[TP] C_2 is diamagnetic. 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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Lecture 36 CH101 A2 (MWF 11:15 am)

Friday, December 7, 2018

For today:

- Complete: B_2 to Ne_2
- When atoms are different, use Symmetry, Overlap, Energy (SOE) to decide which AOs combine, http://goo.gl/oYEf3b

Next lecture: AO relative energies affect MO composition ; Covalent versus ionic character ; MO description of hydroxide, OH^-, and HOH (water)

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[TP] B_2 is paramagnetic. From this we can conclude the following about the relative stability of the 2p 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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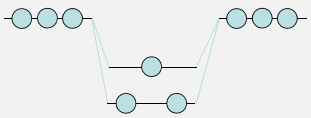
Only valence AO's affect bonding/antibonding

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



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[TP] C_2 is diamagnetic. From this we can conclude the following about the relative stability of the 2p 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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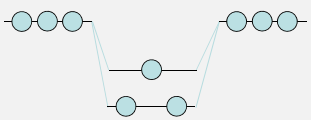
Only valence AO's affect bonding/antibonding

C_2 is diamagnetic. From this we can conclude the following about the relative stability of the 2p bonding MO's.



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[Quiz] N_2 is diamagnetic. From this we can conclude the following about the relative stability of the 2p 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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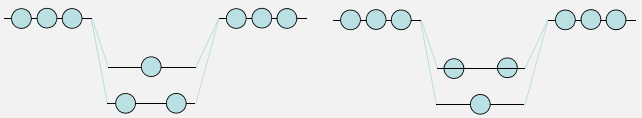
Only valence AO's affect bonding/antibonding

N_2 is diamagnetic. From this we can conclude the following about the relative stability of the 2p bonding MO's.



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Homonuclear diatomics, up to Ne_2

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

Let's see how we can use the magnetic properties O_2, F_2, and Ne_2 to determine the ordering.

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[TP] O_2 is paramagnetic. From this we can conclude the following about the relative stability of the 2p antibonding 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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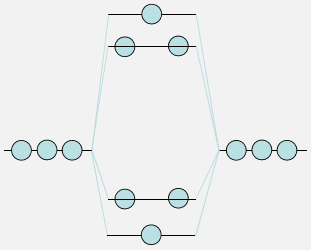
Only valence AO's affect bonding/antibonding

O_2 is paramagnetic. From this we can conclude the following about the relative stability of the 2p antibonding MO's.



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[TP] F_2 is diamagnetic. From this we can conclude the following about the relative stability of the 2p antibonding 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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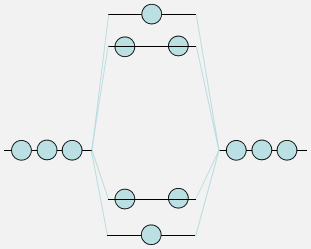
Only valence AO's affect bonding/antibonding

F_2 is diamagnetic. From this we can conclude the following about the relative stability of the 2p antibonding MO's.



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[TP] If Ne_2 were to exist it would diamagnetic. From this we can conclude the following about the relative stability of the 2p antibonding MO's.

0% 1. 2pσ* is more stable than 2pπ*
0% 2. 2pπ* is more stable than 2pσ*
0% 3. Further information is still required

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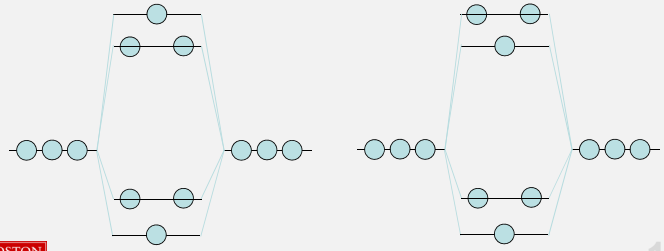
Only valence AO's affect bonding/antibonding

If Ne_2 were to exist it would diamagnetic. From this we can conclude the following about the relative stability of the 2p antibonding MO's.



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Homonuclear diatomics

TABLE 10.7
Order of Energies of Molecular Orbitals, Electron Configurations, and Physical Data for Homonuclear Diatomic Molecules of Second-Period Elements

	B_2	C_2	N_2	O_2	F_2
σ^*_{2p}	□	□	□	□	□
π^*_{2p}	□□	□□	□□	↑ ↑	↑↓ ↑↓
σ_{2p}	□	□	↑↓	↑↓ ↑↓	↑↓ ↑↓
π_{2p}	↑ ↑	↑↓ ↑↓	↑↓ ↑↓	↑↓	↑↓
σ^*_{2s}	↑↓	↑↓	↑↓	↑↓	↑↓
σ_{2s}	↑↓	↑↓	↑↓	↑↓	↑↓
Bond order	One	Two	Three	Two	One
Bond-dissociation energy (kJ/mol)	290	620	945	498	155
Bond distance (pm)	159	131	110	121	143
Observed magnetic behaviour (paramagnetic or diamagnetic)	Para	Dia	Dia	Para	Dia

Mahaffy et al., 2e, Figure 10.17, page 404

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When atoms are different, which AO's combine?

As example, let's consider HO^-.

What AO's on O combine with H 1s to form the MO's of HO^-?

The possibilities O 1s, O 2s, O $2p_x$, O $2p_y$, and O $2p_z$.

To decide the optimum pairing, ...

When atoms are different, which AO's combine?

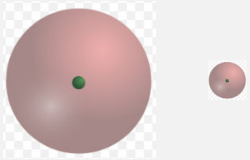
Use SOE: Symmetry, Overlap, Energy

- Symmetry: AO's must have nonzero overlap
- Overlap: AO's with greatest overlap form MO's with the greatest bonding/antibonding effect
- Energy: AO's closest in energy form MO's with the greatest bonding/antibonding effect

When atoms are different, which AOs combine?

They must have appreciable overlap.

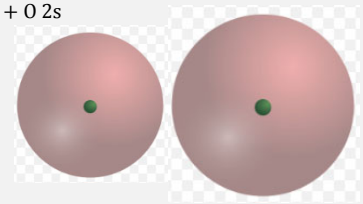
Not OK example: H 1s + O 1s



When atoms are different, which AOs combine?

They must have appreciable overlap.

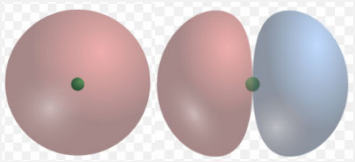
OK example: H 1s + O 2s



When atoms are different, which AO's combine?

They must have the correct symmetry.

OK example: H 1s + O $2p_z$ (z is bond axis)



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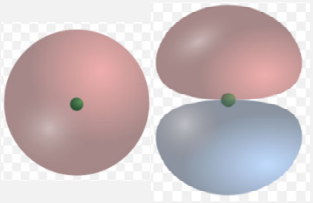
When atoms are different, which AO's combine?

They must have the correct symmetry.

Not OK example: H 1s + O $2p_x$ (x is perpendicular to bond axis)



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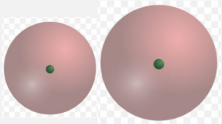
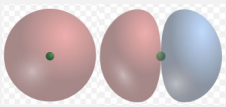
When atoms are different, which AOs combine?

Based on overlap and symmetry, we need to decide between the two pairings

H 1s + O 2s



H 1s + O $2p_z$



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When atoms are different, which AOs combine?

The way to select the optimum pairing is the pairing that is closest in energy.

Here is why.

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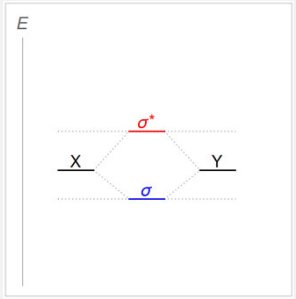
Energy: Closer the better

http://quantum.bu.edu/CDF/101/CorrDiagXY2s.cdf



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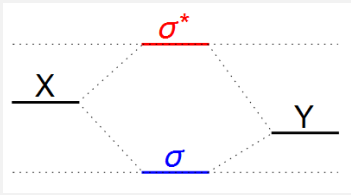
When atoms are different, which AOs combine?

They must be close in energy.

OK example: H 1s (−13.59 eV) + O $2p_z$ (−13.62 eV)



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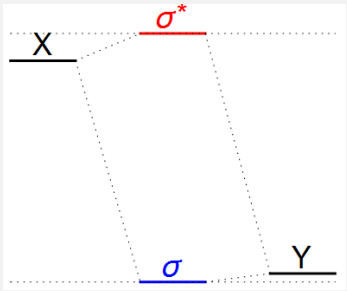
When atoms are different, which AOs combine?

They must be close in energy.

Not OK example: H 1s (−13.59 eV) + O 2s (−35.12 eV)



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When atoms are different, which AOs combine?

They must be close in energy.

OK example: H 1s (−13.59 eV) + O $2p_z$ (−13.62 eV)

Not OK example: H 1s (−13.59 eV) + O 2s (−35.12 eV)

So in HO^- form MO's from

H 1s and O $2p_z$ ($2p_x$ and $2p_y$ have the wrong symmetry) ...

rather than from

H 1s and O 2s.

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