

[TP] Atom X have IE_1 = 17 eV and atom Y has IE_1 =12 eV. Compared to molecule X:H, ...

20% 1. molecule Y:H has a greater dipole moment
20% 2. molecule Y:H has the same dipole moment
20% 3. molecule Y:H has a smaller dipole moment
20% 4. Neither molecule is polar
20% 5. Cannot know relative polarity without knowing the electronegativities of atoms H, X, and Y.

Lecture 37 CH101 A1 (MWF 9 am)

Monday, December 12, 2016

- Evaluation
- When atoms are different, which AO's make MO's
- Origin of polarity
- 2p MO's https://goo.gl/2MEiRA
- B_2 to Ne_2

Bonding in diatomic molecules http://goo.gl/1h0S9C
Questions on Symmetry, Overlap, Energy (SOE) http://goo.gl/oYEf3b

Evaluation

C A S / G R S C H 1 0 1 Section: A 1

Course Title, Instructor, or Semester/Year: Not needed

4. [Do not answer, not applicable]

5. [Do not answer, not applicable]

Reverse side: Comments section: Clear detail will be most helpful

When atoms are different, which AO's combine?

SOE: Symmetry, Overlap, Energy

- Symmetry: Which AO's are able to combine to form MO's?
- Overlap: Which AO's combine with the greatest bonding/antibonding effect?
- Energy: How does relative AO energy affect composition of MO's?

Symmetry: Net overlap or not?

- For a pair of AO's to give a (bonding/antibonding) pair of MO's, there must be net overlap (net in-phase or net out-of-phase).
- If in-phase and out of phase overlap exactly cancel, the AO's remain uncombined, as nonbonding orbitals.

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Overlap: Greater the better

- The more net overlap, the greater the bonding/antibonding effect.
- Core AO's have least overlap
- Valence AO's have greatest overlap
- Bonding due to MO's made from valence AO's

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Energy: Closer the better

- The closer AO's are in energy, the greater the bonding/antibonding effect.
- If AO's have same energy (identical atoms, homonuclear bond), MO's will be 50% of each AO.
- If AO's have different energy (different atoms, heteronuclear bond), ...
  - Bonding MO → contains more of the lower energy AO
  - Antibonding MO → contains more of the higher energy AO

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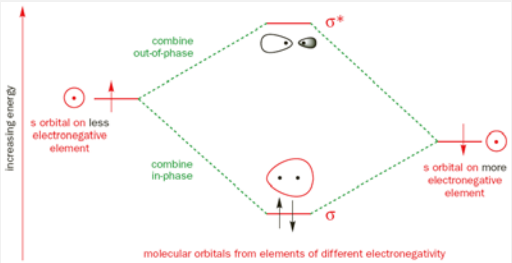
Energy: Closer the better



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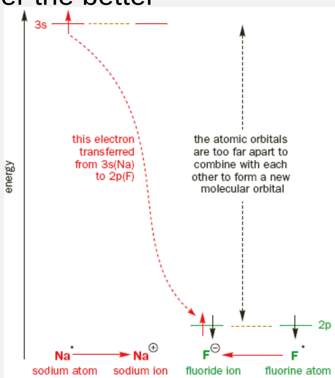
Energy: Closer the better



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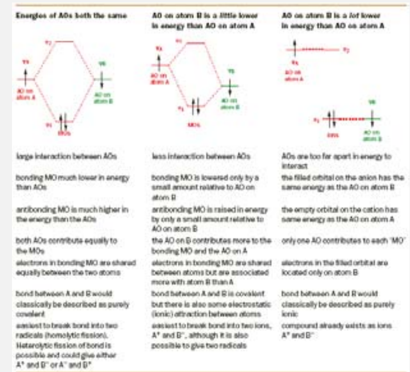
Energy: Closer the better



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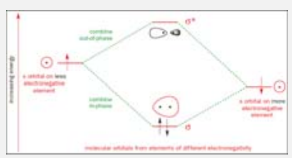
[TP] Assume AO_1 and AO_2 have correct relative symmetry, greatest overlap, and are closest in energy. AO_1 has $IE = 5$ eV and AO_2 has $IE = 6$ eV. Which of the following is true?

17% 1. Bonding MO has more AO_1 than AO_2
17% 2. Bonding MO has more AO_2 than AO_1
17% 3. Antibonding MO is almost entirely AO_1
17% 4. Antibonding MO is almost entirely AO_2
17% 5. 1 and 4
17% 6. I do not know how to tell.



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[Quiz] Atom X have $IE_1 = 17$ eV and atom Y has $IE_1 = 12$ eV. Compared to molecule X:H, …

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Practice

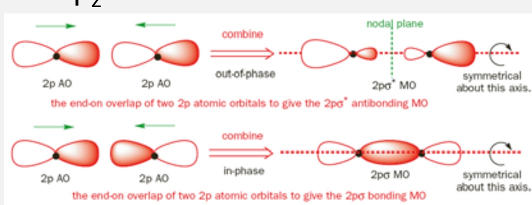
Questions on Symmetry, Overlap, Energy

http://goo.gl/oYEf3b

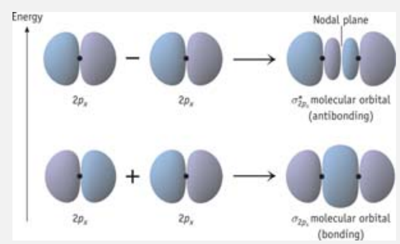
MO's in B_2, C_2, etc.

Build MOs from 2p AO's

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



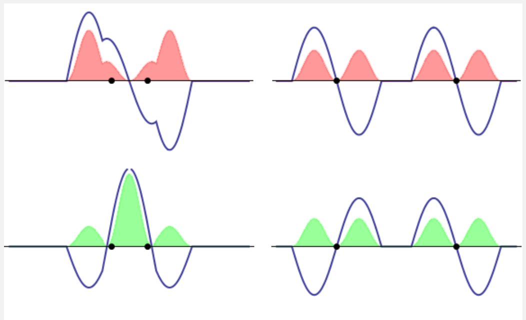
$2p_z\sigma$ and $2p_z\sigma^*$



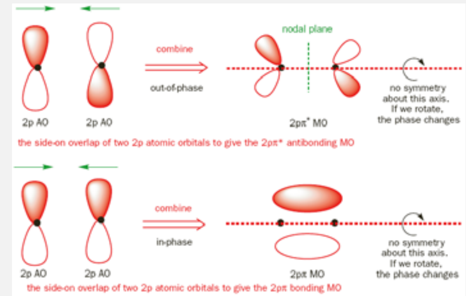
Mahaffy et al., Figure 10.23, p. 403

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

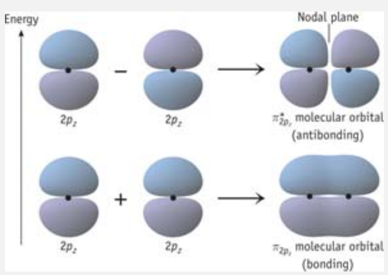
$2p_z$ molecular orbitals:
http://quantum.bu.edu/CDF/101/2pMolecularOrbitals.cdf



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



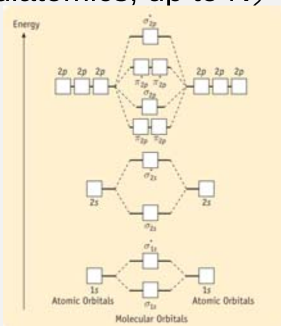
$2p_x\pi$ and $2p_x\pi^*$



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

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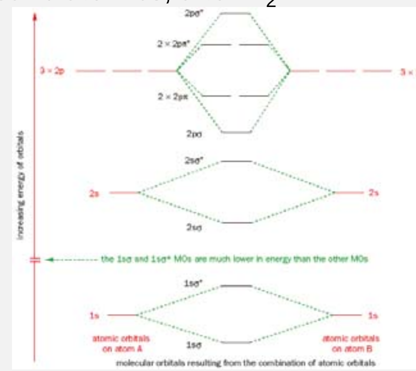
Homonuclear diatomics, after N_2



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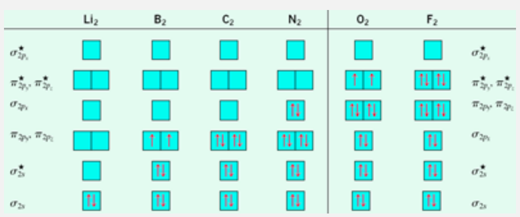
Homonuclear diatomics



Laird, University Chemistry, Figure 3.4

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