

Saitechinfo NEET-JEE Academy



Here is a bullet-point summary of **Molecular Orbital Theory (MOT)** based on **Chemical Bonding**:

- **Molecular Orbital Theory (MOT)** describes chemical bonding in molecules by considering the molecular orbitals formed from the atomic orbitals of the constituent atoms.
- **Linear Combination of Atomic Orbitals (LCAO):**
 - Atomic orbitals from each atom combine to form molecular orbitals.
 - The number of molecular orbitals formed equals the number of atomic orbitals combined.
- **Types of Molecular Orbitals:**
 - **Bonding Molecular Orbital:** Constructive interference of atomic orbitals, results in increased electron density between nuclei, which stabilizes the molecule.
 - **Antibonding Molecular Orbital:** Destructive interference, leads to a node between nuclei and less electron density, making the molecule less stable.
- **Bond Order Calculation:**
 - Bond order = (Number of electrons in bonding orbitals - Number of electrons in antibonding orbitals) / 2.
 - Higher bond order implies stronger and shorter bonds.
- **Orbital Energy:**
 - Bonding orbitals are lower in energy than the original atomic orbitals, while antibonding orbitals are higher.
- **Filling of Molecular Orbitals:**
 - Molecular orbitals are filled according to the **Aufbau Principle, Pauli Exclusion Principle, and Hund's Rule**.
 - Electrons first fill the lowest energy bonding orbitals before moving to higher energy antibonding orbitals.
- **Bonding in Diatomic Molecules:**
 - For homonuclear diatomic molecules (e.g., H_2 , O_2 , N_2), molecular orbitals are formed from s and p atomic orbitals.
 - The sequence of energy levels for molecular orbitals depends on the atomic number (Z). For molecules with atomic numbers less than 8 (like N_2), the σ_{2p} orbital is higher in energy than the π_{2p} orbital, but for atoms with $Z \geq 8$ (like O_2), σ_{2p} is lower than π_{2p} .
- **Paramagnetism and Diamagnetism:**
 - Molecules with unpaired electrons in molecular orbitals exhibit paramagnetism (e.g., O_2 is paramagnetic because it has two unpaired electrons in its π^*_{2p} orbitals).

- o Molecules where all electrons are paired are diamagnetic.

- **Comparison with Valence Bond Theory (VBT):**

- o VBT explains bond formation through overlap of atomic orbitals, while MOT uses molecular orbitals formed from the entire molecule.
- o MOT provides better explanations for phenomena like bond order, bond energy, and magnetism (especially for diatomic molecules like O₂).

This summary captures the key points of Molecular Orbital Theory for your study on chemical bonding. If you need more specific examples or diagrams, feel free to ask!

