Lecture Notes J: Molecular Orbital Theory

1) Bond formation

Bonding between two 1s orbitals in H₂

H₂ versus He₂ (definition of bond order)

Bond order = (number of bonding electrons – number of antibonding electrons)/2

If atom B is more electronegative than atom A
2) **Sigma (σ) versus pi (π) bonding**

Sigma bonding between s orbitals

Sigma bonding between p orbitals

Sigma bonding between s and p orbital

Pi bonding
3) **Hybrid orbitals in polyatomic molecules**

\[ \text{H}_2\text{CCH}_2 \]

\[ \text{HCCH} \]
4) **Terminal heavy (non-hydrogen) atom**

Orbitals on a terminal atom do not hybridize

For B₂, C₂, N₂

For O₂, F₂

Why does the order switch for O₂ and F₂?
**Exercise**

Draw the molecular orbital diagram for $\text{C}_2$

What is the bond order for $\text{C}_2$, $\text{C}_2^+$ and $\text{C}^-$?

- $\text{C}_2$
  - a) 1
  - b) $1\frac{1}{2}$
  - c) 2
  - d) $2\frac{1}{2}$

- $\text{C}_2^+$
  - a) 1
  - b) $1\frac{1}{2}$
  - c) 2
  - d) $2\frac{1}{2}$

- $\text{C}_2^-$
  - a) 1
  - b) $1\frac{1}{2}$
  - c) 2
  - d) $2\frac{1}{2}$

Which of the following are paramagnetic?

- $\text{C}_2$
  - a) paramagnetic
  - b) not paramagnetic

- $\text{C}_2^+$
  - a) paramagnetic
  - b) not paramagnetic

- $\text{C}_2^{+2}$
  - a) paramagnetic
  - b) not paramagnetic

- $\text{C}_2^-$
  - a) paramagnetic
  - b) not paramagnetic

- $\text{C}_2^{-2}$
  - a) paramagnetic
  - b) not paramagnetic
5) *Diatomice molecules: hydrides*

HF