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Lecture 36 CH101 A1 (MWF 9 am)

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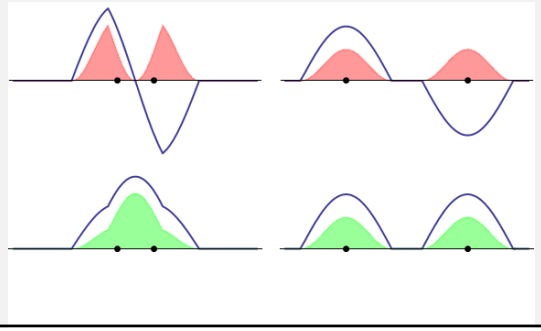
1s molecular orbitals:
http://quantum.bu.edu/CDF/101/1sMolecularOrbitals.cdf



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

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Atoms interact by mixing waves

AO "+" AO → 2 MO's

"+" means mixing (not addition!)

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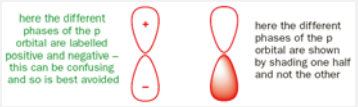
Relative AO phase determines MO character



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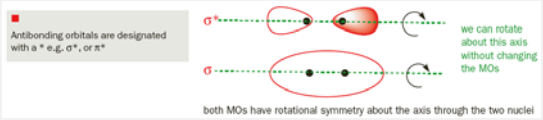
σ MO's have cylindrical symmetry



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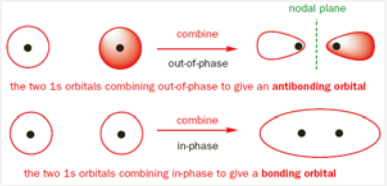
1sσ and 1sσ*



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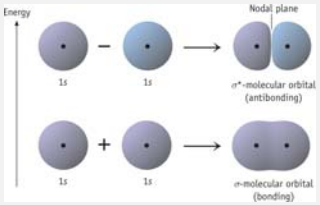

Mahaffy et al., Figure 10.20, p. 400

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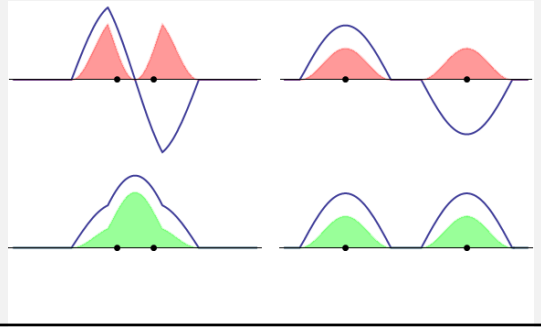
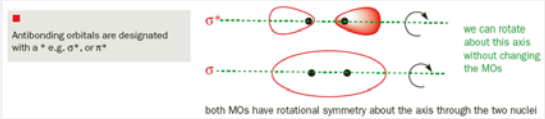
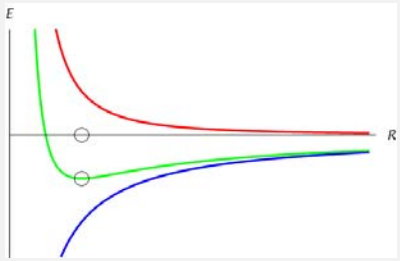


σ is “bonding” and σ* is “antibonding”



AO-MO correlation diagrams

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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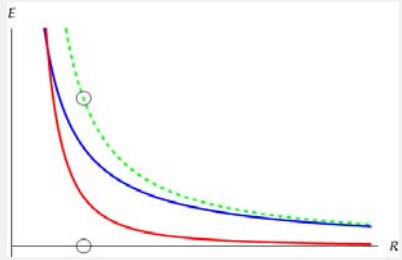
Antibonding *PE*, *KE* and total *E*



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

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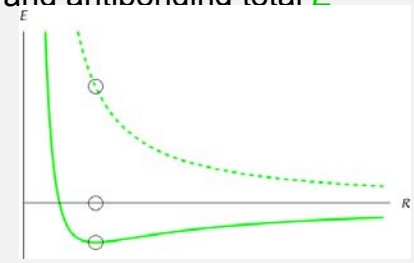
Bonding and antibonding total *E*



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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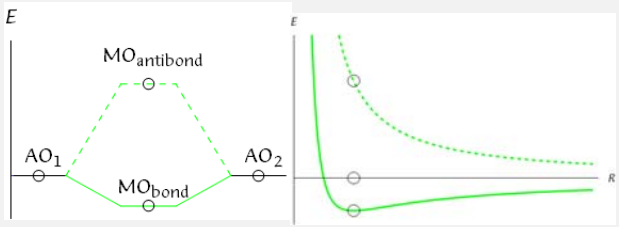
Correlation diagrams …



… summarize
bonding and antibonding effects

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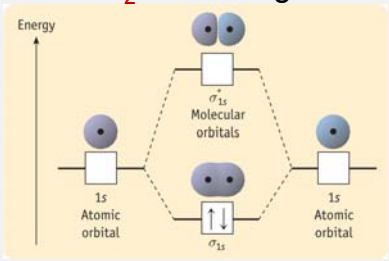
Bond order: H_2^+ to Be_2 (!)

Filling of MO's → H_2 MO configuration



Mahaffy et al., Figure 10.20, p. 400

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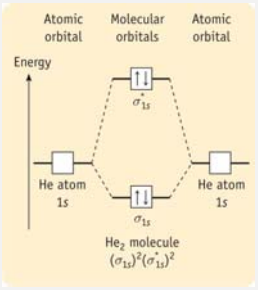


Mahaffy et al., Figure 10.21

Bond order

(bonding e⁻'s – antibonding e⁻'s)/2

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

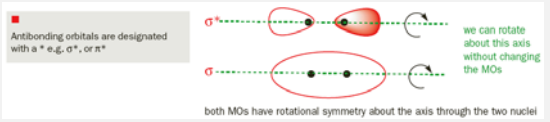
$H_2^+ = H{\cdot}H^+ \rightarrow$ bond order = 1/2

$H_2 = H{:}H \rightarrow$ bond order = 1

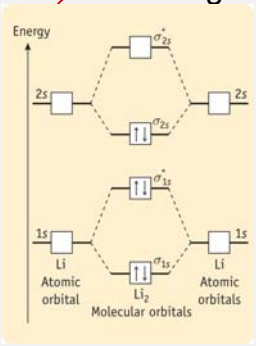
$He_2 \rightarrow$ bond order = 0

$He_2^+ \rightarrow$ bond order = ...?

1s (and 2s) σ and σ*



Filling of MO's → Li_2 MO configuration



Mahaffy et al., Figure 10.22