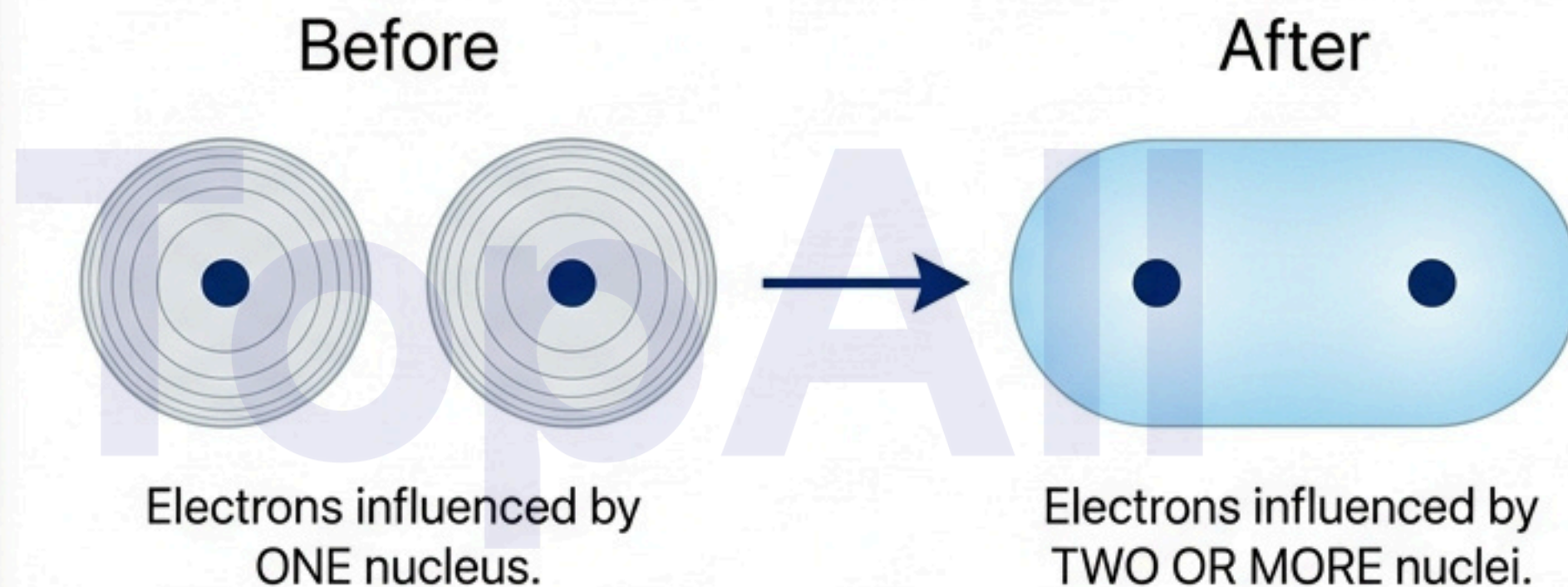


Molecular Orbital Theory

The Paradigm Shift

- Developed by F. Hund and R.S. Mulliken (1932).
- The Core Concept: Electrons in molecules do not belong to individual atoms. They belong to the molecule as a whole.
- The Mechanism: Atomic orbitals of comparable energy and symmetry combine to form entirely new Molecular Orbitals.



Defining the Domain: AO vs. MO

How electron probability shifts from isolated atoms to unified molecules.

Atomic Orbital (AO)



- **Center of Influence:** Monocentric (Influenced by 1 nucleus)
- **Nature:** Exists independently in isolated atoms
- **Nomenclature:** Designated as s, p, d, f
- **Shape:** Simple, symmetrical geometries (e.g., spherical, dumbbell)



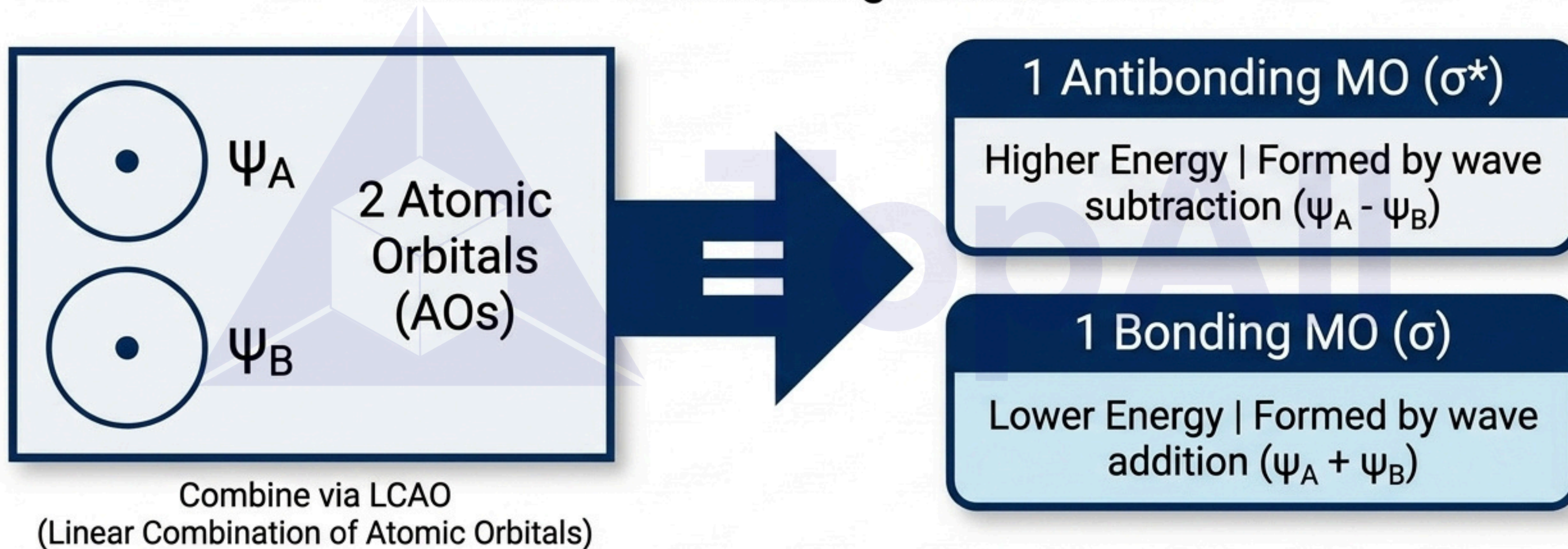
Molecular Orbital (MO)



- **Center of Influence:** Polycentric (Influenced by ≥ 2 nuclei)
- **Nature:** Formed via Linear Combination of Atomic Orbitals (LCAO)
- **Nomenclature:** Designated as σ , π , δ
- **Shape:** Complex contours depending on constructive/destructive interference

The Conservation of Orbitals

The number of molecular orbitals formed precisely equals the number of combining atomic orbitals.



Rule of Thumb: The total energy of the two new molecular orbitals remains exactly the same as the two original atomic orbitals.



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$$E=mc^2$$



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Key Highlights

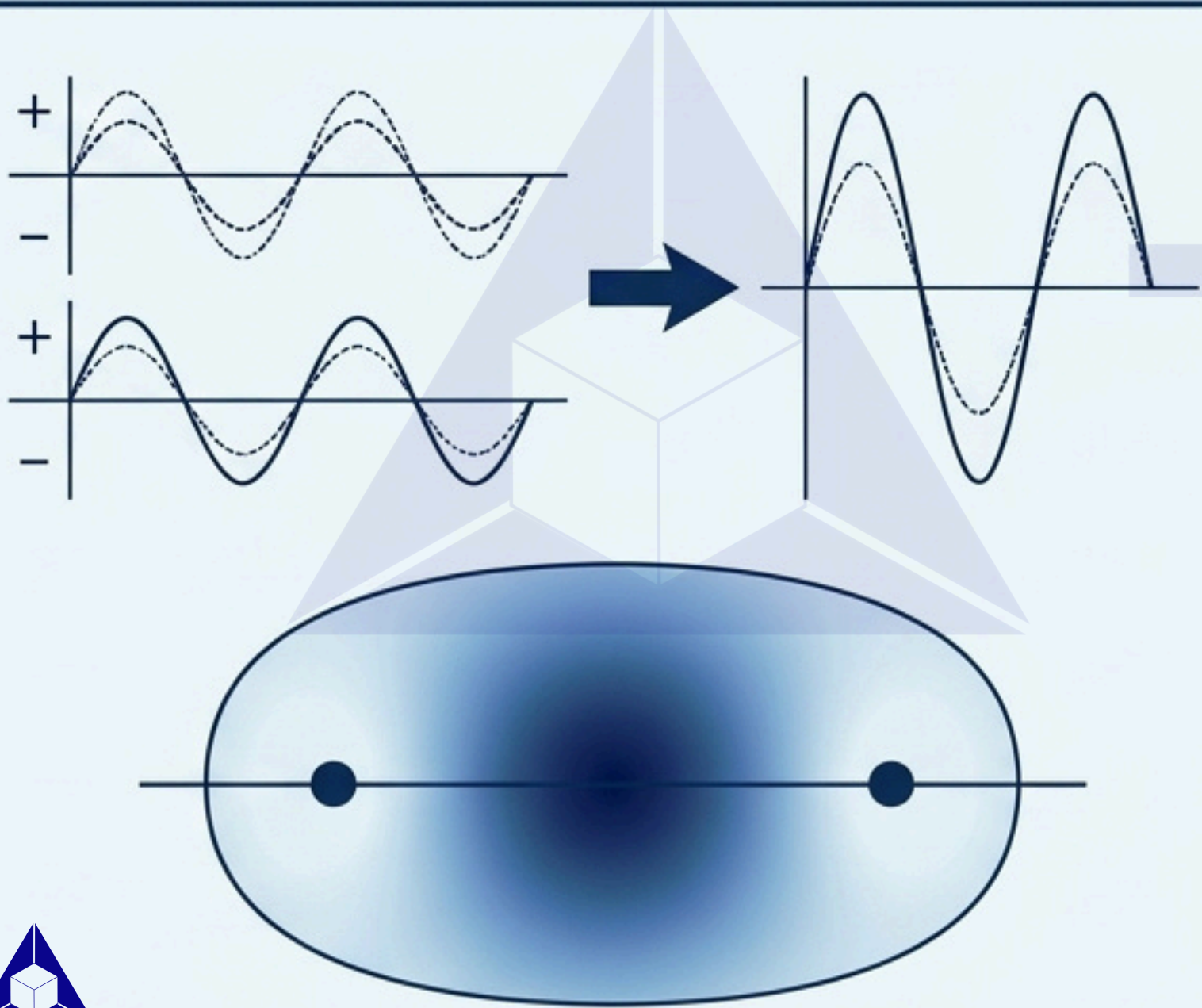
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The Stabilizer: Bonding MO

Forged through the constructive interference of electron waves.

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



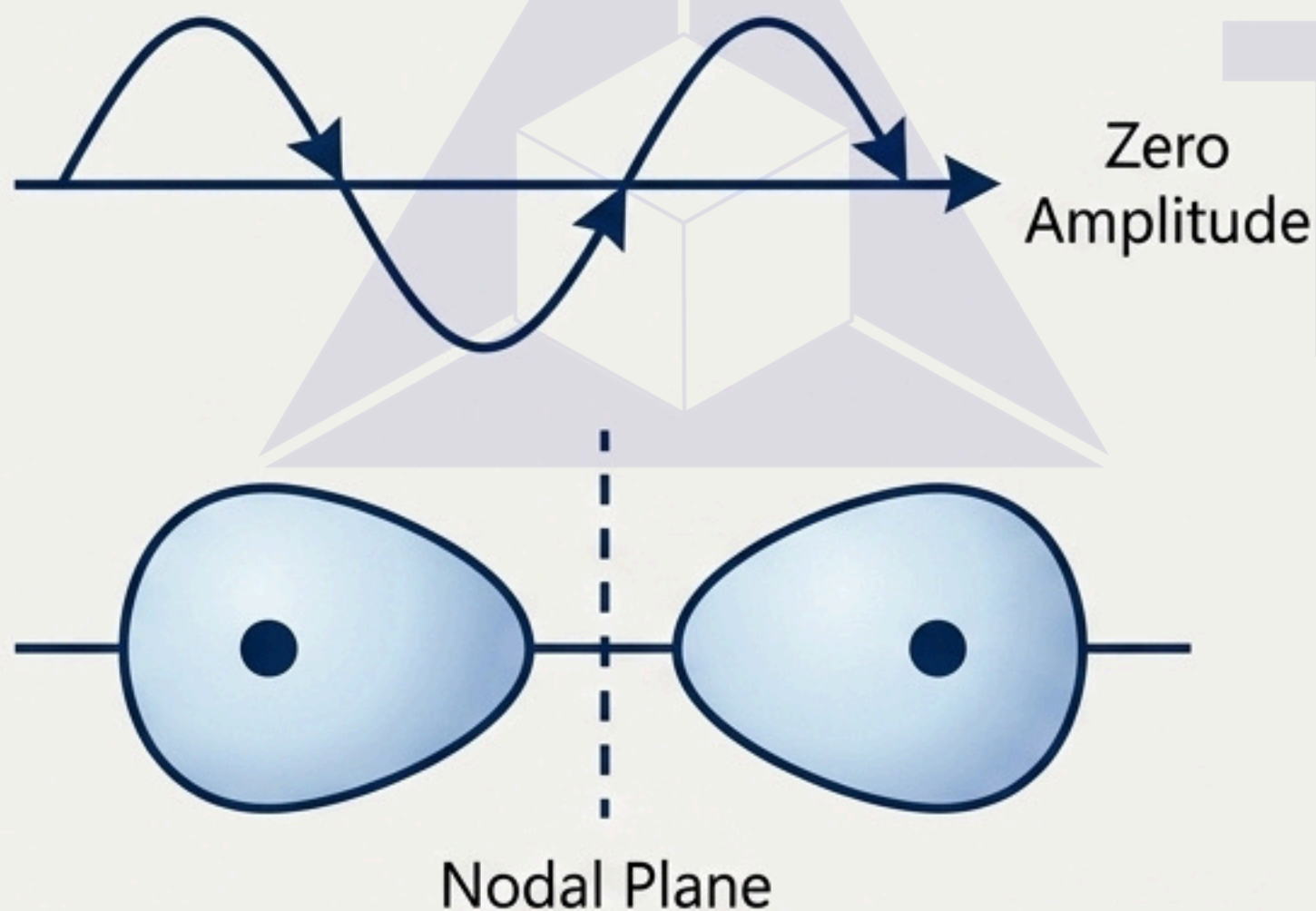
- **Wave Addition:** Electron waves reinforce each other.
- **Electron Density:** Highly concentrated in the space between the bonded nuclei.
- **Nuclear Repulsion:** Minimized, as the concentrated electrons act as a stabilizing 'glue' between the positively charged nuclei.
- **Energy State:** Lower energy than the parent atomic orbitals, resulting in Greater Stability.

The Destabilizer: Antibonding MO

Forged through the destructive interference of electron waves.

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

Left Visual (Destructive Interference)



Right Text (Key Insights)

- **Wave Subtraction:** Electron waves completely cancel each other out.
- **Electron Density:** Concentrated away from the space between the nuclei.
- **The Nodal Plane:** Creates a zone of zero electron density between the nuclei, leading to high mutual nuclear repulsion.
- **Energy State:** Raised above the energy of parent orbitals, which Destabilizes the molecule.

Revision Frame: MO Theory

Core principles and stability rules for quick reference.

The Core Math (LCAO)

- **Bonding MO:** $\sigma = \psi_A + \psi_B$ (Constructive)
- **Antibonding MO:** $\sigma^* = \psi_A - \psi_B$ (Destructive)
- **Conservation:** **N** of Combining AOs = **N** of Resulting MOs

Energy & Stability



BMO: Lower energy, holds nuclei together.
ABMO: Higher energy, pushes nuclei apart.

Predicting Stability (Bond Order)

Let **N_b** = Electrons in Bonding MOs

Let **N_a** = Electrons in Antibonding MOs

- If **N_b > N_a**: Molecule is **Stable** (Positive Bond Order).
- If **N_b ≤ N_a**: Molecule is **Unstable** (Zero/Negative Bond Order).

Conditions for LCAO

1. **Energy:** Combining orbitals must have the same or nearly the same energy.
2. **Symmetry:** Orbitals must have the same symmetry about the molecular axis (z-axis).
3. **Overlap:** Must overlap to the maximum extent to ensure high electron density.



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