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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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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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7

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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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11

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Bond order: H_2^+ to Be_2 (!)

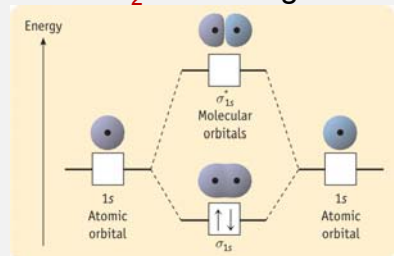


12

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Filling of MO's → H_2 MO configuration



Mahaffy et al., Figure 10.20, p. 400

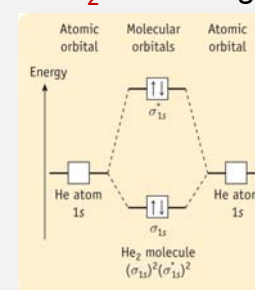


13

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Filling of MO's → He_2 MO configuration



Mahaffy et al., Figure 10.21



14

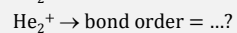
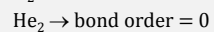
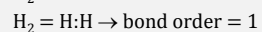
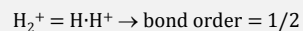
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Bond order

(bonding e⁻s - antibonding e⁻s)/2

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

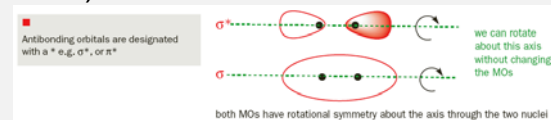


15

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1s (and 2s) σ and σ^*

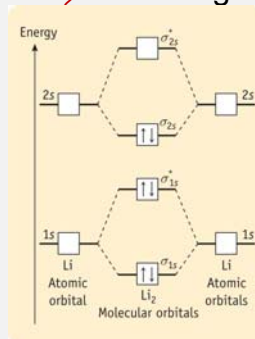


16

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Filling of MO's \rightarrow Li₂ MO configuration



Mahaffy et al., Figure 10.22



17

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MO's in B₂, C₂, etc.

Build MOs from 2p AO's



18

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

combine out-of-phase $2p_z\sigma^*$ MO symmetrical about this axis.
the end-on overlap of two $2p$ atomic orbitals to give the $2p_z\sigma^*$ antibonding MO

combine in-phase $2p_z\sigma$ MO symmetrical about this axis.
the end-on overlap of two $2p$ atomic orbitals to give the $2p_z\sigma$ bonding MO

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

Energy

$2p_z$ $2p_z$ $2p_z\sigma^*$ molecular orbital (antibonding)

$2p_z$ $2p_z$ $2p_z\sigma$ molecular orbital (bonding)

Nodal plane

Mahaffy et al., Figure 10.23, p. 403

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

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

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

combine out-of-phase $2p_x\pi^*$ MO no symmetry about this axis. If we rotate, the phase changes.
the side-on overlap of two $2p$ atomic orbitals to give the $2p_x\pi^*$ antibonding MO

combine in-phase $2p_x\pi$ MO no symmetry about this axis. If we rotate, the phase changes.
the side-on overlap of two $2p$ atomic orbitals to give the $2p_x\pi$ bonding MO

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

Energy ↑

$2p_z$ $2p_z$ π_{2p}^* molecular orbital (antibonding)

$2p_z$ $2p_z$ π_{2p} molecular orbital (bonding)

Nodal plane

Mahaffy et al., Figure 10.24, p. 403

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B_2 to Ne_2 (!)

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Homonuclear diatomics, up to N_2

Energy ↑

Atomic Orbitals Molecular Orbitals

Mahaffy et al., 1e, Figure 10.25

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Homonuclear diatomics, after N_2

Increasing energy of orbitals ↑

atomic orbitals on atom A atomic orbitals on atom B

molecular orbitals resulting from the combination of atomic orbitals

the $1s$ and $1s^*$ MOs are much lower in energy than the other MOs

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Homonuclear diatomics

	Li ₂	B ₂	C ₂	N ₂	O ₂	F ₂	
σ_{2p}^*							σ_{2p}^*
π_{2p}^*, π_{2p}^*							π_{2p}^*, π_{2p}^*
σ_{2p}							π_{2p}, π_{2p}
π_{2p}, π_{2p}							σ_{2p}
σ_{2s}^*							σ_{2s}^*
σ_{2s}							σ_{2s}

Laird, University Chemistry, Figure 3.4

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27

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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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29