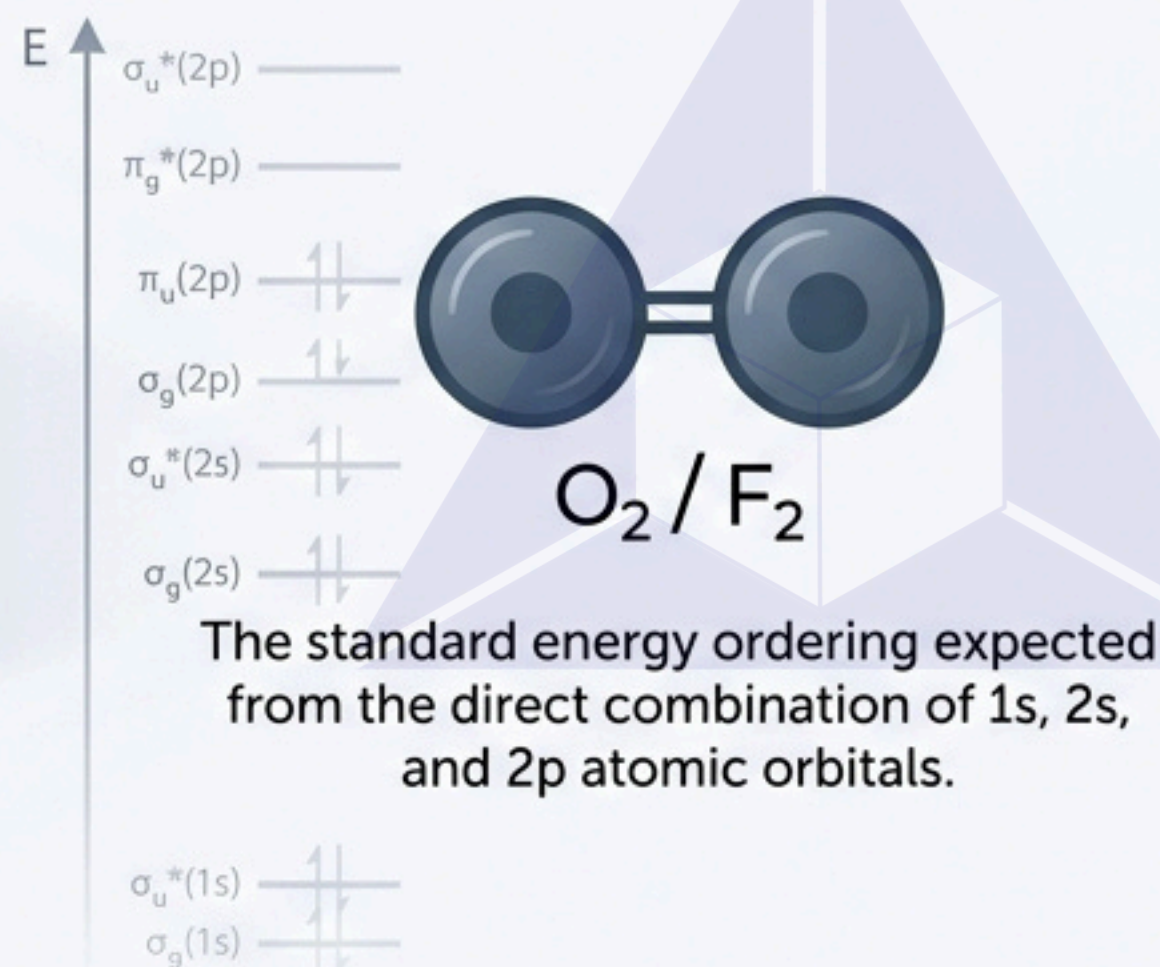


The Two Paradigms of Molecular Orbitals

Spectroscopic data reveals that homonuclear diatomic molecules of the second row do not all follow a single energy level sequence. They are governed by two distinct molecular orbital (MO) blueprints.

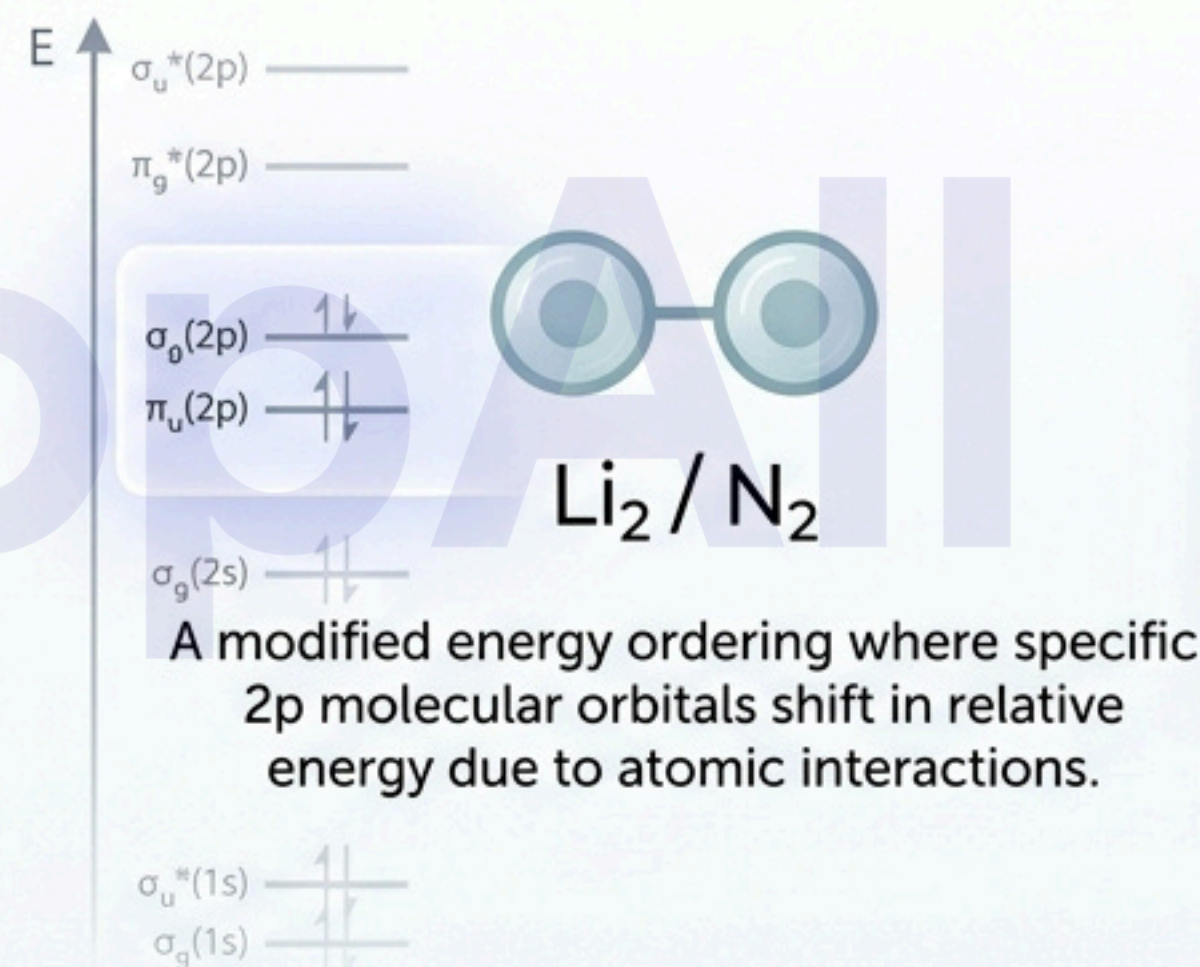
The O₂ / F₂ Sequence



The standard energy ordering expected from the direct combination of 1s, 2s, and 2p atomic orbitals.

Applies to Oxygen (O₂) and Fluorine (F₂)

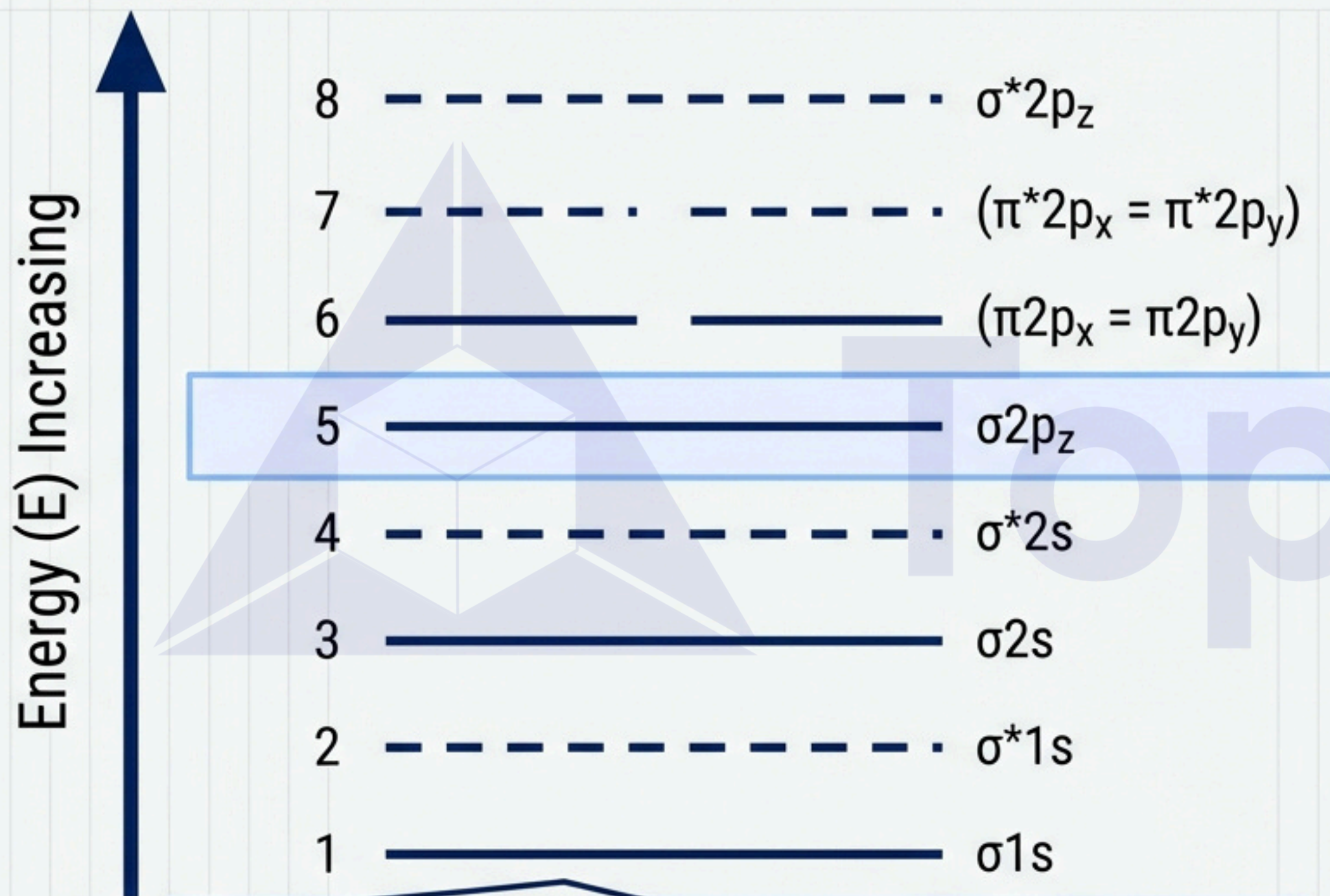
The Li₂ to N₂ Sequence



A modified energy ordering where specific 2p molecular orbitals shift in relative energy due to atomic interactions.

Applies to Lithium (Li₂) through Nitrogen (N₂)

The Standard Ordering: O₂ & F₂

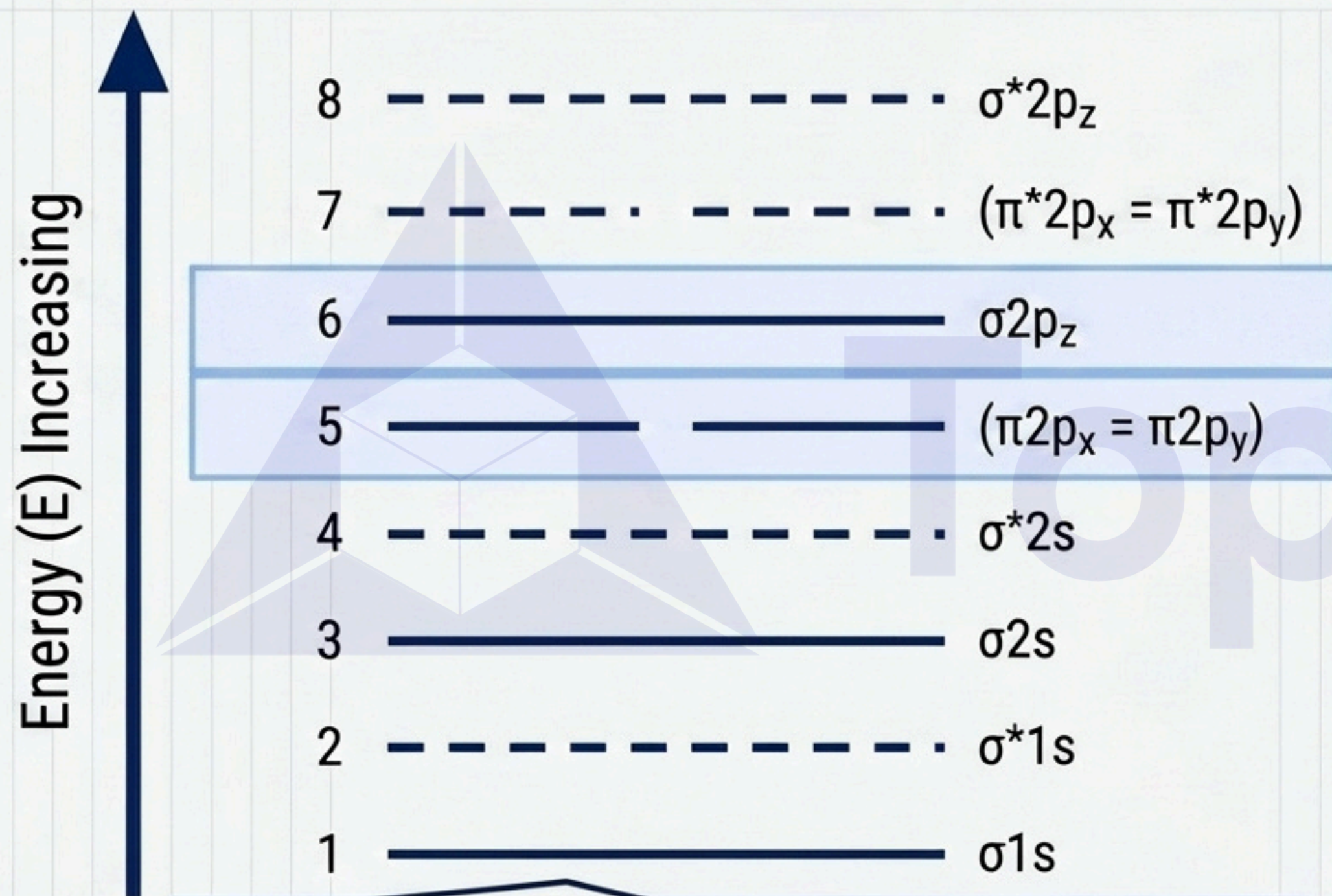


For Oxygen and Fluorine, molecular orbitals fill sequentially based on the energy of their parent atomic orbitals.

The $\sigma2p_z$ orbital sits lower in energy than the $\pi2p$ orbitals.

Full Sequence: $\sigma1s < \sigma^*1s < \sigma2s < \sigma^*2s < \sigma2p_z < (\pi2p_x = \pi2p_y) < (\pi^*2p_x = \pi^*2p_y) < \sigma^*2p_z$

The Modified Ordering: Li_2 to N_2



For molecules from Lithium (Li_2) through Nitrogen (N_2), experimental data dictates a structural shift in the 2p orbital region.

Full Sequence: $\sigma1s < \sigma^*1s < \sigma2s < \sigma^*2s < \sigma^*2s < (\pi2p_x = \pi2p_y) < \sigma2p_z < (\pi^*2p_x = \pi^*2p_y) < \sigma^*2p_z$



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The Point of Divergence

The defining characteristic distinguishing the two blueprints is the relative energy of the $2p_z$ molecular orbital compared to the $2p_x$ and $2p_y$ orbitals.

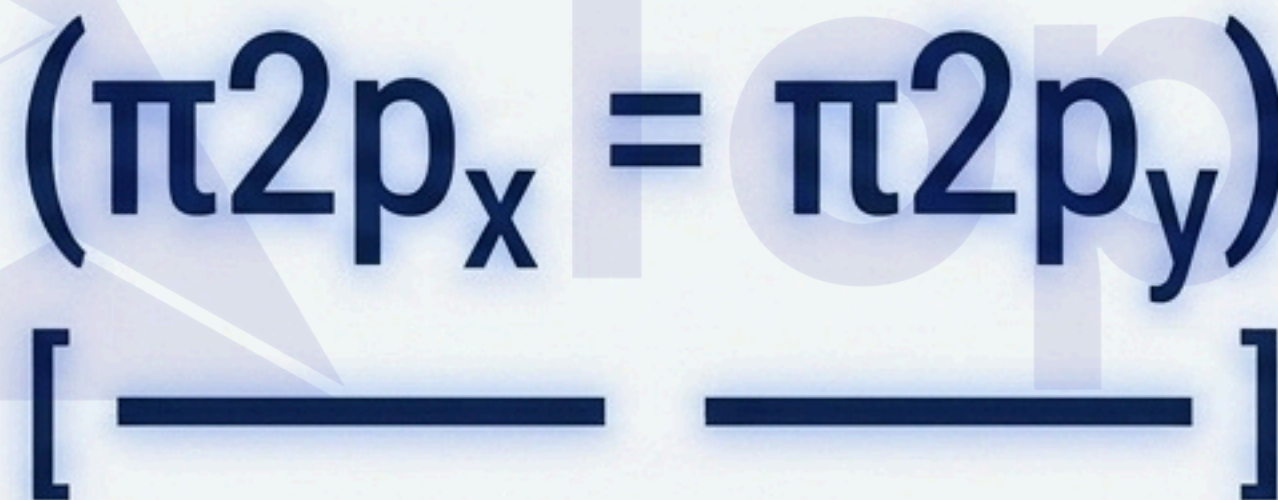


Understanding Degenerate π Orbitals

In both orderings, the notation includes an equals sign: ($\pi 2p_x = \pi 2p_y$). This is not a placeholder—it defines a critical physical property of the molecule.

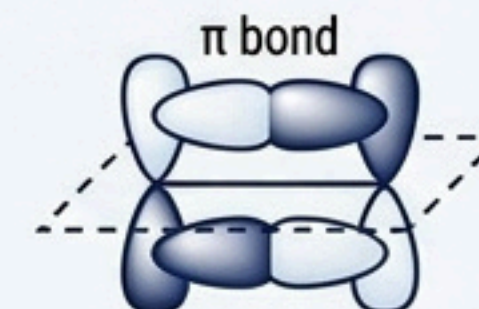
Equal Energy

These two pi molecular orbitals are “degenerate,” meaning they possess the exact same energy level on the diagram.



Symmetry & Shape

Formed from $2p_x$ and $2p_y$ atomic orbitals, they are not symmetrical around the bond axis (unlike sigma bonds). They feature saucer-type positive and negative lobes above and below the inter-nuclear plane (a node is present).

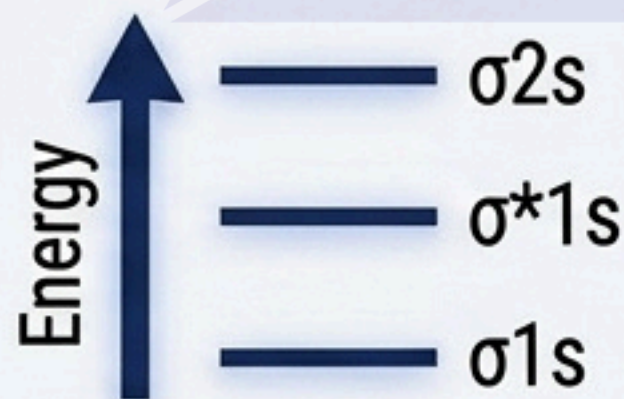


Rules of Engagement: Filling the Orbitals

Once the correct molecular orbital blueprint is selected, electrons must be distributed according to three fundamental principles, just like atomic orbitals.

1. Aufbau Principle

Molecular orbitals must be filled in order of increasing energy levels. Always start at the bottom ($\sigma 1s$) and work your way up the ladder.



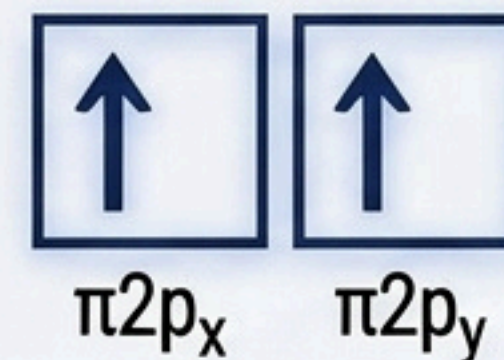
2. Pauli Exclusion Principle

A single molecular orbital can hold a maximum of two electrons, and they must have opposite spins (represented as $\uparrow\downarrow$).



3. Hund's Rule

For degenerate orbitals (like $\pi 2p_x = \pi 2p_y$), each orbital must receive one electron (singly occupied) before any pairing occurs.



Stability Check: A molecule is stable if Bonding Electrons (N_b) > Antibonding Electrons (N_a).

Revision Frame: MO Energy Levels

O ₂ , F ₂ (Standard)	Li ₂ to N ₂ (Modified)	Filling Rules & Notation
σ^*2p_z	σ^*2p_z	The Rules Aufbau: Lowest energy first. Pauli: Max 2 e⁻ per MO, opposite spins. Hund: Fill degenerate orbitals singly first. Nomenclature σ = Symmetrical around bond axis. π = Not symmetrical (node present). $*$ = Antibonding (higher energy, destabilizing).
$(\pi^*2p_x = \pi^*2p_y)$	$(\pi^*2p_x = \pi^*2p_y)$	
$(\pi2p_x = \pi2p_y)$	$\sigma2p_z$ (Higher)	
$\sigma2p_z$ (Lower)	$(\pi2p_x = \pi2p_y)$	
σ^*2s	σ^*2s	
$\sigma2s$	$\sigma2s$	
σ^*1s	σ^*1s	
$\sigma1s$	$\sigma1s$	



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