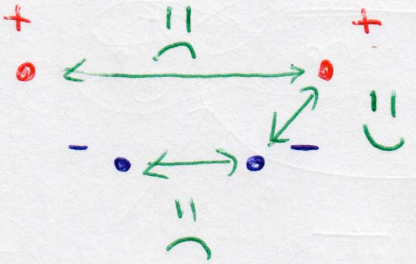
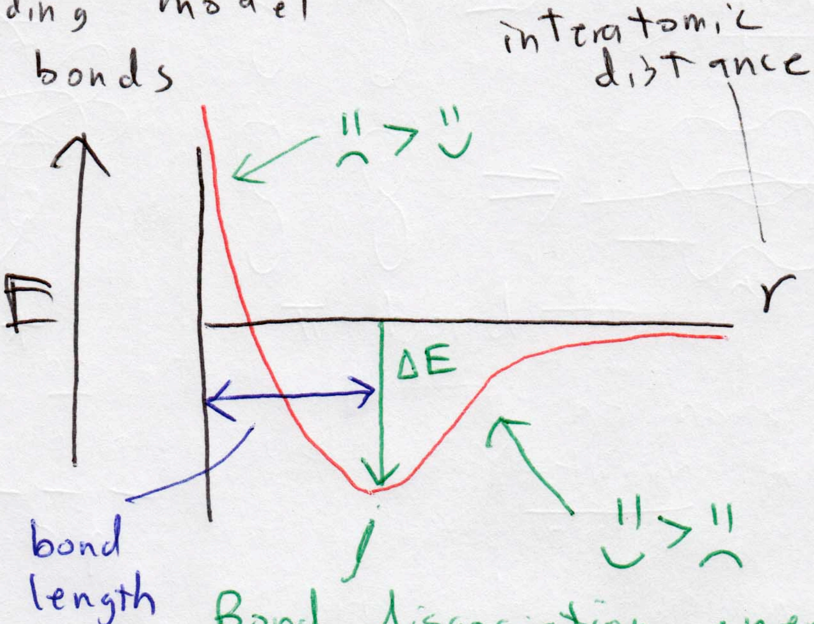
9/30/11 classical bonding model

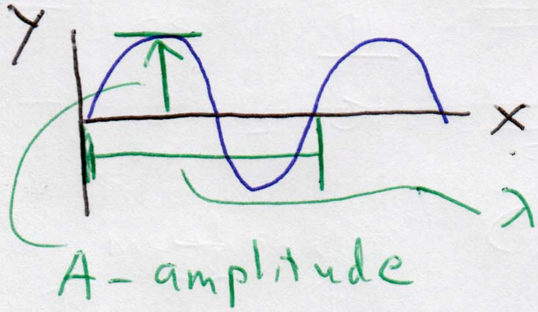
quantum bonding model

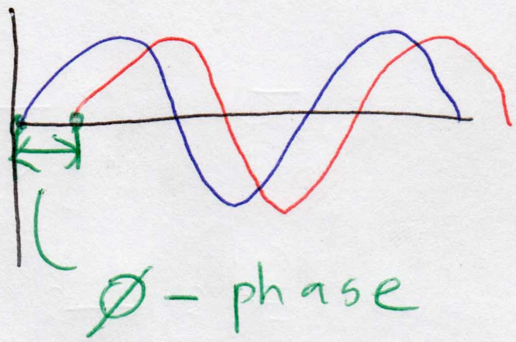
sigma + pi bonds

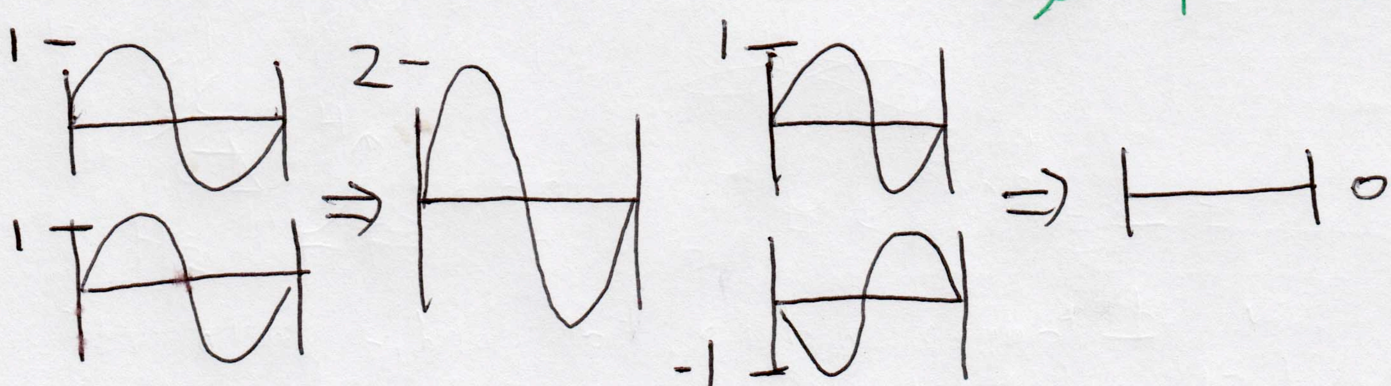




This classical model of bonding as able to describe H_2, but it fails to describe He_2 because it treats electrons as particles and does not take into account their wave behavior.





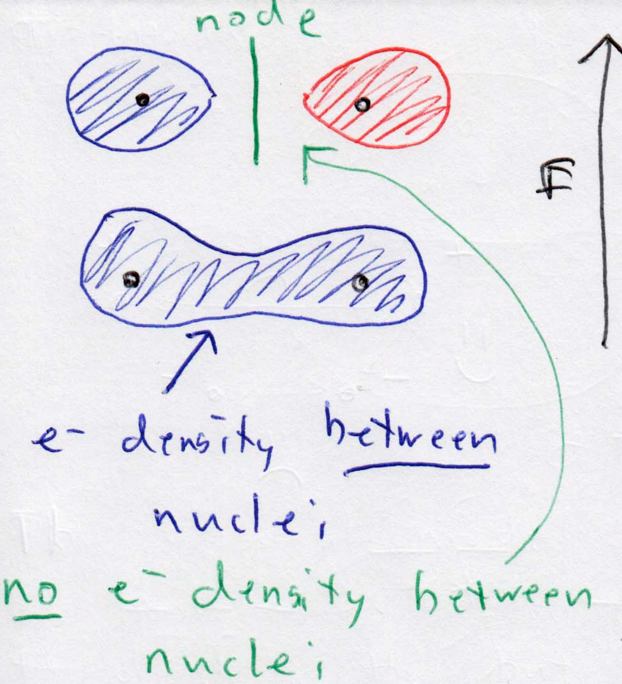


same A, λ, ∅

constructive interference

same A, λ
opposite ∅

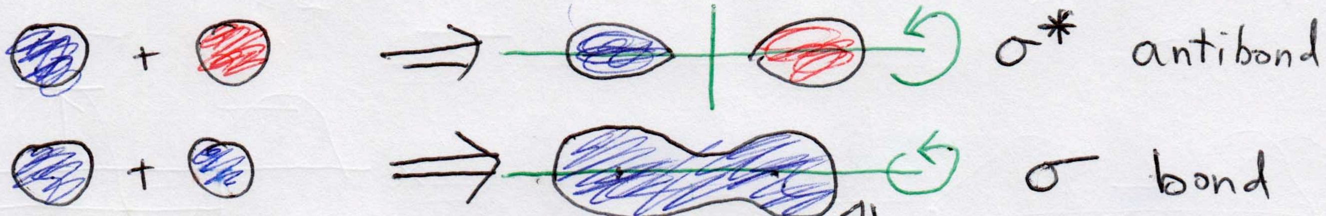
deconstructive interference

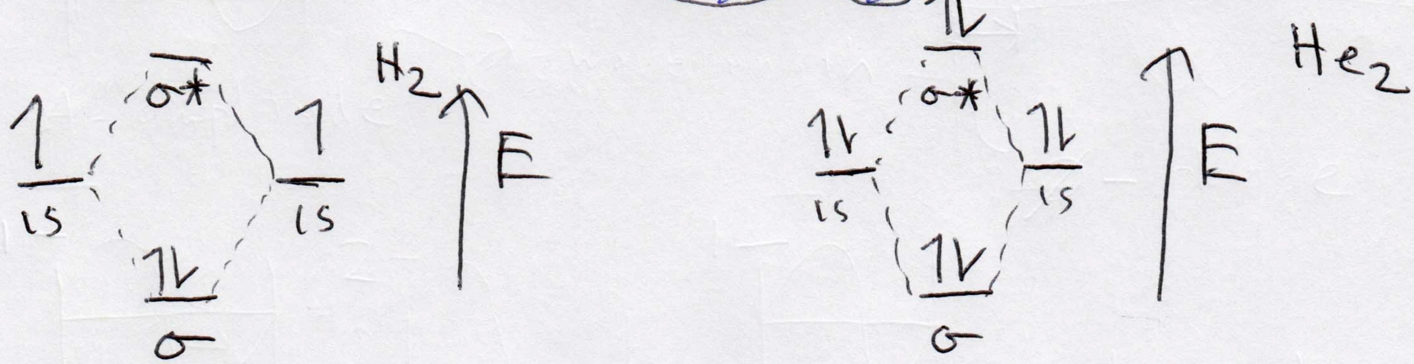


This orbital is an antibond because the energy is higher than if the atoms had not interacted.

This orbital is a bond because the energy is lower than if the atoms had not interacted.

LCAO - linear combination of atomic orbitals
atomic orbitals are added and subtracted to produce a new set of molecular orbitals (MO)

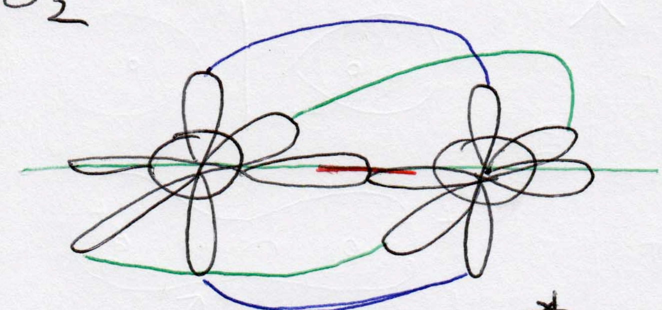


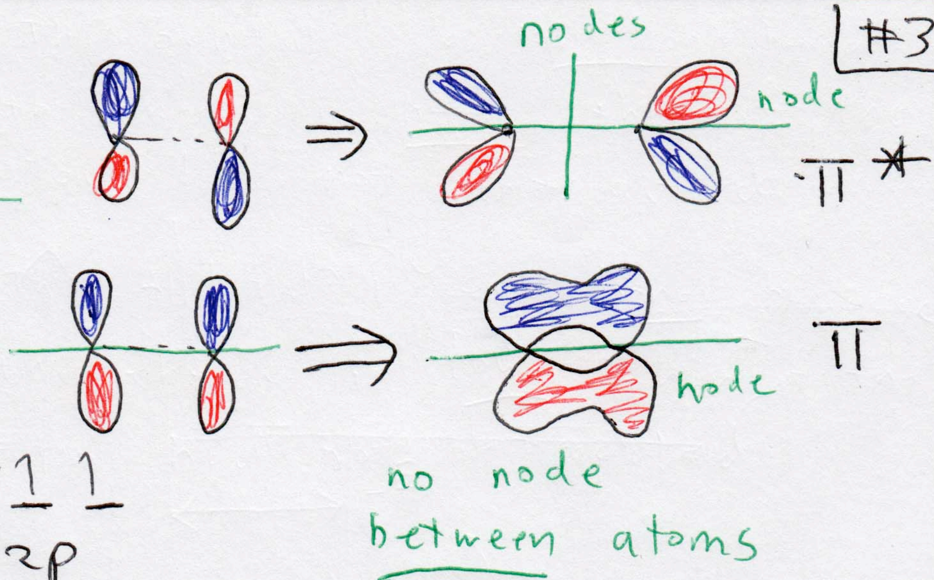


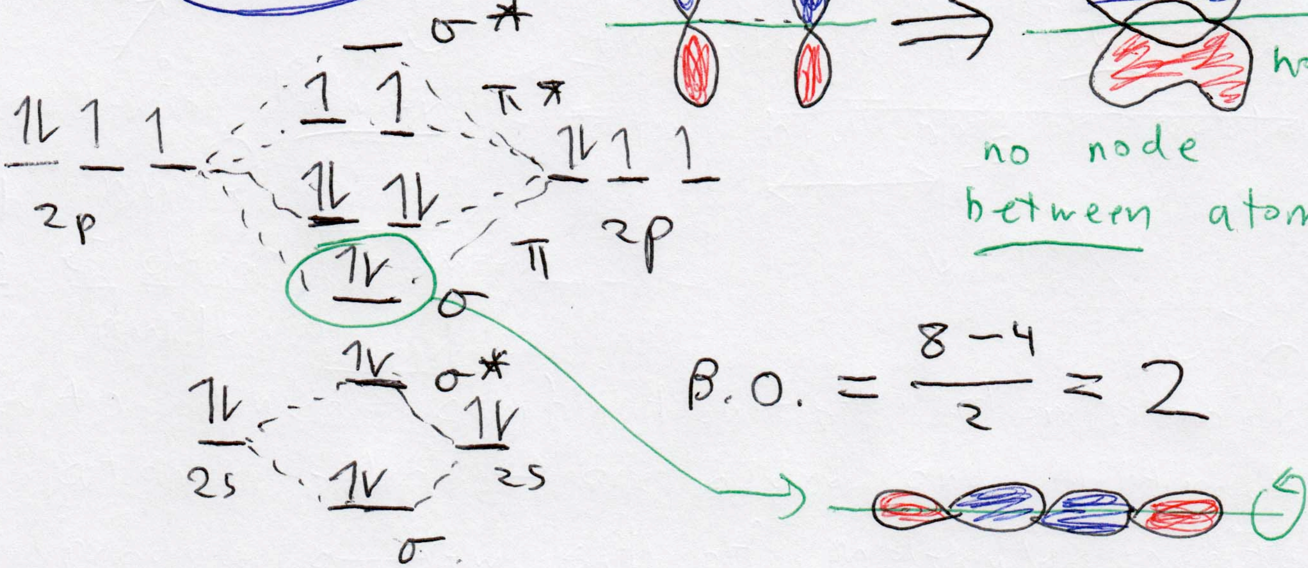
$$\text{Bond order} \equiv \frac{\#\text{ of bonding } e^- - \#\text{ of antibond } e^-}{2}$$

Each antibonding e^- causes a destabilization (increase in energy) that negates the stabilization (decrease in energy) provided by a bonding electron.

O_2







$$B.O. = \frac{8-4}{2} = 2$$

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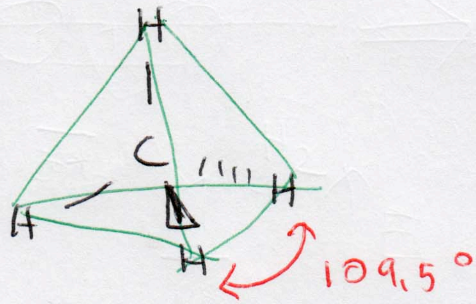
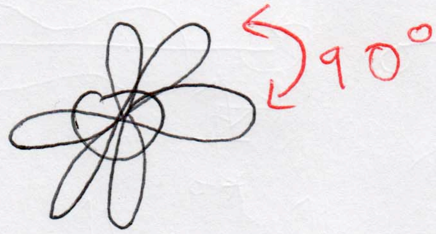
methane CH_4





The atomic orbitals of carbon cannot directly be used to describe the molecule methane since the geometry of the orbitals is incorrect and energy of the orbitals is not the same. To describe methane, a set of hybrid orbitals is created by adding and subtracting atomic orbitals on the same atom (LCAO).