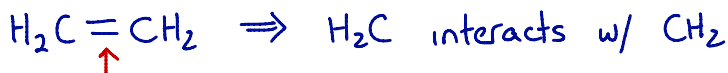
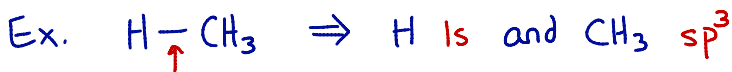


Day 5 - How to draw an "MO" orbital mixing diagram

Step 1. Identify the interacting atoms or "molecular fragments"



Step 2. Identify the atomic/hybrid orbitals that describe the interacting electrons on each fragment.



Step 3. Draw one fragment's interacting orbital(s) on the side of the diagram. Draw the other fragment's orbital(s) on the right side. Leave space in the middle for the MO's. The vertical axis is an energy axis and orbitals should be positioned correctly relative to each other. Label each orbital and draw the fragment at the bottom underneath its orbital(s).

Ex.

$1s +$

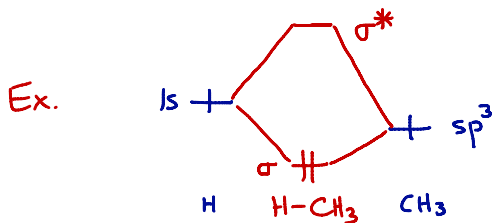
H

$+ sp^3$

CH_3

Step 4. Count the electrons contributed by each fragment and assign them to the fragment's orbital(s).

Step 5. For each pair of interacting orbitals, one on each fragment, draw 2 MOs in the blank space in the center of the diagram. Position one MO (BMO) at a lower energy than either fragment orbital. Position the second MO (ABMO) at a higher energy than either fragment orbital. Label the BMO as σ or π depending on the type of overlap. Label the ABMO as σ^* or π^* . Draw the molecule at the bottom underneath the MO's. Draw lines from the fragment orbitals to the 2 MO's. Draw the electrons in the lowest energy MO's available.



Step 5 adjustments.

- ① The ABMO goes up more than the BMO goes down.
- ② Both MO's are positioned according to the strength of the overlap between the fragment orbitals. σ overlap is always stronger than π overlap. Overlap falls as fragments move farther apart.

