) - (anti\text{-}bonding\ e^-)}{2}$$

(MO Theory.1)

If bond order = 1, there is a single bond (H_2, for instance). If bond order = 0, we expect no bond. If bond order = 0.5, we have a 1-electron bond or a half bond. It's approximately half as strong as a 2-electron bond.

Outside Link

- ChemSurvival: A Brief Introduction to Molecular Orbital Theory (10 min)

Contributors

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