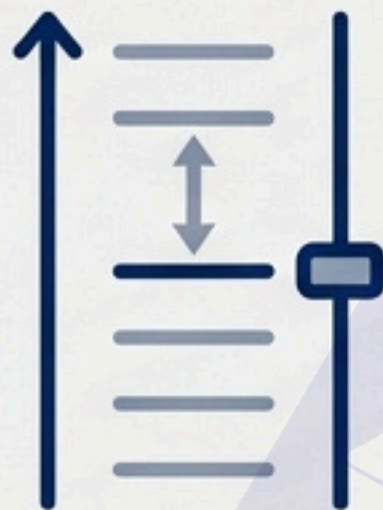


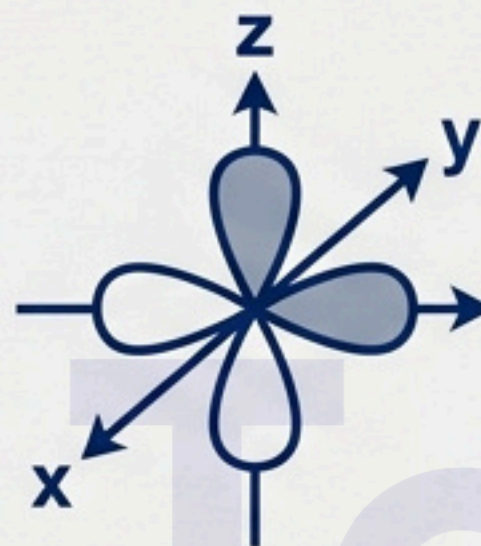
The Three Gates of LCAO

For atomic orbitals to combine and form molecular orbitals, they must satisfy three strict conditions.



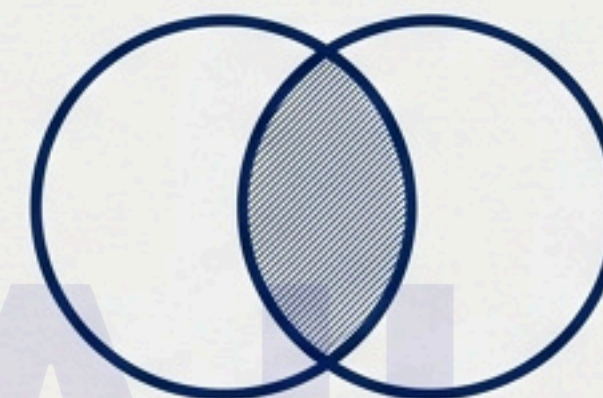
1. Energy Match

Combining atomic orbitals must possess the same, or nearly the same, energy levels.



2. Axial Symmetry

Orbitals must share the exact same spatial symmetry around the inter-nuclear axis.



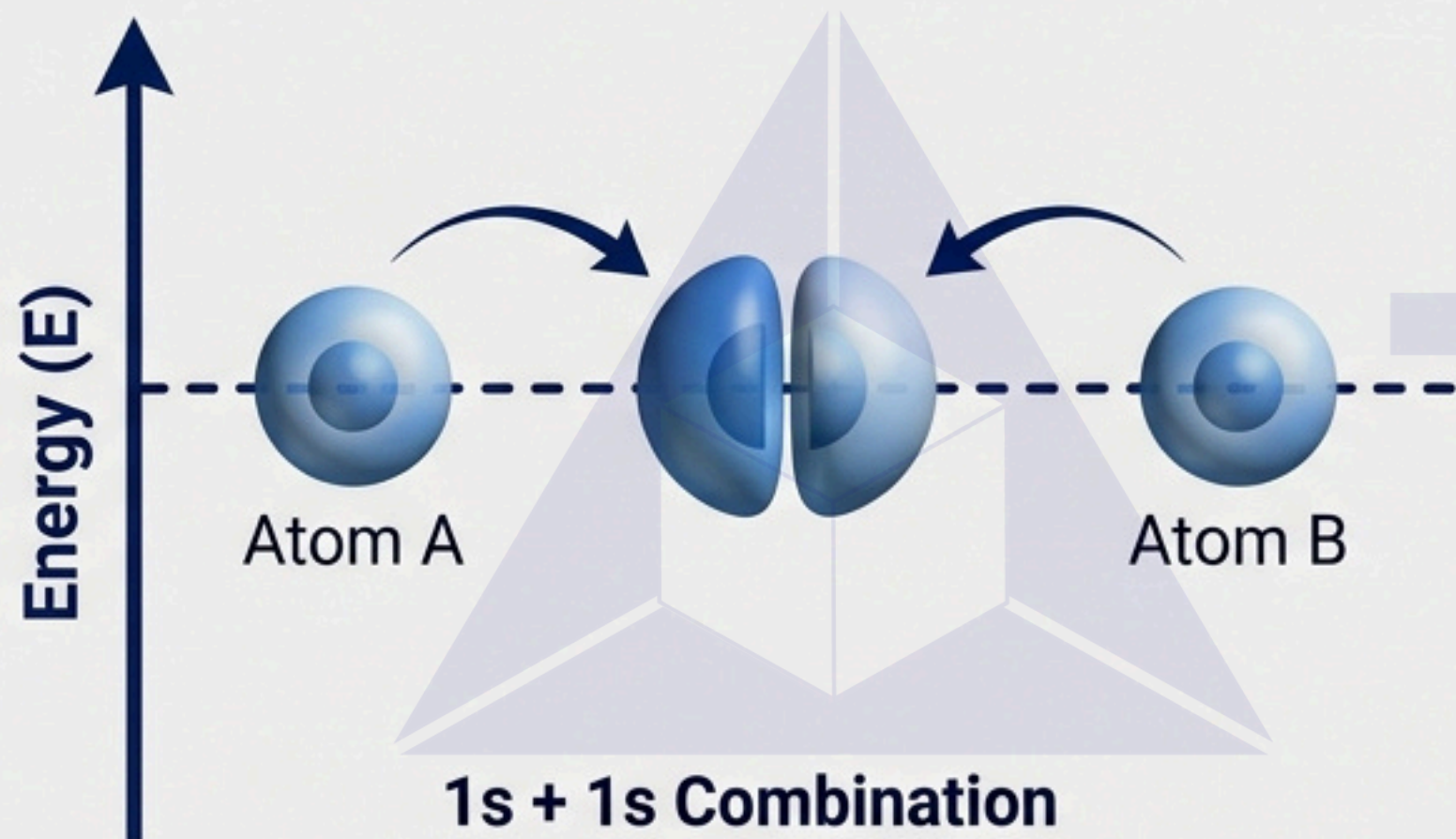
3. Maximum Overlap

Orbitals must physically overlap to the maximum extent to ensure high electron density.

The LCAO Principle: Molecular orbitals are mathematically formed by the **constructive addition (σ)** or **destructive subtraction (σ^*)** of individual atomic wave functions—but only if all three security gates are passed.

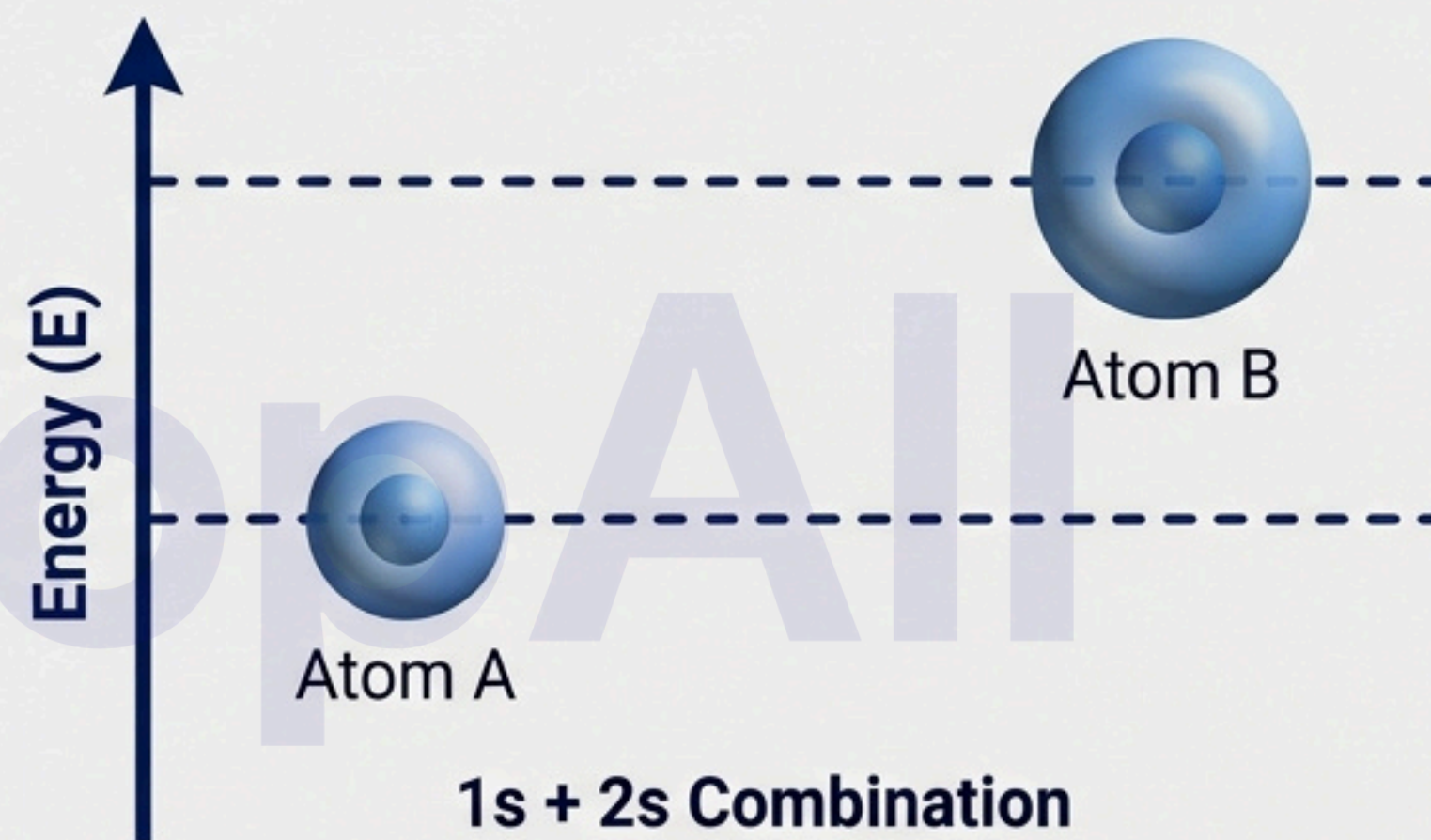
Gate 1: The Energy Condition

Orbitals must exist on comparable energy planes to interact.



✓ **VALID**

The 1s orbital of Atom A has the exact same energy as the 1s orbital of Atom B. Their wave functions successfully combine.



✗ **INVALID**

The energy of the 2s orbital is appreciably higher than that of the 1s orbital. This energy gap prevents linear combination.



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Key Highlights

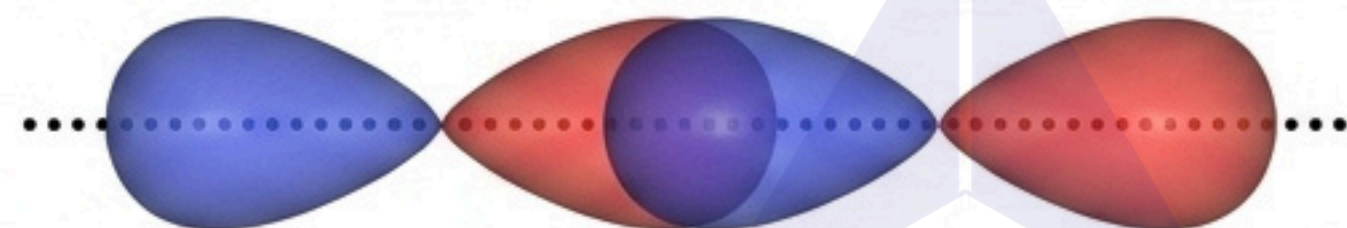
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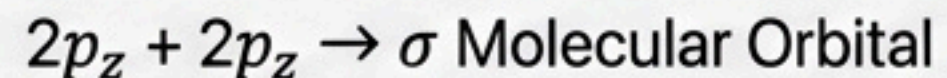
Gate 2: The Symmetry Condition

By convention, the z-axis is the molecular axis. Orbitals must align symmetrically along it.

Symmetrical Match



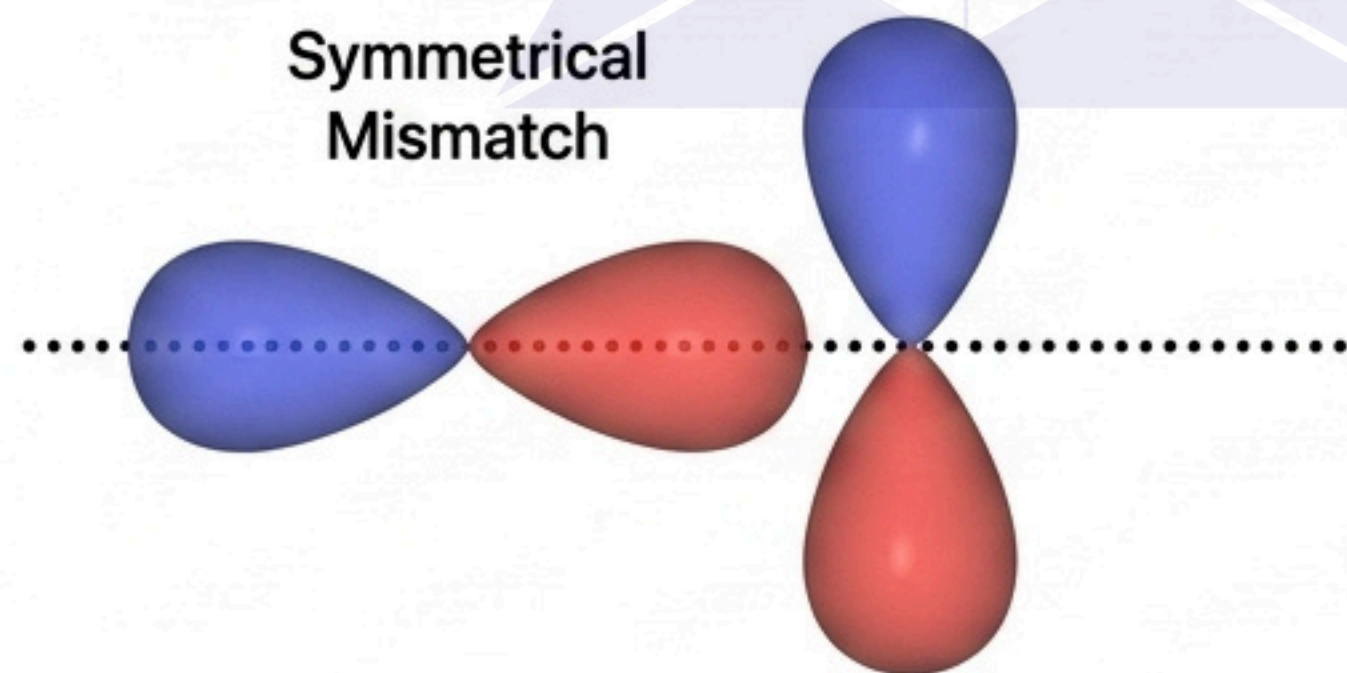
z-axis (molecular axis)



✓ CONSTRUCTIVE OVERLAP

Both orbitals share the same symmetry around the z-axis, allowing their electron waves to reinforce each other constructively.

Symmetrical Mismatch

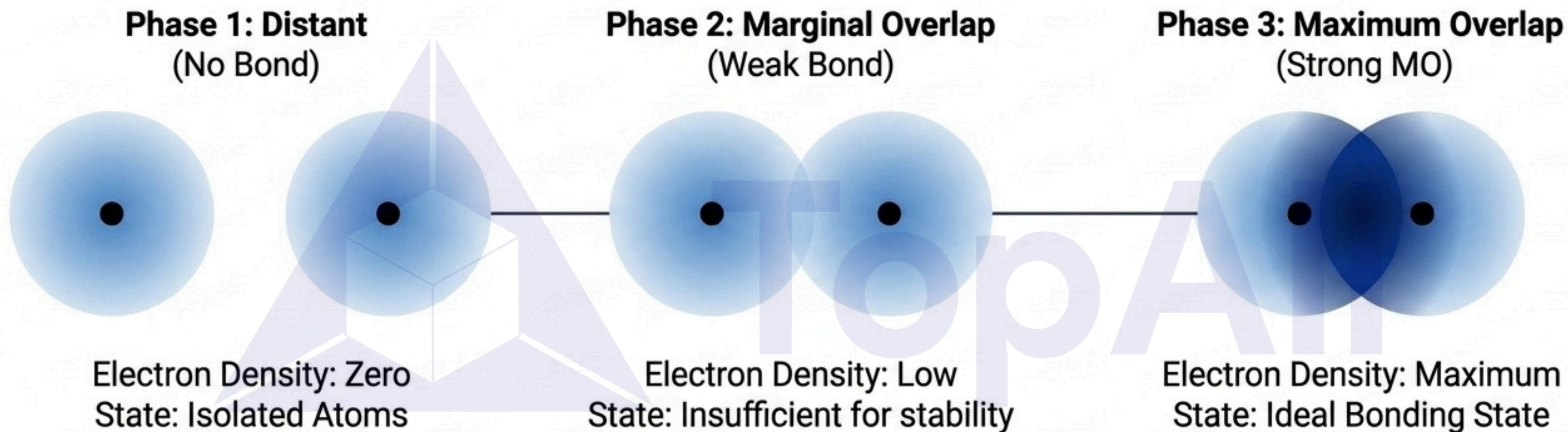


✗ ZERO OVERLAP

A p_z orbital cannot combine with p_x or p_y orbitals. Differing spatial symmetries result in a net-zero overlap, meaning no bond is formed.

Gate 3: The Overlap Condition

Greater physical interpenetration yields higher electron density and stronger chemical bonds.



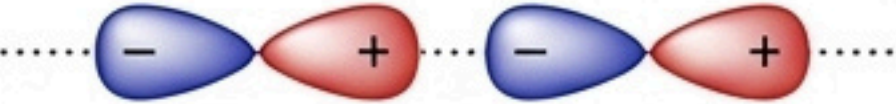
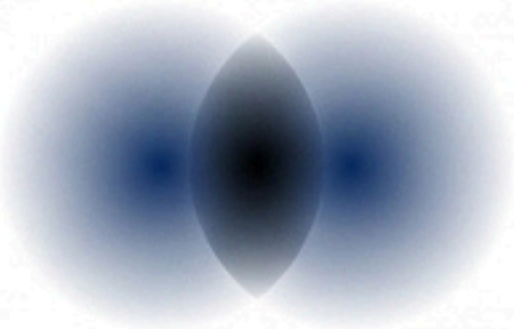
The high electron density between the nuclei perfectly shields and overcomes nuclear repulsion.

The LCAO method relies on finding the optimal internuclear distance where this overlap peaks.

Revision Frame: Conditions for AO Combination



The Linear Combination of Atomic Orbitals (LCAO) Checklist.

ENERGY	SYMMETRY	OVERLAP
Rule: Same or Nearly Same Energy The “Why”: Wave functions cannot effectively mix if their initial energy states are vastly different. Pass/Fail: 1s + 1s (Pass) 1s + 2s (Fail) 	Rule: Same Symmetry on Molecular Axis The “Why”: Electron wave amplitudes must geometrically align to constructively interfere and avoid zero-overlap nodes. Pass/Fail: 2p_z + 2p_z (Pass) 2p_z + 2p_x (Fail) 	Rule: Maximum Physical Overlap The “Why”: High electron density between the nuclei is required to overcome nuclear repulsion and stabilize the structure. Metric: Greater Overlap = Stronger Covalent Bond. 

Note: Satisfying all three conditions allows atomic orbitals to successfully split into both lower-energy Bonding MOs (σ , π) and higher-energy Antibonding MOs (σ^* , π^*).



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