Dr. Sandblom's Fill-in Notes for MO Model…

What

-

Where

-

-

When

-

Why

-

-

How

-

-

-

10.6 The Molecular Orbital Model

MOs are like AOs:

-
    - o
    - o
-

We will not talk about the math to get these functions, instead we will use a qualitative approach to understand the results.

Since the orbitals are wavefunctions → combining them can result in constructive and destructive interference of the waves
Figure 10.22

Start with simplest molecule - H_2

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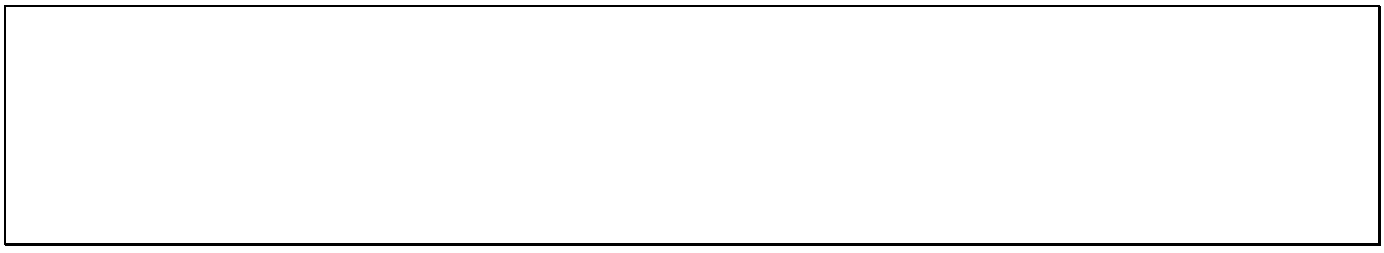
To make MOs: mix together or "overlap" AOs by adding and by subtracting the functions.



So:

-
- MO_{σ} is called a σ **bonding** orbital
    - o
- MO_{σ^*} is called a σ^* **antibonding** orbital
    - o

Energy level diagram:

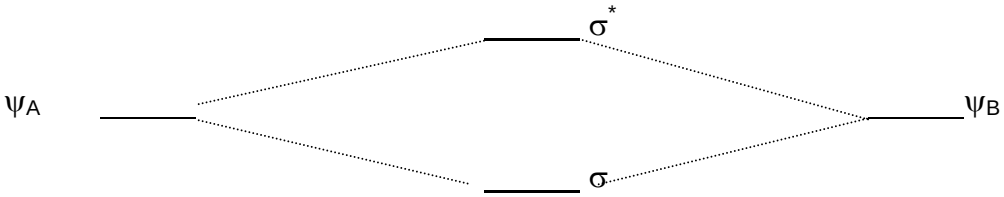


Figure 10.23a

Last step:

- add electrons
    - o for ground state:
        -
        -

Examples

- H_2
- H_2^-
- He_2

Bond Order

$$BO = \frac{\#\ of\ e^-\ in\ bonding - \#\ of\ e^-\ in\ antibonding}{2}$$

- H_2 BO
- H_2^- BO
- He_2

What will the MOs look like?

$\psi_A + \psi_B = MO_\sigma$

$\psi_A - \psi_B = MO_{\sigma^*}$

Figure 10.23b

We can use the M.O. model for any molecule, but for this course we will only look at simple homonuclear diatomics - the ones we have already considered and O_2.

Important guidelines for building MO diagram:
1.

-

2.

-
-
-

3.

As with H_2 - To make MOs: mix together valence AOs

So: $\psi_{2s} + \psi_{2s} = \sigma_{2s}$ and $\psi_{2s} - \psi_{2s} = \sigma_{1s}^*$

-

What happens for the p orbitals?
Figure 10.24b

- $2p_x$ and $2p_x$ make σ_{2p} and σ_{2p}^*
- $2p_y$ and $2p_y$ make π_{2p} and π_{2p}^*
- $2p_z$ and $2p_z$ make π_{2p} and π_{2p}^*

How do the energies compare?

Now, the electrons can be added - 12 e^-:

-
-
-

Bond Order:

Prediction: Is O_2 diamagnetic or paramagnetic?

OBSERVATION:
MODEL:

What about O_2^-?

If I told you that F_2 had the same MO diagram based on the same valence MOs, what would be the Bond Order?

The MO diagram provides some information about a compound's reactivity: the HOMO reacts with electrophiles, the LUMO reacts with nucleophiles.

Remember a π bond is not as strong as a σ bond - this affects the reactivity.
After a reaction begins by reacting with (and breaking) a π bond, there are two possibilities to consider:

A. The σ bond is left intact.
B. The σ bond is reacts and breaks as well.

(more about this later)
Earlier: VSEPR prediction of structure of NH_3 and PH_3… trigonal pyramidal!
incorrect prediction for angles in PH_3
better prediction (closer to experiment) with M.O. model
How about trying to construct MO diagram for PH_3? Or CH_3CN? Or $CH_3CH_2CH_2CH_2Br$?

MO is a ***good*** model, but we need a ***simple*** model! Exercises: 46, 47, 48, 52, 58