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[TP] When atomic orbitals (AO's) on different atoms combine, the resulting molecular orbital (MO) ...

17% 1. less stable than the AO's
 17% 2. has the same energy as the AO's
 17% 3. more stable than the AO's
 17% 4. 1 and 2
 17% 5. 1 and 3
 17% 6. 2 and 3

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Friday, December 9, 2016

Begin ch 10: Modeling bonding in molecules

- Mixing AO's makes MO's <https://goo.gl/eliM2a>
- AO-MO correlation diagrams
- Bond order: H_2^+ to Be_2 (!)

Next (final) lecture: 2p MO's <https://goo.gl/2MEiRA>; B_2 to Ne_2 (!);
 When atoms are different, which AO's make MO's: Symmetry, overlap, energy (SOE)

Bonding in diatomic molecules <http://goo.gl/1h0S9C>
 Questions on Symmetry, Overlap, Energy (SOE) <http://goo.gl/oYef3b>

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1s molecular orbitals:
<http://quantum.bu.edu/CDF/101/1sMolecularOrbitals.cdf>

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Bonding in diatomic molecules
<http://goo.gl/1h0S9C>

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Atoms interact by mixing **waves**

AO "+" AO \rightarrow 2 MO's

"+" means **mixing** (not addition!)


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
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Relative AO phase determines MO character

here the different phases of the p orbital are labelled positive and negative – this can be confusing and so is best avoided



here the different phases of the p orbital are shown by shading one half and not the other



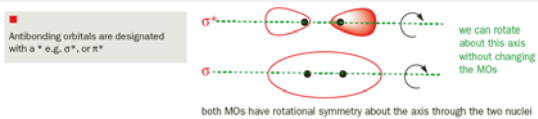
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σ MO's have cylindrical symmetry

Antibonding orbitals are designated with a * e.g. σ^* , or π^*



we can rotate about this axis without changing the MOs

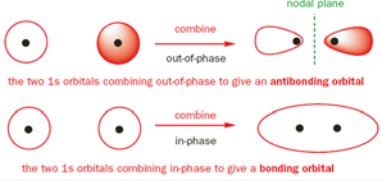
both MOs have rotational symmetry about the axis through the two nuclei

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$1s\sigma$ and $1s\sigma^*$



nodal plane

combine out-of-phase

the two 1s orbitals combining out-of-phase to give an antibonding orbital

combine in-phase

the two 1s orbitals combining in-phase to give a bonding orbital

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1s and 1s*

Mahaffy et al, Figure 10.20, p. 400

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1s molecular orbitals:
<http://quantum.bu.edu/CDF/101/1sMolecularOrbitals.cdf>

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σ is “bonding” and σ^* is “antibonding”

Antibonding orbitals are designated with a * e.g. σ^* , or π^*

we can rotate about this axis without changing the MOs

both MOs have rotational symmetry about the axis through the two nuclei

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AO-MO correlation diagrams

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Bonding PE, KE and total E

Attractive (< 0) PE is opposed by repulsive (> 0) KE.
Molecular size is at minimum of total E.

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Antibonding PE, KE and total E

Repulsive (> 0) PE enhanced by repulsive (> 0) KE.
No minimum of total E --- atoms fly apart!

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Bonding and antibonding total E

What matters are the total bonding and antibonding E at the bonding minimum versus the AO energies---the energy at infinite separation.

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Correlation diagrams ...

... summarize bonding and antibonding effects

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Bond order: H_2^+ to Be_2 (!)

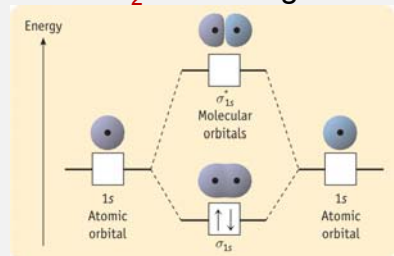


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Filling of MO's → H_2 MO configuration



Mahaffy et al., Figure 10.20, p. 400

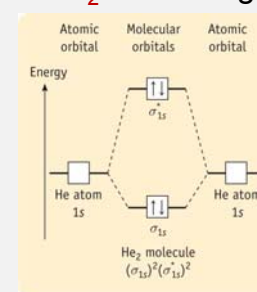


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Filling of MO's → He_2 MO configuration



He₂ molecule
(σ_{1s})²(σ_{1s}^*)²



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Bond order

$(\text{bonding } e^-s - \text{antibonding } e^-s)/2$

Division by two is because a single "bond" shares a pair of electrons

$H_2^+ = H:H^+ \rightarrow \text{bond order} = 1/2$
 $H_2 = H:H \rightarrow \text{bond order} = 1$
 $He_2 \rightarrow \text{bond order} = 0$
 $He_2^+ \rightarrow \text{bond order} = \dots?$

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1s (and 2s) σ and σ^*

Antibonding orbitals are designated with a * e.g. σ^* , or π^*

we can rotate about this axis without changing the MOs

both MOs have rotational symmetry about the axis through the two nuclei

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Filling of MO's $\rightarrow Li_2$ MO configuration

Mahaffy et al., Figure 10.22

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