[TP] In Li_2 which MO makes the greatest contribution to the bond strength?

33% 1. 1sσ
33% 2. 2sσ
33% 3. 1 and 2 contribute equally

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Lecture 35 CH101 A1 (MWF 9:05 am)

Wednesday, December 5, 2018

For today:

- Only valence AO's affect bonding/antibonding: CDF: https://goo.gl/QLHdRf
- Bond order: Li_2^+ to Be_2 (!)
- 2p MO's: CDF https://goo.gl/2MEiRA
- B_2 to Ne_2

Next lecture: When atoms are different, use Symmetry, Overlap, Energy (SOE) to decide which AOs combine ; Covalent versus ionic character ; MO description of hydroxide, OH^-, and HOH (water)

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Filling of MO's → Li_2 MO configuration

In Li_2 each atom has electrons in 1s and 2s AO's.

Which AO's interact?

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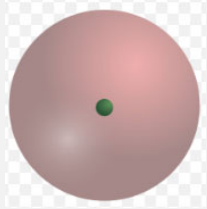
Only valence AO's affect bonding/antibonding

Here 2s AO of Li. Recalling that diameter ≈ 0.10 nm $\frac{n^2}{Z_{\text{eff}}}$, sketch below it on the same scale the 1s AO of Li.



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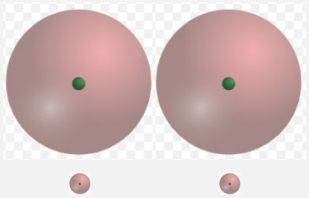
Only valence AO's affect bonding/antibonding

Here are the 1s and 2s AO's Li_2 .



The 1s AO's are $\frac{1}{Z_{\text{eff}}} \times \frac{1}{n^2} \approx \frac{1}{3} \times \frac{1}{4} = \frac{1}{12}$ the size of the 2s AO's and so overlap negligibly.

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Only valence AO's affect bonding/antibonding

http://quantum.bu.edu/CDF/101/Li2Bonding1sAnd2sElectronClouds.cdf

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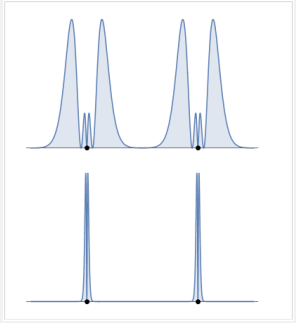
At $R = \infty$, no 1s or 2s bonding

http://quantum.bu.edu/CDF/101/Li2Bonding1sAnd2sElectronClouds.cdf



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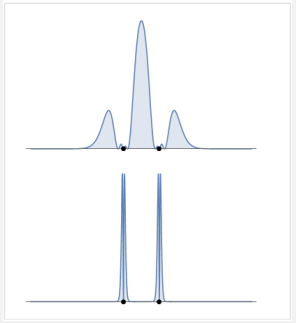
At maximum 2s bonding, $R = R_e$, no 1s bonding

http://quantum.bu.edu/CDF/101/Li2Bonding1sAnd2sElectronClouds.cdf



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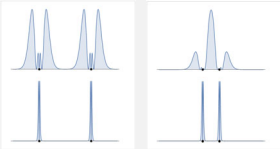
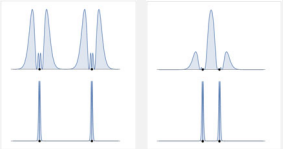
Only valence AO's affect bonding/antibonding

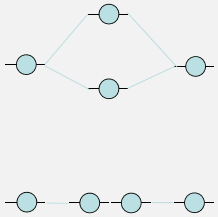
Sketch the correlation diagram that correspond to these figures.



Only valence AO's affect bonding/antibonding

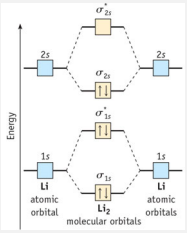
Sketch the correlation diagram that correspond to these figures.





Only valence AO's affect bonding/antibonding

Here is the correlation diagram we have seen for Li_2 (fig 10.22, p 402).



Sketch a more correct version.

[TP] In Li_2 which MO makes the greatest contribution to the bond strength?

33% 1. 1sσ
33% 2. 2sσ
33% 3. 1 and 2 contribute equally

Bond order: Li_2^+ to Be_2 (!)

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MO's in B_2, C_2, etc.

Build MO's from 2p AO's

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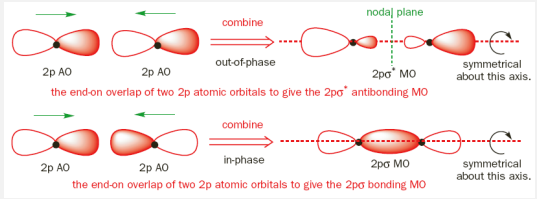
$2p_z\sigma$ and $2p_z\sigma^*$



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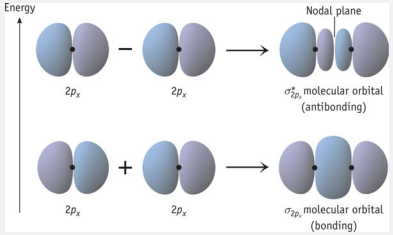
$2p_z\sigma$ and $2p_z\sigma^*$



Mahaffy et al., Figure 10.23, p. 403

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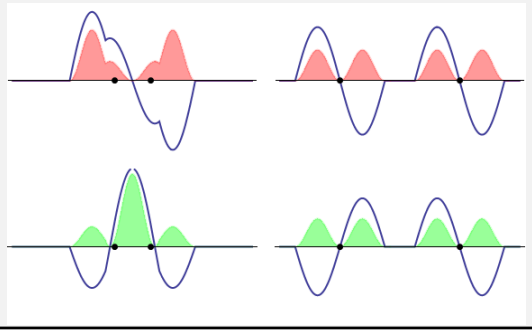
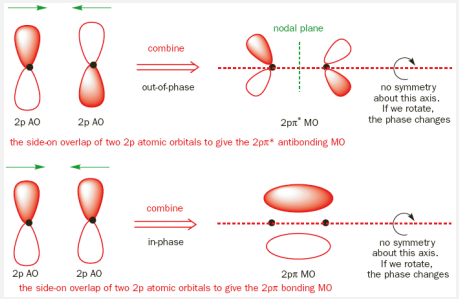
$2p_z\sigma$ (lower) and $2p_z\sigma^*$ (upper)

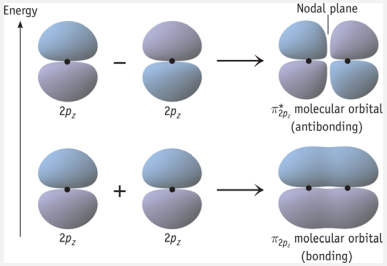
$2p_z$ molecular orbitals:
http://quantum.bu.edu/CDF/101/2pMolecularOrbitals.cdf



$2p_x\pi$ 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

Sketch the portion of the correlation diagram for MO's built from 2s and 2p AO's

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Homonuclear diatomics, up to N_2

The relative stability of the 2pσ and 2pπ bonding MO's is uncertain.

Let's see how we can use the magnetic properties B_2, C_2, and N_2 to determine the ordering.

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[TP] B_2 is paramagnetic. From this we can conclude the following about the relative stability of the $n = 2$ bonding MO's.

33% 1. 2pσ is more stable than 2pπ
33% 2. 2pπ is more stable than 2pσ
33% 3. Further information is still required

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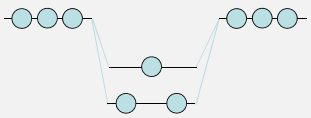
Only valence AO's affect bonding/antibonding

B_2 is paramagnetic. From this we can conclude the following about the relative stability of the $n = 2$ bonding MO's.



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