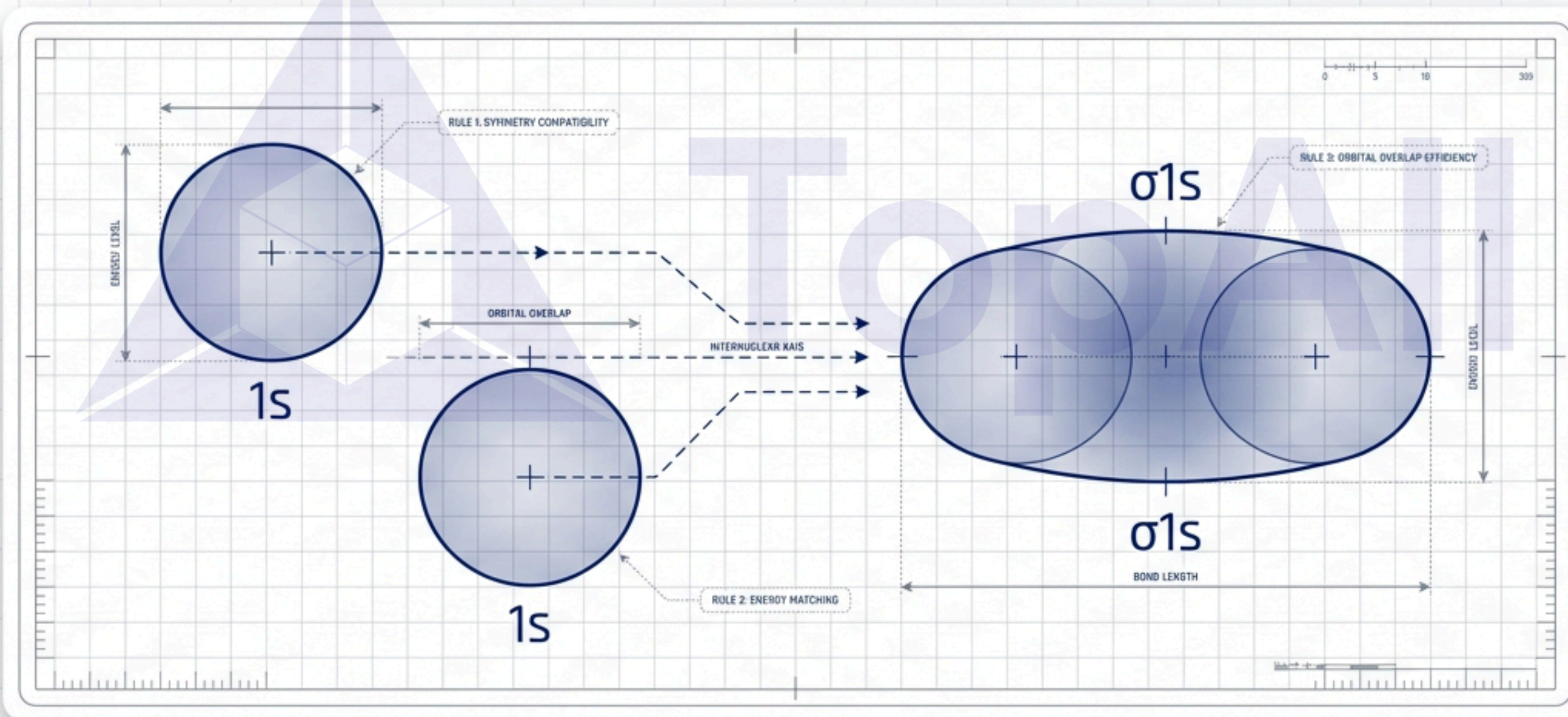


4.7.2 Conditions for the Combination of Atomic Orbitals

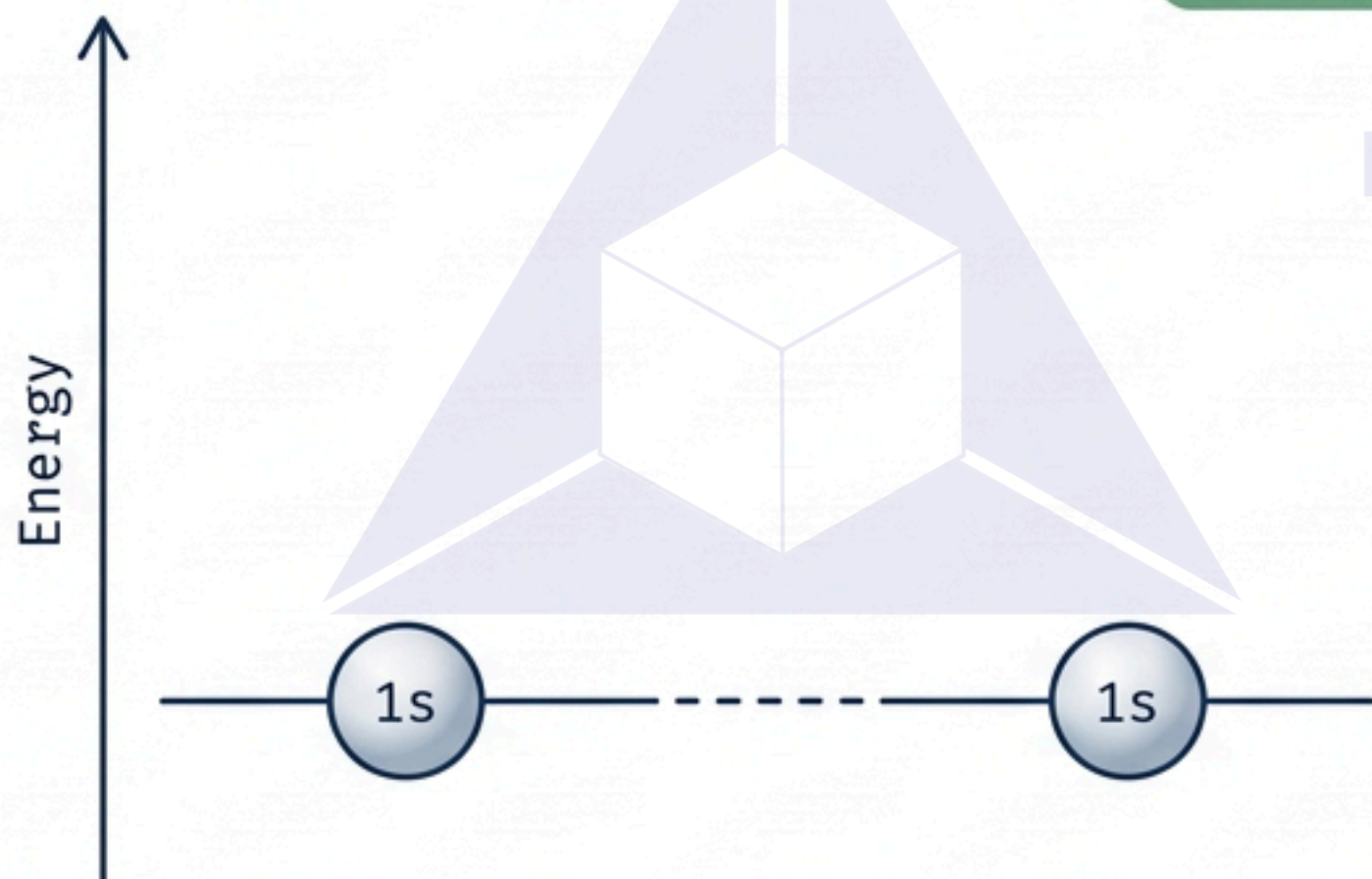
The three mandatory rules an atomic orbital pair must pass to form a stable molecular orbital.



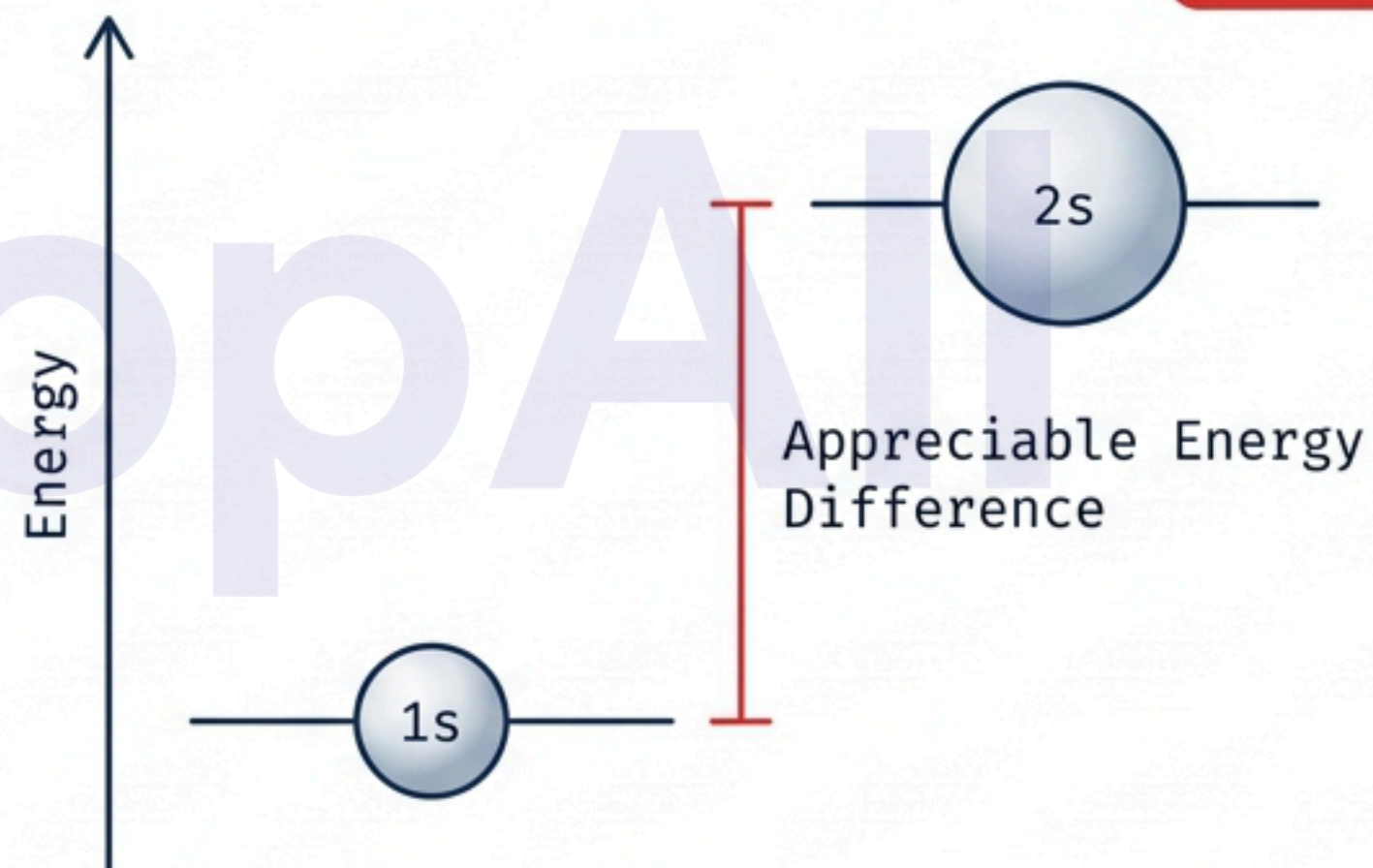
Comparable Energies

The combining atomic orbitals must have the same or nearly the same energy.

✓ PASS



✗ FAIL



1s can combine with 1s, but not with 2s.



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$$E=mc^2$$



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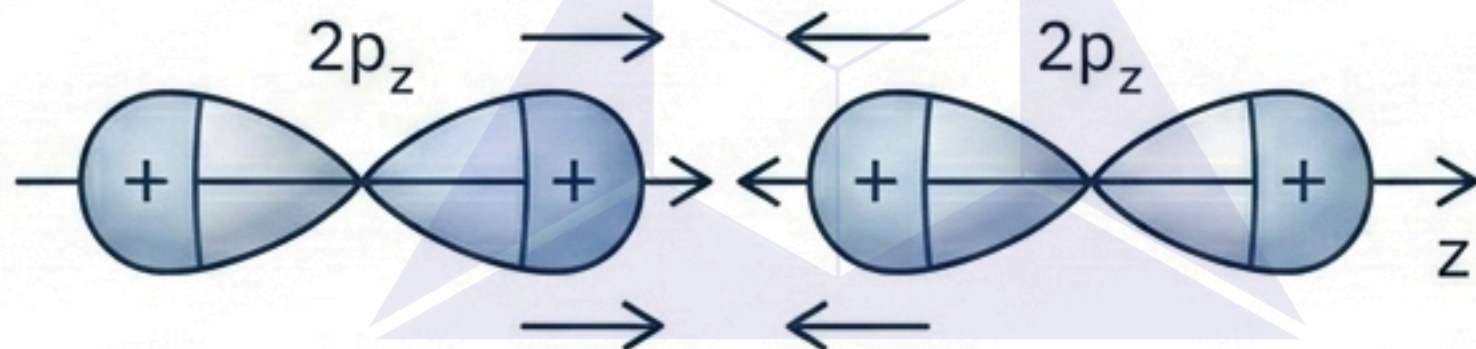


Proper Symmetry

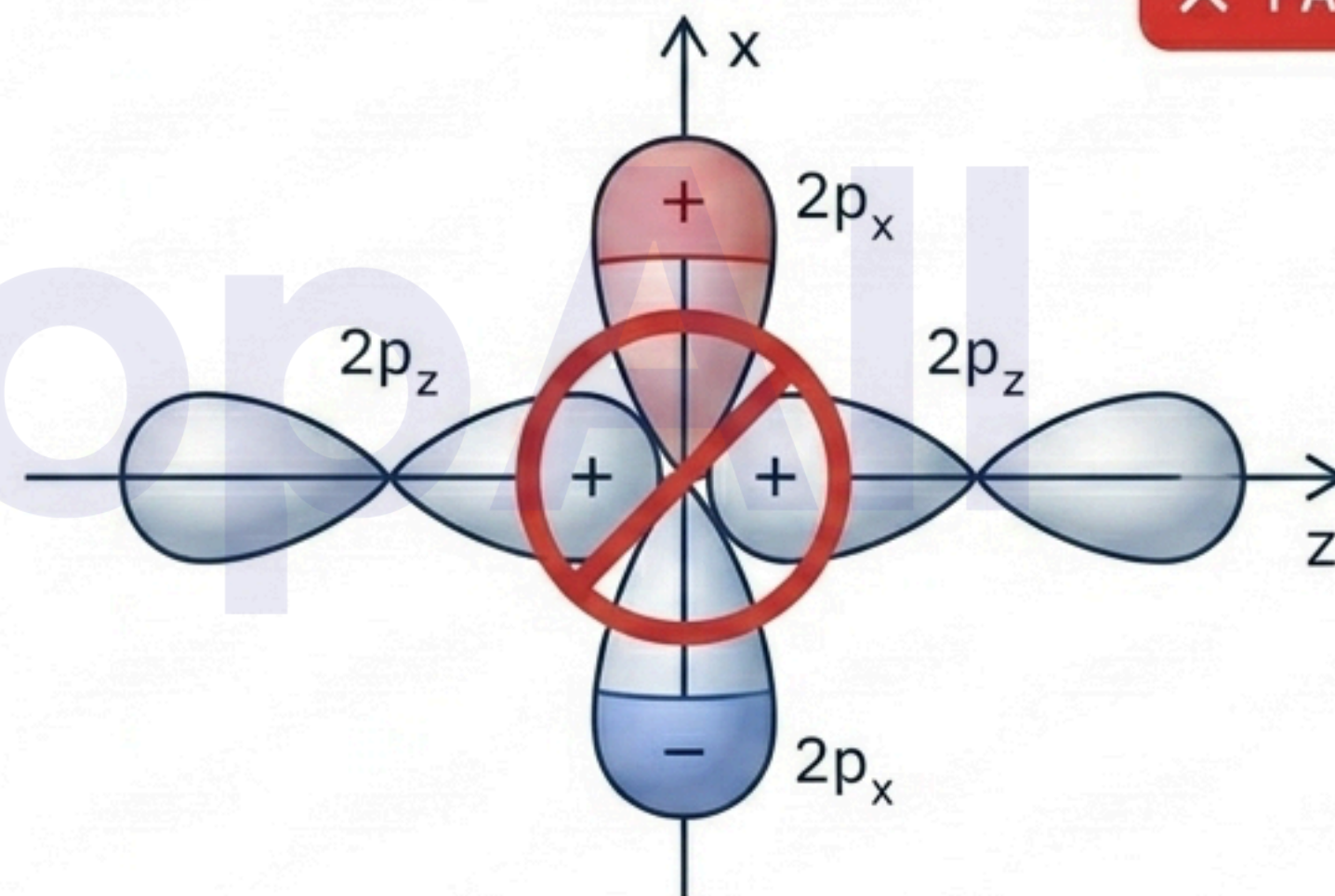
The combining atomic orbitals must have the same symmetry about the molecular axis.

Z-axis = Internuclear Axis

✓ PASS



✗ FAIL

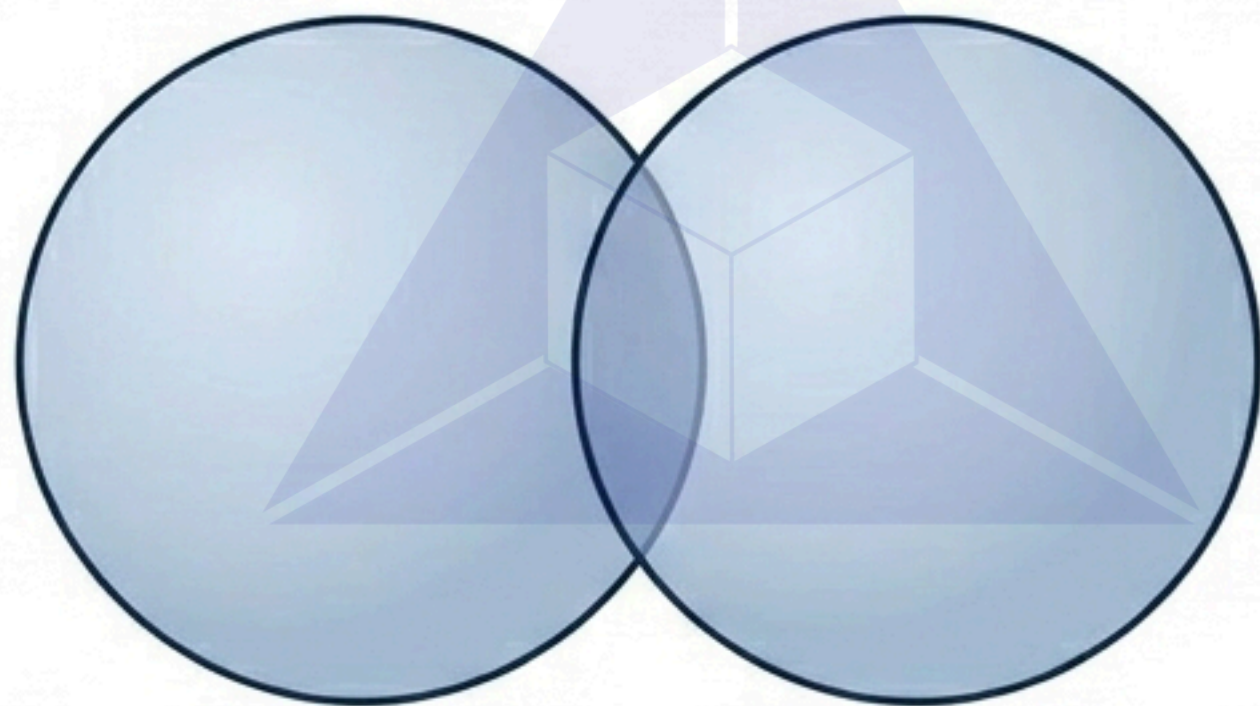


$2p_z$ combines with $2p_z$, but fails with $2p_x$ or $2p_y$.

Maximum Overlap

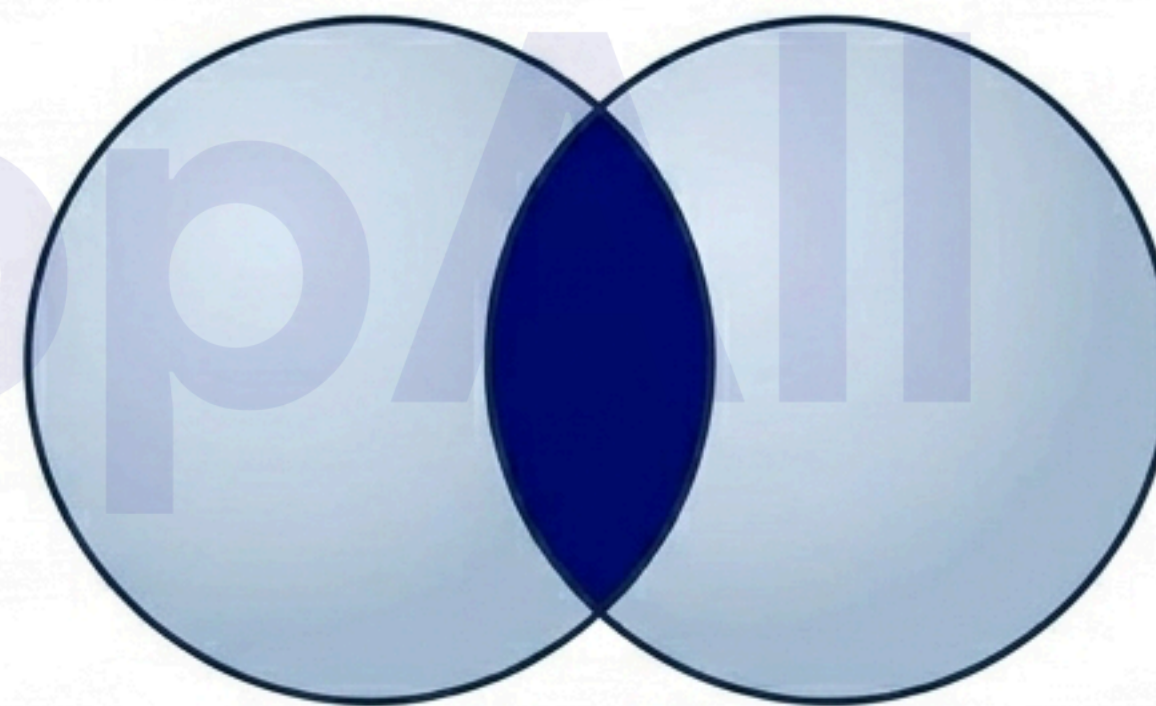
The combining atomic orbitals must overlap to the maximum extent. Greater overlap equals greater electron density between the nuclei.

✗ POOR OVERLAP



Low electron density = Weak/No bond.

✓ MAXIMUM OVERLAP



High electron density = Stable bond.

Extent of Overlap $\propto$ Bond Stability

Final Recap

ENERGY



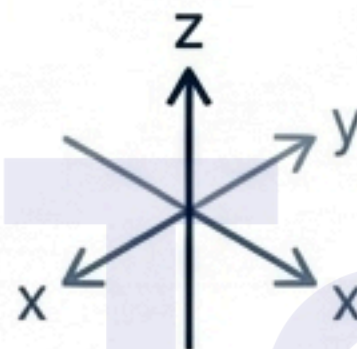
Must be comparable.

✓ $1s + 1s$

✗ $1s + 2s$



SYMMETRY



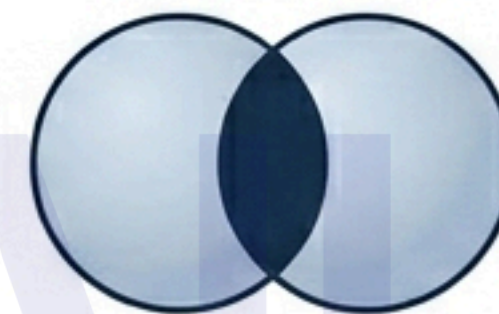
Must align on the molecular axis.

✓ $2p_z + 2p_z$

✗ $2p_z + 2p_x$



OVERLAP



Must be maximized for electron density.

✓ Deep intersection

✗ Shallow intersection



Only suitable AOs combine effectively



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