Guidelines on Orbital Interactions: G1 & G2

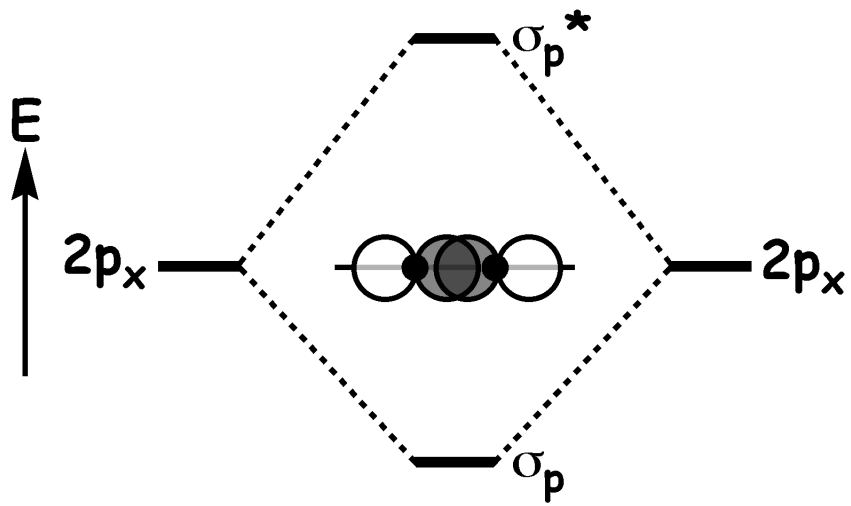
Four rules (guidelines G1 - G4) govern the interaction of two atomic orbitals (ψ_1 and ψ_2) to form two molecular orbitals (Ψ_1 and Ψ_2). These generalizations are useful for constructing "orbital interaction diagrams".

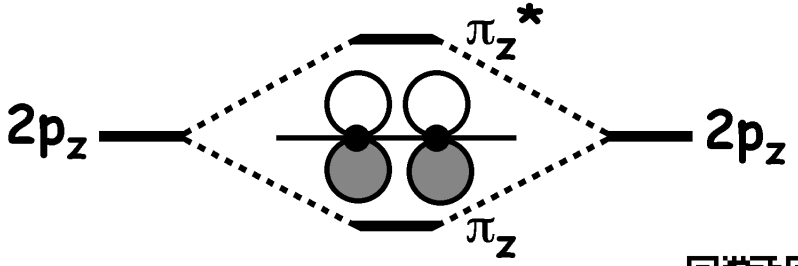
G1 - The overlap of two atomic orbitals depends on:

- symmetry of the orbitals
- distance between orbitals
- spatial extent of the orbitals
- the energy difference between orbitals (E_1-E_2)

G2 -The stabilization of the bonding MO (Ψ_1) and destabilization of the antibonding MO (Ψ_2) increase as the overlap increases.

These orbital interaction diagrams apply G1 and G2 to explain why a pair of 2p orbitals that come together in the sigma mode (left) produce a stronger interaction than in the pi mode (right).





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G3 - As the energy difference between ψ_1 and ψ_2 increases (assume $E_1 < E_2$), the magnitude of the stabilization decreases, the contribution of ψ_1 to the bonding MO Ψ_1 increases, and the contribution of ψ_2 to the antibonding MO Ψ_2 increases.

G4 - The antibonding MO Ψ_2 is slightly more destabilized than the bonding MO Ψ_1 is stabilized.

These diagrams represent the interaction of two generic atomic orbitals, ψ_1 and ψ_2, that differ in energy. For the case on the left, the AOs have nearly equal energy and interact strongly. For the case on the right, the AO energies differ significantly and the interaction is weak. It can be seen that $\Delta E_{destab} > \Delta E_{stab}$ (i.e., G_4).