sp hybridization

ex. acetylene

\[ \text{H-C=C-H} \]

Molecular Orbital Theory

Some assumptions (MO)

1) Molecular orbitals form from linear combinations of atomic orbitals (AO's)
2) MO's are to molecules what AO's are to atoms.
3) Addition combinations \( \rightarrow \) bonding MO's
   Subtractive \( \rightarrow \) antibonding MO's

\[ \sigma_{\text{antibonding}} \quad 1\alpha_e - 1\alpha_e \]

\[ E \quad 1\alpha_e \quad 1\alpha_e \quad 1\alpha_e \quad \text{H}_2 \quad \text{H}_2 \]

\[ \sigma_{\text{bonding}} \quad 1\alpha_e + 1\alpha_e \quad 1\alpha_e + 1\alpha_e \quad \text{H}_2 \quad \text{H}_2 \]

Bond Order: 

\[ \text{# bonds} \times \text{antibond} = \text{pairs} \]

Topics

Form of MO Theory
Drawing Chemical Structures
Isomers
Representative Org. Compounds
Functional Groups
in gas phase under \( A_2 \xrightarrow{e^-} H_2 \) 

\[
\begin{align*}
H_2 & \quad \text{of} \\
\text{ib} & \\
\text{value} & = \frac{1}{2}
\end{align*}
\]

- 3 types of MO's:
  1. Bonding - lower in energy than corresponding atomic orbitals. Result in increase in \( \epsilon^- \) density between atoms.
  2. antibonding - higher in energy than corresponding atomic orbitals. Result in decrease in \( \epsilon^- \) density between atoms.
  3. Nonbonding - about same energy as corresponding atomic orbitals. No change in \( \epsilon^- \) density between atoms.

Ex. \( O_2 \)

- Valence bond predicts \( \epsilon^2 = 0 \).
- MO predicts \( \epsilon^2 = 0 \) (also predicts paramagnetism)
- Bond order = 2

\[
\begin{align*}
\text{O} & \quad 2\epsilon \quad \text{ib} \\
\text{O} & \quad 2\epsilon \quad \text{ib}
\end{align*}
\]
- Drawing Chemical Structures

**Ex. Propene** \( \text{C}_3\text{H}_6 \)  \hspace{2cm} **Butane** \( \text{C}_4\text{H}_{10} \)

\[
\begin{align*}
\text{Propene} &: H \quad H \quad H \\
&: H - C - C - H \\
&: H \quad H
\end{align*}
\]

\[
\begin{align*}
\text{Butane} &: H \quad H \quad H \quad H \\
&: H - C - C - C - C \quad H \\
&: H \quad H \quad H
\end{align*}
\]

**Condensed -**

\[
\begin{align*}
\text{Propene} &: \text{CH}_3\text{CH}_2\text{CH}_3 \\
\text{Butane} &: \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \\
\text{CH}_3\text{C}_2\text{H}_5 &: \text{CH}_3\text{C}_2\text{H}_5
\end{align*}
\]

- Thin bond -
  - Hydrogens assumed
  - Carbon at corner

- Represents 3 dimensions

**Ex. Methane**

1) make 2 bonds coplanar

\[
\begin{align*}
\text{Methane} &: H \quad H \\
&: H - C - H \\
&: H
\end{align*}
\]

2) wedge bonds coming out of plane of paper

3) dashed line going back into plane of paper

**Ex. Propene (or other chain):**

- Put backbone in plane of paper
- Isomers.

- Pentane $C_5H_{12}$

- $C_5H_{11}Cl$

- Functional Group - atom or group of atoms expected of a molecule characterized by its structure and type of reactivity.

- Hydrocarbons - contain only $C$ and $H$

  - Alkanes $C_nH_{2n+2}$
    - $CH_4$ - methane
    - $C_2H_6$ - ethane
    - $C_3H_8$ - propane
    - $C_4H_{10}$ - butane (2 isomers)
    - $C_5H_{12}$ - pentane (3 isomers)