# Mixing Orbitals to Make MOs

**Skills to Develop**

- Describe and illustrate MOs in a molecule

**Molecular Orbitals** or MOs are orbitals in a molecule. Remember that atomic orbitals (AOs) are "electron probability clouds." We can't know exactly where an electron is or what path it follows, because of the Uncertainty Principle, but we can find a mathematical function that tells us how likely we are to find the electron at each position around an atom. If we think of electrons behaving like waves, which they do, the wavefunction $\Psi$ tells us the amplitude of the "electron wave" at each point around the atom. $\Psi^2$ tells us the probability of finding the electron there. When we combine atoms to make molecules, there's wave interference between the electron waves on different atoms. The electrons in a molecule occupy molecular orbitals, or MOs, that are combinations of the atomic orbitals made using the basic rules of wave interference.

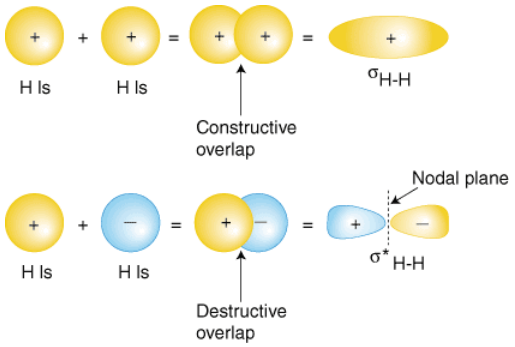
MOs have the same basic properties that atomic orbitals have. Each MO can hold 2 electrons with opposite spins. $\Psi^2$ still represents the probability of finding the electron. Each MO has a specific energy, and removing an electron from that MO requires that much energy. However, MOs can have very different shapes compared to MOs, and they can be spread out over many atoms in a molecule.

We make MOs in a way similar to how we made hybrid orbitals. If we combine 2 AOs (call them $\varphi_A$ and $\varphi_B$) on different atoms, we will make 2 new MOs (call them $\psi_1$ and $\psi_2$).

$$\Psi_1 = C\left(\varphi_A + \varphi_B\right) \tag{1}$$

$$\Psi_2 = C\left(\varphi_A - \varphi_B\right) \tag{2}$$

We will make one MO by adding the AOs and the other by subtracting the AOs. C is a constant that "normalizes" the wavefunction so that the total probability of finding the electron over the whole atom is 1.




An example of making one MO by adding AOs, top, and another by subtracting AOs, bottom.

## Contributors and Attributions

- Emily V Eames (City College of San Francisco)

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