

CLASS 11 CHEMISTRY • SECTION 4.7

Molecular Orbital Theory

A Quantum Mechanical Approach to Chemical Bonding

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R.S. Mulliken

1932



Beyond Valence Bond Theory

The Limitation

VB Theory successfully explained molecular shapes but failed on key properties. It assumed electrons remain strictly localized between two specific atoms.

It completely failed to explain the paramagnetic nature of O_2 .



The Requirement

A new mathematical model was required that treated the entire molecule as a single quantum mechanical entity, rather than just two discrete atoms pushed together.

Bonding is nature's way of lowering the energy of a system to attain stability.
MO theory provides the most accurate mathematical model for this stabilization.

Main Postulates of MO Theory



Polycentric Nature

Unlike an atomic orbital (monocentric), a molecular orbital is polycentric. Electrons are influenced by two or more nuclei depending on the molecule's size.



Orbital Conservation

Number of MOs formed = Number of combining Atomic Orbitals (AOs). Two combining AOs always yield one Bonding MO and one Antibonding MO.



Energy & Symmetry

AOs must have comparable energy and proper symmetry to combine (e.g., a 1s orbital cannot combine with a 2p if the energy gap is too wide or the symmetry does not match the z-axis).



Standard Filling Rules

MOs are filled in order of increasing energy, strictly obeying the Aufbau principle, Pauli's exclusion principle, and Hund's rule.



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$$E=mc^2$$



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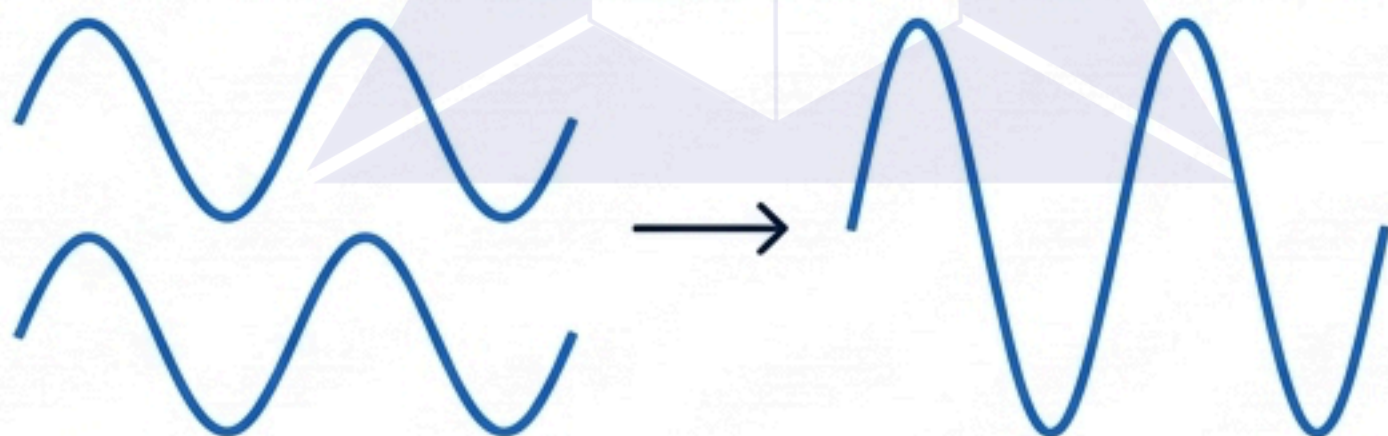


Linear Combination of Atomic Orbitals (LCAO)

Molecular orbitals are obtained approximately by the linear combination (addition or subtraction) of individual atomic orbital wave functions (ψ).

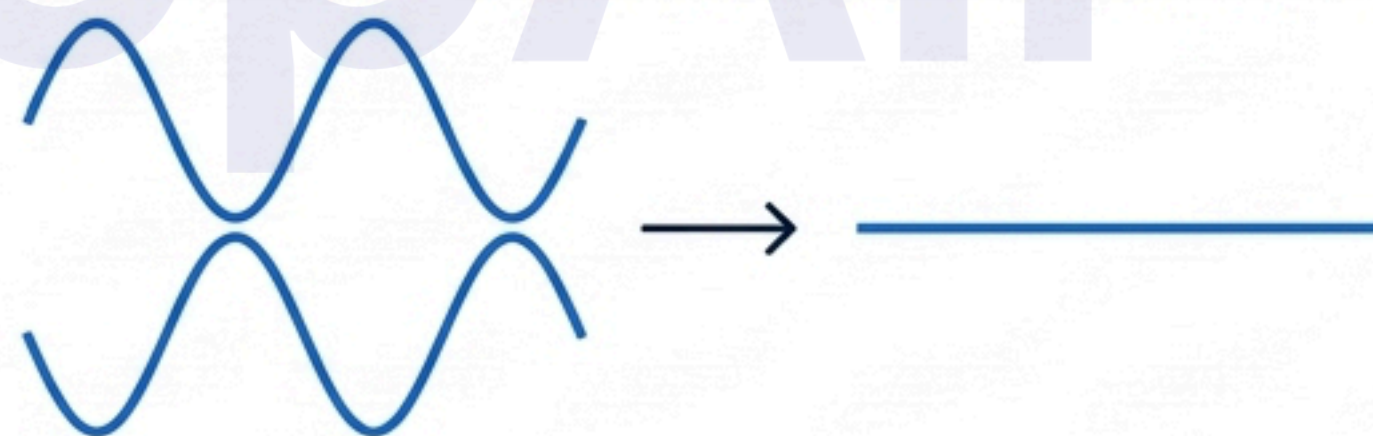
$$\psi_{MO} = \psi_A \pm \psi_B$$

$$\sigma = \psi_A + \psi_B$$



Addition of wave functions.
Waves reinforce each other $\rightarrow$ Forms a Bonding MO.

$$\sigma^* = \psi_A - \psi_B$$



Subtraction of wave functions.
Waves cancel each other $\rightarrow$ Forms an Antibonding MO.

Bonding vs Antibonding MOs

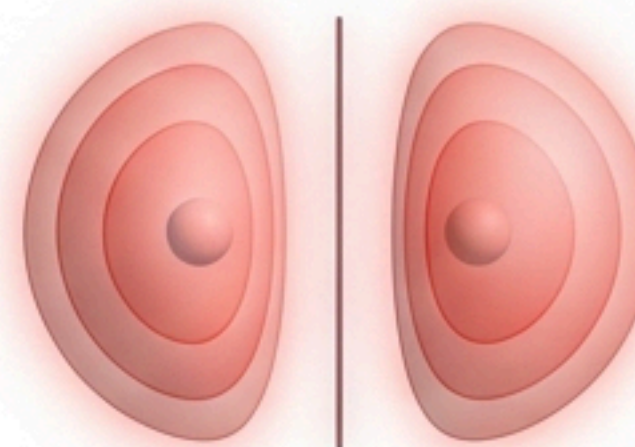
Bonding Molecular Orbital (BMO)

- **Notation:** σ , π
- **Formation:** Constructive interference (electron waves reinforce).
- **Electron Density:** Located between the nuclei. Shields internuclear repulsion.
- **Energy Level:** **Lower Energy** More stable than the parent AOs.



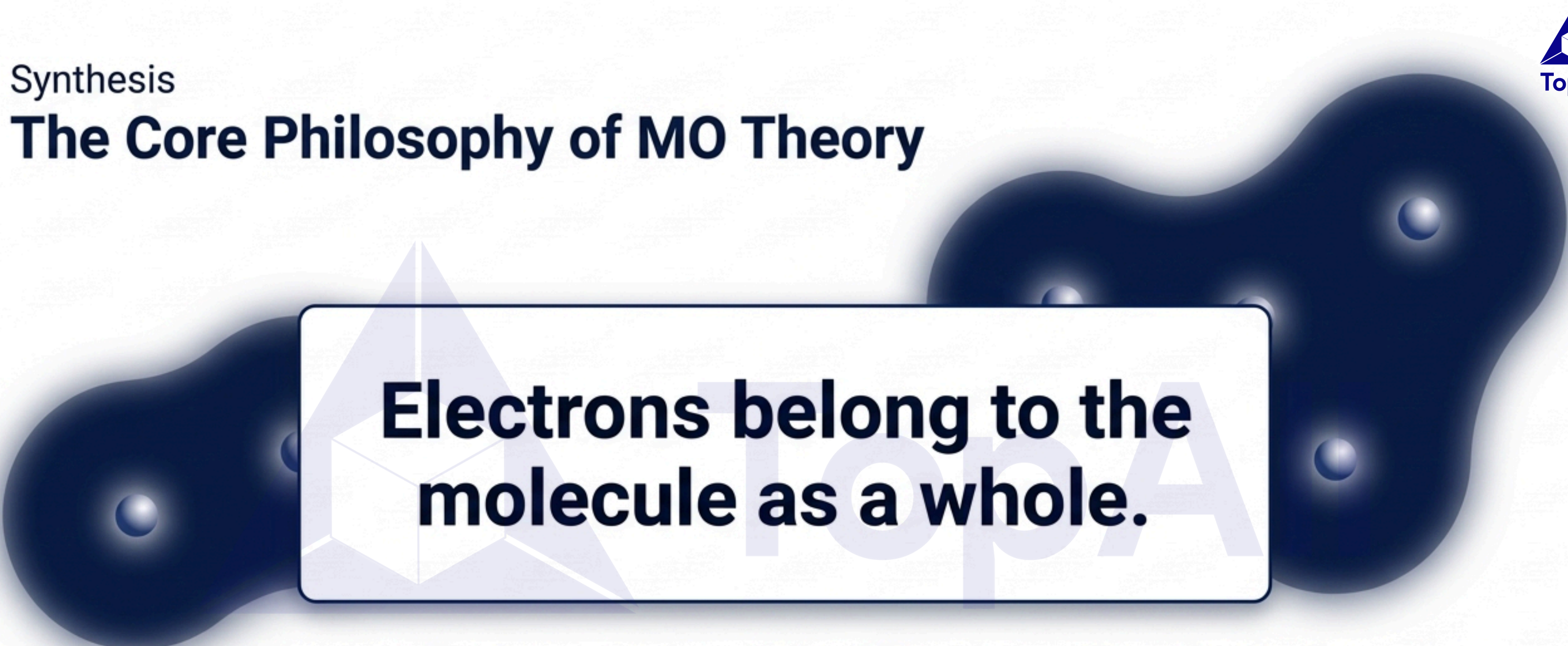
Antibonding Molecular Orbital (AMO)

- **Notation:** σ^* , π^*
- **Formation:** Destructive interference (electron waves cancel).
- **Electron Density:** Located away from the internuclear space. Features a distinct nodal plane.
- **Energy Level:** **Higher Energy** Destabilizes the molecule.



Synthesis

The Core Philosophy of MO Theory



Electrons belong to the molecule as a whole.

Just as an atomic orbital describes the electron probability distribution around a single nucleus, a molecular orbital gives the electron probability distribution around a group of nuclei. The identity of the individual atom is fundamentally merged into the identity of the molecule.

Monocentric → Polycentric

AOs → Linear Combination → MOs

Bonding = Stabilization



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