Orbital Overlap, Sigma and Pi Bonds, and Formation of H_2, F_2, HF, O_2 Molecules - Lecture Notes

---

1. Orbital Overlap and Bond Formation:

- **Orbital Overlap** is a fundamental concept in **Valence Bond Theory** (VBT), which explains how atoms in a molecule share electrons to form covalent bonds.
- A **covalent bond** forms when two atomic orbitals from different atoms overlap, resulting in a region of increased electron density between the two nuclei. The overlapping orbitals allow for the sharing of electrons.
- The strength of the bond depends on the extent of overlap. Greater overlap results in a stronger bond.

There are two types of bonds based on the nature of orbital overlap:

---

2. Sigma (σ) Bond:

- A **sigma (σ) bond** is formed by the **head-on overlap** of atomic orbitals.
- The electron density in a sigma bond is concentrated along the axis connecting the two nuclei (internuclear axis).
- Sigma bonds are stronger than pi bonds because the overlap is more extensive.

  Examples:
  - Overlap of two **s orbitals** (as in H_2 molecule).
  - Overlap of an **s orbital** and a **p orbital** (as in HF molecule).
  - Overlap of two **p orbitals** head-to-head (as in F_2 molecule).

---

3. Pi (π) Bond:

- A **pi (π) bond** is formed by the **side-to-side overlap** of two **p orbitals**.
- The electron density in a pi bond is concentrated **above and below** the internuclear axis.
- Pi bonds are generally weaker than sigma bonds due to less overlap.
- Pi bonds always accompany sigma bonds in multiple bonds (double or triple bonds).

  Example:

- In O_2 (oxygen molecule), there is a sigma bond and a pi bond between the two oxygen atoms (double bond).

---

4. Formation of Molecules:

a) Formation of H_2 Molecule:

- In an H_2 molecule, the bond is formed by the overlap of two 1s orbitals, one from each hydrogen atom.
- This results in the formation of a **sigma bond** along the internuclear axis.
- The molecular orbital formed has increased electron density between the two hydrogen nuclei, stabilizing the molecule.

  H_2 bond type: Sigma bond.

b) Formation of F_2 Molecule:

- In an F_2 molecule, each fluorine atom has a half-filled 2p orbital.
- A sigma bond is formed by the **head-on overlap** of these two **2p orbitals**.
- Fluorine has a stable octet, and the bond strength comes from the sharing of one electron from each atom.

  F_2 bond type: Sigma bond (from 2p-2p overlap).

c) Formation of HF Molecule:

- In HF, the bond forms between the hydrogen atom's 1s orbital and the fluorine atom's 2p orbital.
- The bond is a **sigma bond** resulting from the overlap of the **1s** orbital of hydrogen and the **2p** orbital of fluorine.
- Since fluorine is highly electronegative, the shared electron pair is drawn closer to fluorine, resulting in a **polar covalent bond**.

  HF bond type: Polar sigma bond (from 1s-2p overlap).

d) Formation of O_2 Molecule:

- In O_2, each oxygen atom forms one sigma bond and one pi bond with the other oxygen atom.
- The sigma bond results from the **head-on overlap** of two **2p orbitals** (one from each oxygen).
- The pi bond results from the **side-to-side overlap** of another set of **2p orbitals** (perpendicular to the sigma bond axis).
- This leads to a **double bond** between the oxygen atoms, with one sigma and one pi bond.

O_2 bond type: One sigma bond (from 2p-2p head-on overlap) and one pi bond (from 2p-2p side-to-side overlap).

---

5. Bond Characteristics in Different Molecules:

- **H_2 Molecule**: Strong sigma bond formed by the overlap of two 1s orbitals.
- **F_2 Molecule**: Sigma bond formed by 2p-2p overlap, the bond is weaker than in H_2 due to increased repulsion between lone pairs on fluorine atoms.
- **HF Molecule**: Polar sigma bond due to the overlap of a 1s orbital of hydrogen and a 2p orbital of fluorine, with electron density pulled toward fluorine.
- **O_2 Molecule**: Double bond consisting of one sigma and one pi bond, leading to higher reactivity due to the presence of the pi bond.

---

6. Summary of Bond Types and Overlap:

Molecule	Bond Type	Orbital Overlap
H_2	Sigma	1s-1s
F_2	Sigma	2p-2p
HF	Polar Sigma	1s-2p
O_2	Sigma, Pi	2p-2p (Sigma), 2p-2p (Pi)

Understanding the type of bond and the nature of orbital overlap helps explain the molecular structure, bond strength, and reactivity of these molecules.