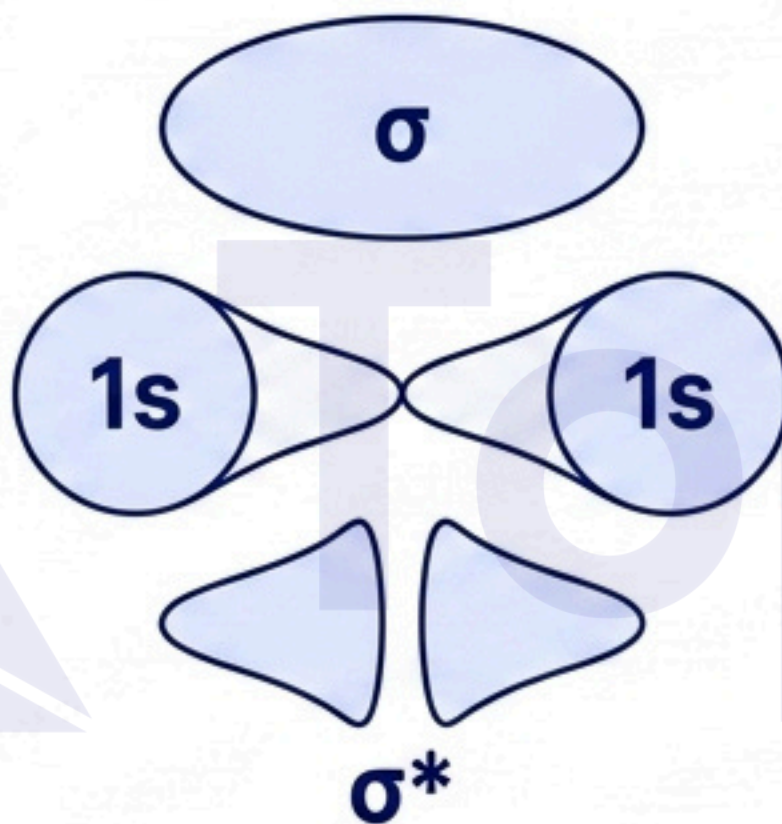


MO Theory Applied to Homonuclear Diatomics

Predicting molecular stability and magnetic behavior through the progressive filling of molecular orbitals.



LCAO Principle

Atomic orbitals combine to form MOs.

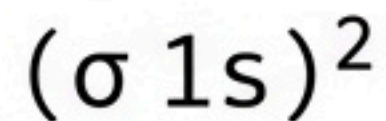
Aufbau & Pauli

Filled lowest energy first, max 2 e⁻ per MO.

Hund's Rule

Degenerate orbitals fill singly first.

Hydrogen (H₂)



Total Electrons: 2

Bond Order:

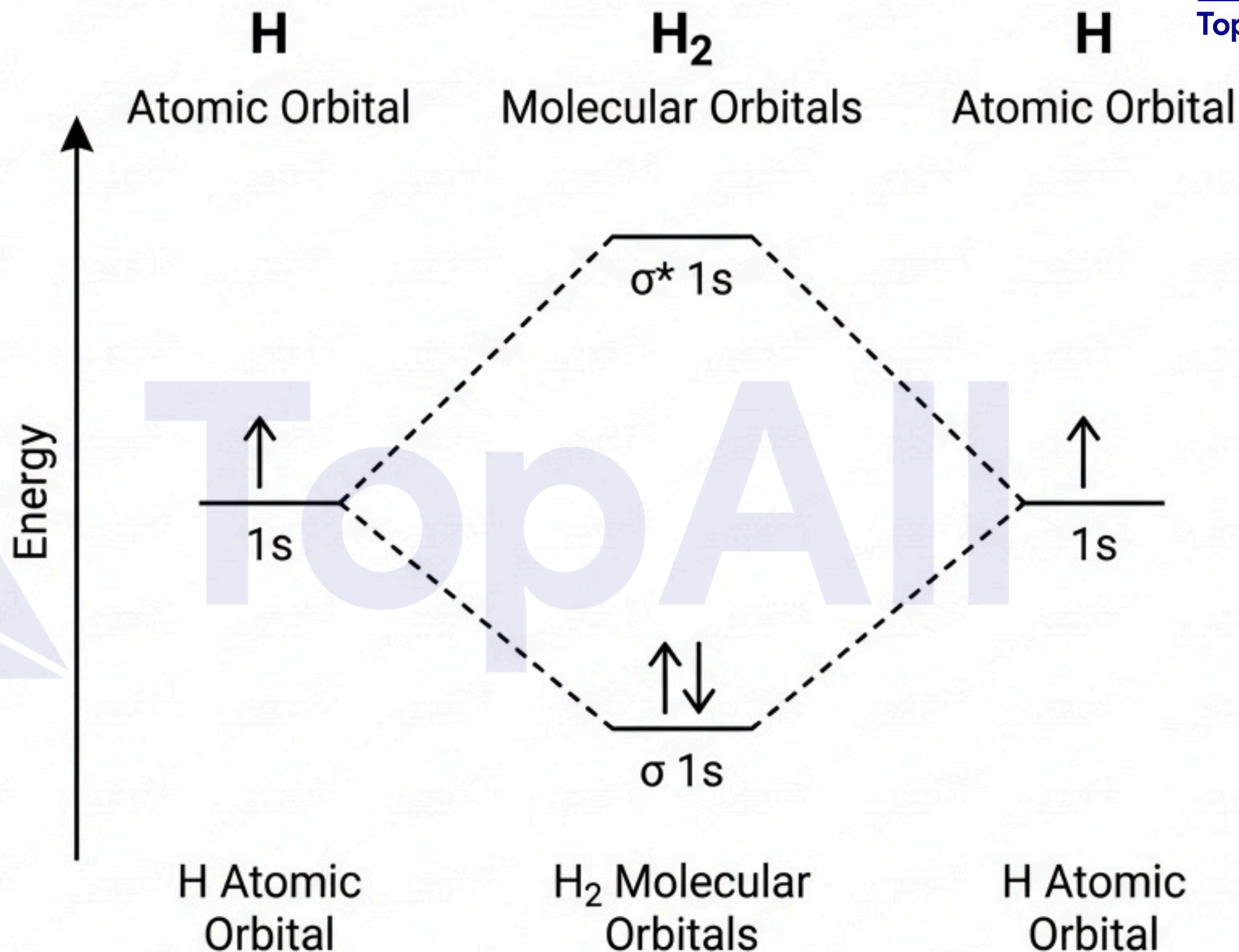
$$BO = \frac{1}{2}(2 - 0) = 1$$

(Single Covalent Bond)

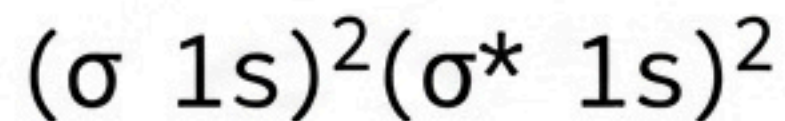
Magnetic Nature: Diamagnetic
(0 unpaired electrons)

Properties:

Bond length 74 pm,
Dissociation energy 438 kJ mol⁻¹



Helium (He₂)



Total Electrons: 4

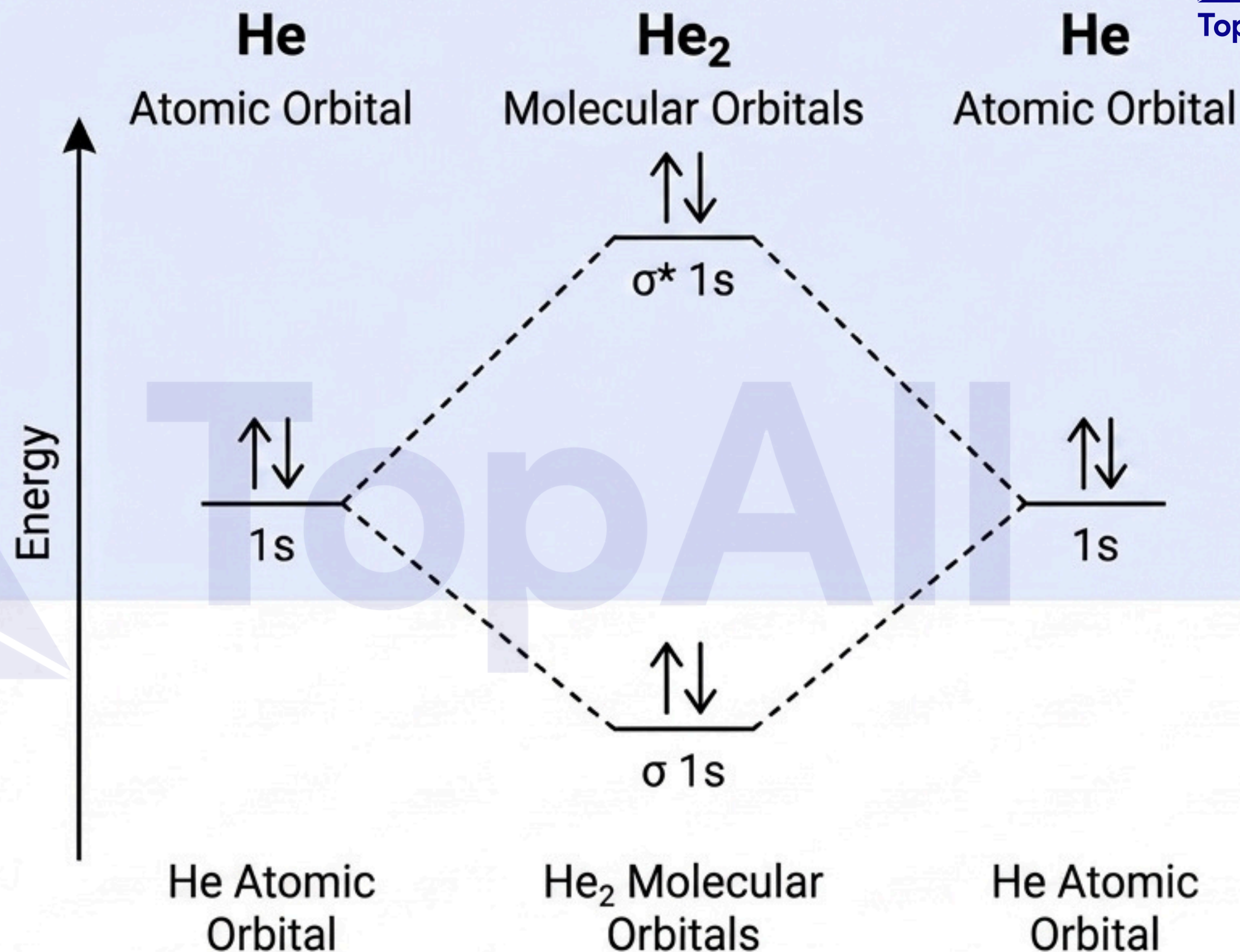
Bond Order: $BO = 1/2(2 - 2) = 0$

Magnetic Nature: N/A

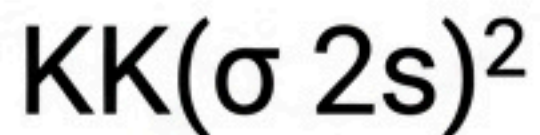
Existence: Unstable / Does not exist.

Insight Callout:

Rule of Stability: When the number of antibonding electrons equals or exceeds bonding electrons ($N_a \geq N_b$), the molecule cannot form.

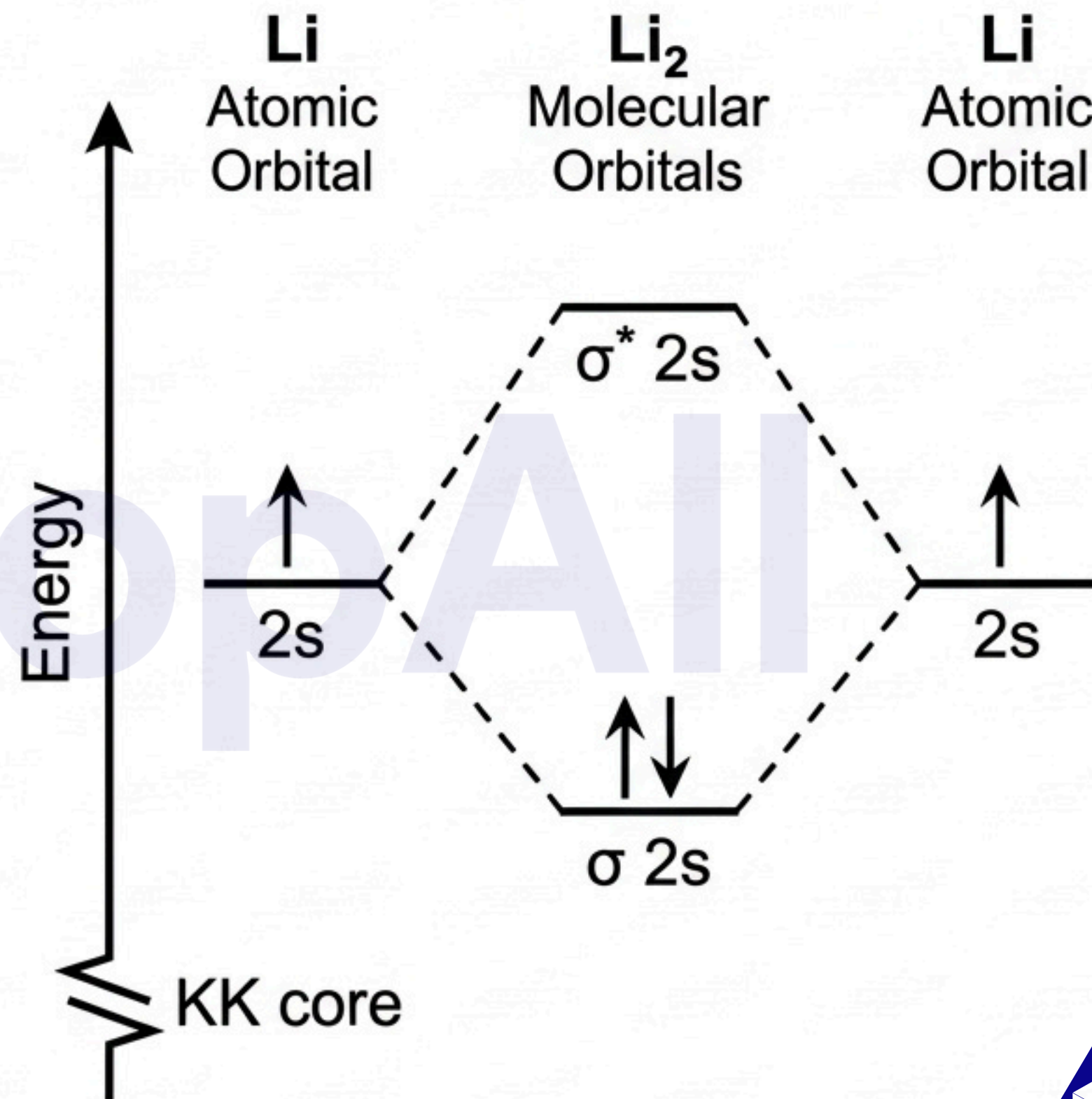


Lithium (Li_2)



1. Total Electrons: 6 (2 valence)
2. Bond Order: $\text{BO} = 1/2(4 - 2) = 1$
3. Magnetic Nature: Diamagnetic
(All electrons paired)
4. Existence: Stable
(Known to exist in the vapor phase)

Molecular Orbital Energy Diagram for Li_2





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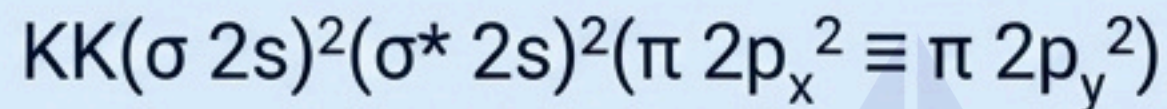
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Molecular Orbital Theory: Carbon (C₂)

Carbon (C₂)



Total Electrons: 12

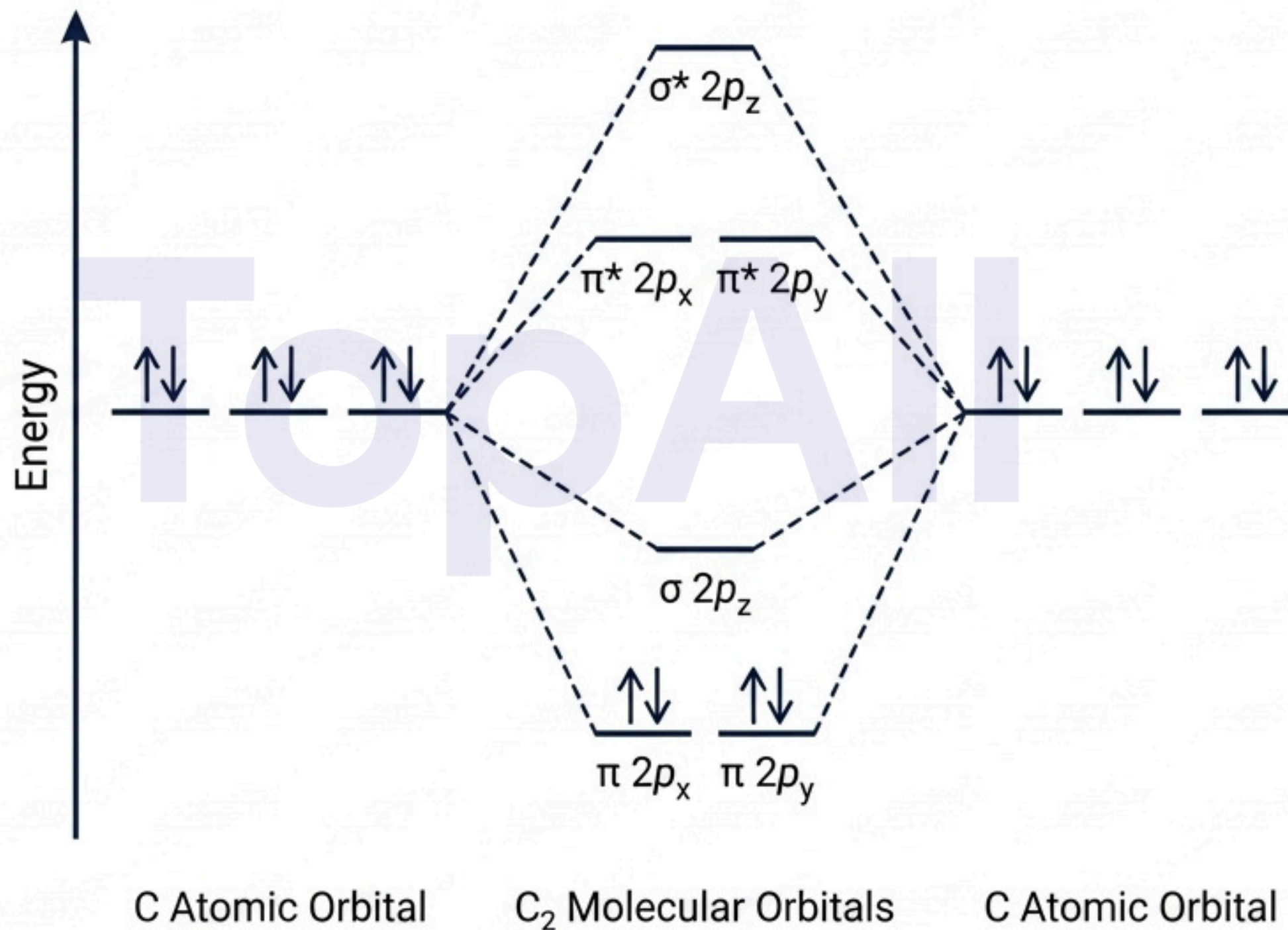
Bond Order: $BO = 1/2(8 - 4) = 2$

Magnetic Nature: Diamagnetic

Structural Anomaly:

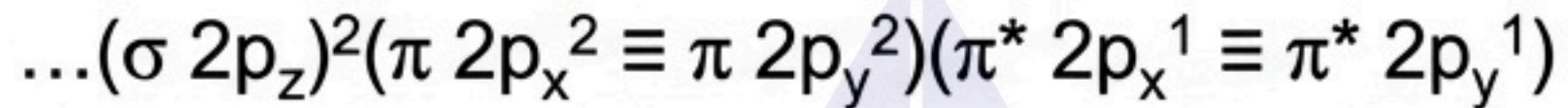
Unlike most double bonds (which feature one σ and one π bond), the C₂ double bond consists of two π bonds. The highest occupied MOs are purely π .

Molecular Orbital Energy Diagram for C₂



Molecular Orbital Theory: Oxygen (O₂)

Oxygen (O₂)



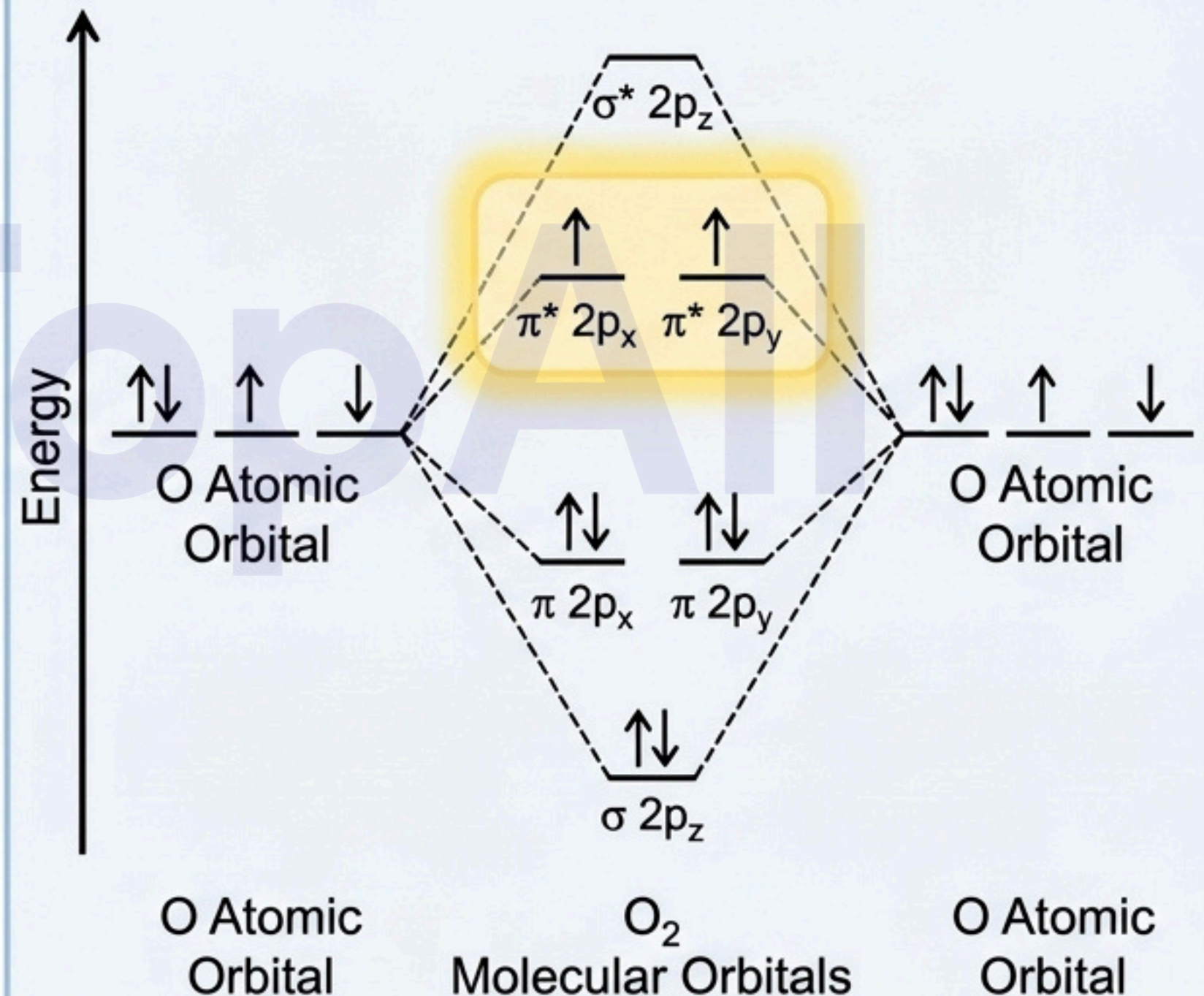
Total Electrons: 16

Bond Order: $BO = \frac{1}{2}(10 - 6) = 2$ (Double Bond)

Magnetic Nature:
Paramagnetic (2 unpaired electrons)

The Triumph of MO Theory: Simple Lewis structures cannot explain oxygen's paramagnetism. MO theory perfectly predicts the two unpaired electrons in the π^* antibonding orbitals.

Molecular Orbital Energy Diagram for O₂



Species Comparison Matrix: Homonuclear Diatomics

Molecule	Total e ⁻	Bond Order (BO)	Magnetic Nature	Existence Status
H ₂	2	1	Diamagnetic (↑↓)	Stable
He ₂	4	0	N/A	Does Not Exist
Li ₂	6	1	Diamagnetic (↑↓)	Exists (Vapor)
C ₂	12	2	Diamagnetic (↑↓)	Exists (Vapor)
O ₂	16	2	Paramagnetic (↑ ↑)	Stable

MO Theory Quick Revision

The Bond Order Formula

$$BO = 1/2(N_b - N_a)$$

N_b = Bonding electrons (lower energy, stable)

N_a = Antibonding electrons (higher energy, unstable, marked with *)

Stability Rules

$N_b > N_a$ ($BO > 0$) → Molecule is Stable

$N_b \leq N_a$ ($BO \leq 0$) → Molecule is Unstable (does not exist)

Higher BO = Shorter bond length, higher bond enthalpy.

Magnetic Nature

All electrons paired → Diamagnetic (Repelled by magnets)

≥ 1 unpaired electron → Paramagnetic (Attracted by magnets)

The 2p Energy Shift

For elements up to N (e.g., B_2 , C_2 , N_2): $\pi 2p_{x,y}$ are LOWER in energy than $\sigma 2p_z$.

For elements past N (e.g., O_2 , F_2): $\sigma 2p_z$ is LOWER in energy than $\pi 2p_{x,y}$.



You've Learned the Theory.

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