[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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Lecture 37 CH101 A1 (MWF 9:05 am)

Monday, December 11, 2017

For today ...

- Special birthday today
- AO-MO correlation diagrams
- Bond order: H_2^+ to Be_2 (!)
- 2p MO's: CDF https://goo.gl/2MEiRA
- B_2 to Ne_2
- Class evaluation: https://bu.campuslabs.com/courseeval

Next lecture: CH102 Spring 2018!

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Today is Max Born's 135th birthday

Max Born proposed the recipe that connects electron wave to electron clouds.

$$|\text{electron wave}|^2 = \text{electron cloud}$$

His birthday is celebrated with today's Google Doodle.

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AO-MO correlation diagrams

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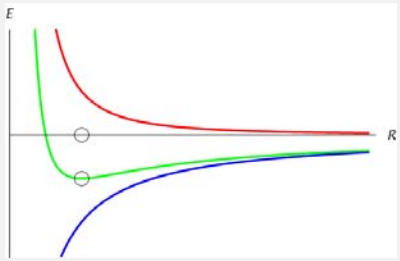
Bonding *PE*, *KE* and total *E*



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

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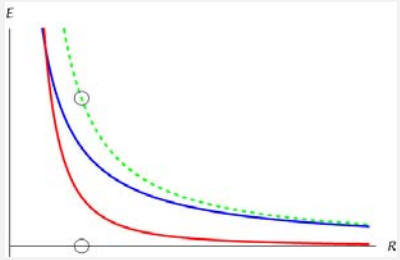
Antibonding *PE*, *KE* and total *E*



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

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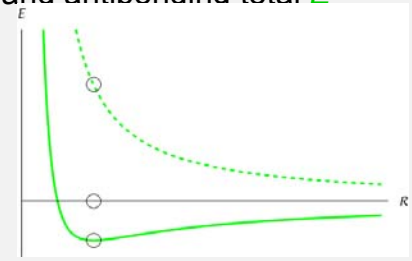
Bonding and antibonding total *E*



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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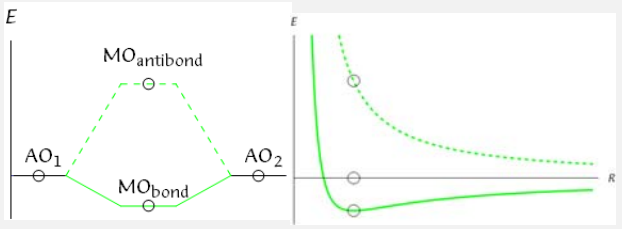
Correlation diagrams …



… summarize
bonding and antibonding effects

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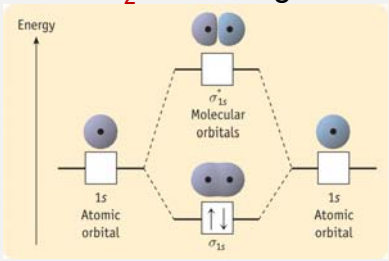
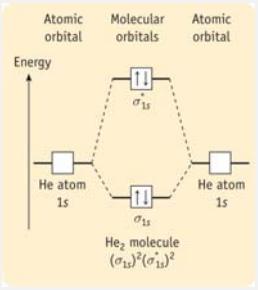
Bond order: H_2^+ to Be_2 (!)

Filling of MO's → H_2 MO configuration



Mahaffy et al., Figure 10.20, p. 400

Filling of MO's → He_2 MO configuration



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

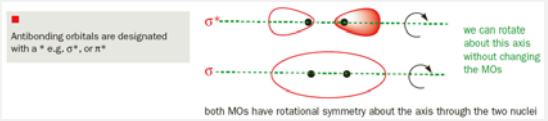
$H_2^+ = H{\cdot}H^+ \rightarrow$ bond order = 1/2

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

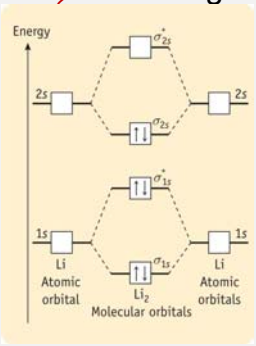
$He_2 \rightarrow$ bond order = 0

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

1s (and 2s) σ and σ*



Filling of MO's → Li_2 MO configuration

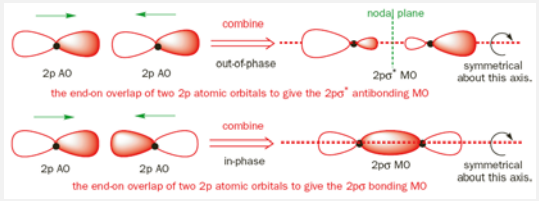


Mahaffy et al., Figure 10.22

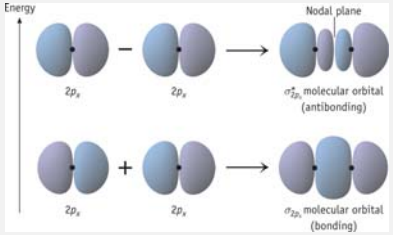
MO's in B_2, C_2, etc.

Build MOs from 2p AO's

$2p_z\sigma$ and $2p_z\sigma^*$



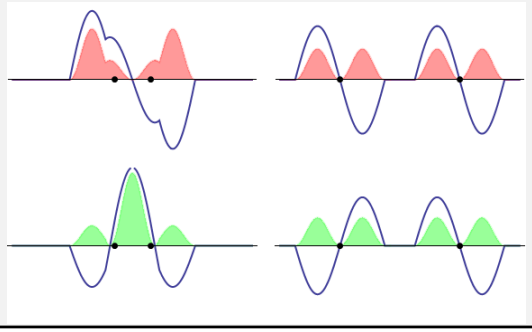
$2p_z\sigma$ and $2p_z\sigma^*$



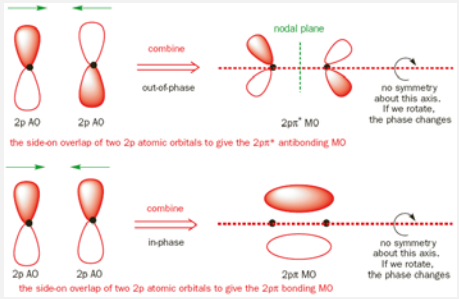
Mahaffy et al., Figure 10.23, p. 403

$2p_z\sigma$ (lower) and $2p_z\sigma^*$ (upper)

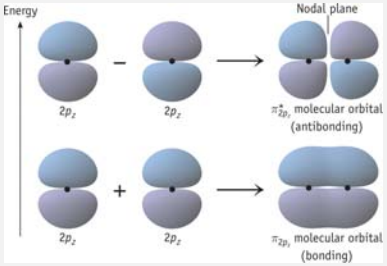
$2p_z$ molecular orbitals:
http://quantum.bu.edu/CDF/101/2pMolecularOrbitals.cdf



$2p_x\pi$ and $2p_x\pi^*$



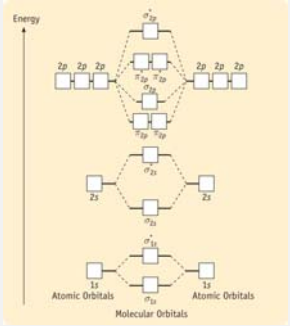
$2p_x\pi$ and $2p_x\pi^*$



Mahaffy et al., Figure 10.24, p. 403

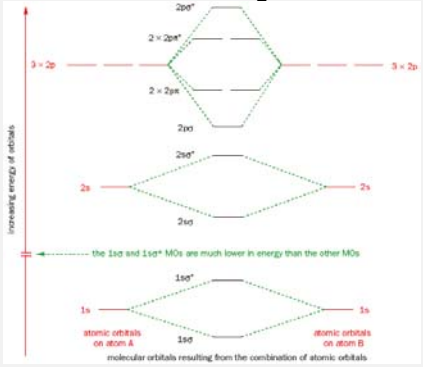
B_2 to Ne_2 (!)

Homonuclear diatomics, up to N_2

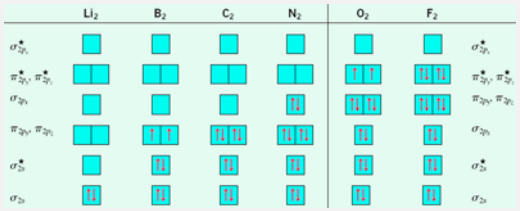


Mahaffy et al., 1e, Figure 10.25

Homonuclear diatomics, after N_2



Homonuclear diatomics



Laird, University Chemistry, Figure 3.4

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Course evaluation

https://bu.campuslabs.com/courseeval

- Lecture, discussion, and lab
- Your responses are anonymous.
- They will be read many people.
- The more thoughtful your responses, the more helpful they will be.
- If more time is needed, you may continue until December 15.

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