

Molecular Orbital (MO) Models for Electrons in Molecules

Quantum Mechanical Picture of Covalent Bonding
Ch 1.5-1.9

“Toy” Quantum Mechanics

- ▶ QM more informative than ad hoc Lewis model
- ▶ QM much, much harder to use
 - ▶ Correct usage requires lots of adv. mathematics
 - ▶ Rigorous QM waaay beyond this course, but “toy” QM ok?

1.
become
mathematician

2.
make computer do
the math

3.
use “toy” QM – just
like “real thing”

- ▶ Even “toy” QM will look *strange*
 - ▶ Choose MO model: similar to atomic orbital (AO) model

Will bonding occur? “How to” guide

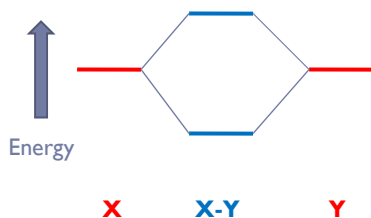
- ▶ Bonding joins 2 atoms, X & Y, to make a molecule, X-Y
 - ▶ X-Y more stable than X + Y → BOND
 - ▶ less stable → NO BOND

1. Describe valence e⁻ w/ orbitals & orbital energies
 - ▶ electron in atom → describe by AO
 - ▶ electron in molecule → describe by MO
2. Compare AO/MO energies of electrons
 - ▶ AO higher energy than MO → BOND
 - ▶ AO lower energy than MO → NO BOND
3. Use “orbital interaction diagram” for comparison

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Interaction Diagram for $X\cdot + Y\cdot \rightarrow X-Y$

Step #1 – position orbitals by energy

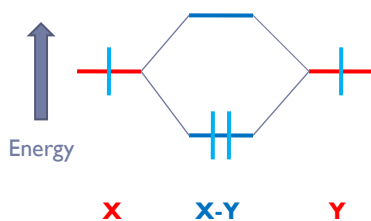


- What color lines show AO energies?
- The valence electrons on X and Y can be described by two AO. How many MO can describe the valence electrons on X-Y?
- Haven't explained why one MO "below" & one MO "above", but ALWAYS this way
- Dashed lines connect AO to the MO that replace them (or *vice versa*)

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Interaction Diagram for $X\cdot + Y\cdot \rightarrow X-Y$

Step #2 – add electrons



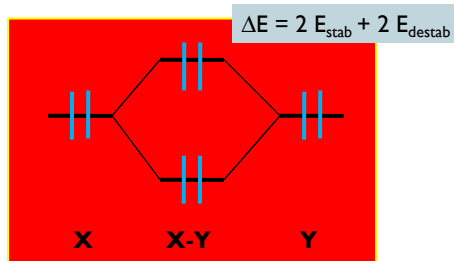
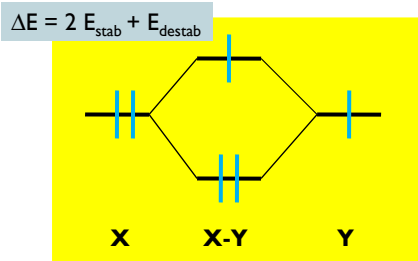
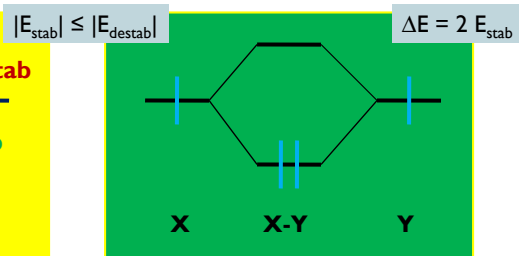
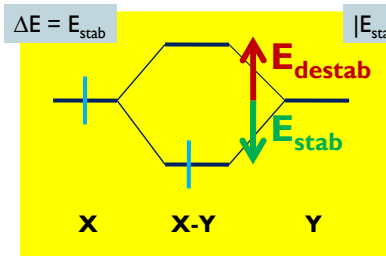
• What happens to energy when electrons move from AO to MO?

• Is a bond expected?

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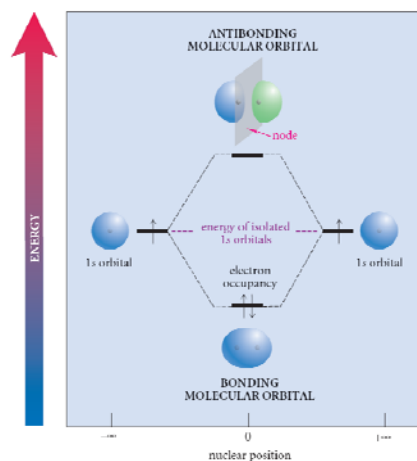
2 Electrons \rightarrow Strongest Bond

4 Electrons \rightarrow No Bond



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Does Loudon's Figure Make Sense?



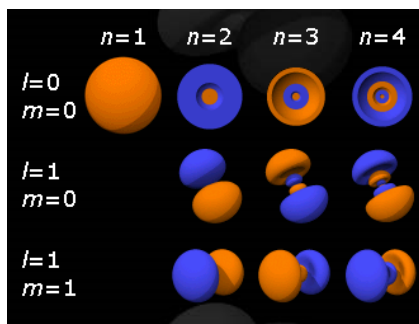
- I haven't examined MO shapes (just hang on)

- I don't understand labeling of axis

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What are orbitals?

- ▶ Source of information
 - ▶ electron location
 - ▶ electron energy



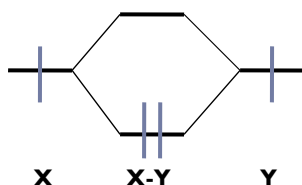
www.orbitals.com/orb/orbtable.htm#table3

- ▶ Atomic orbitals (AO)
 - ▶ quantum numbers
 - ▶ n = principal quantum #
 - ▶ determines energy & size
 - ▶ determines possible l
 - ▶ $n = 1, l = 0$ ($1s$)
 - ▶ $n = 2, l = 0$ ($2s$) or 1 ($2p$)
 - ▶ Symmetry
 - ▶ $l = 0$ spherical
 - ▶ $l = 1$ cylindrical

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Is a 'source of information' a 'thing'?

- ▶ Orbital = Thing
- ▶ 'House w/ rooms' analogy
 - ▶ Rooms are orbitals
 - ▶ Some rooms "occupied"
 - ▶ Some rooms "empty"

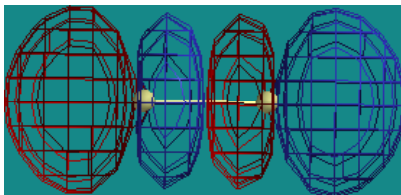


- ▶ Orbital = Possible description
- ▶ 'Part in a play' analogy
 - ▶ Parts (roles) are orbitals
 - ▶ Some roles are taken
 - ▶ Some roles are not
- ▶ All depends on #electrons

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Mathematical "description"

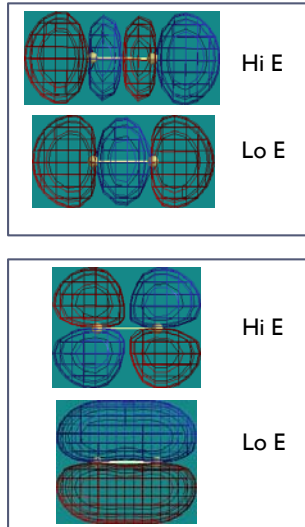
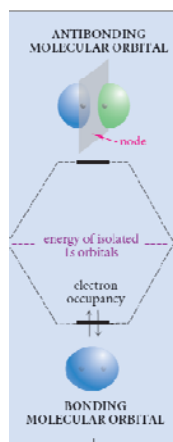
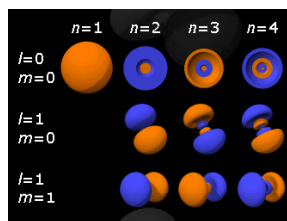
- ▶ Orbital is a "wave function"
 - ▶ put in some numbers, independent variables (x, y, z coords of electron)
 - ▶ get out a new number (value of orbital)
 - ▶ *square* of orbital value is proportional to probability of electron being at x, y, z (orbital called "probability amplitude")



- ▶ 'Wave-particle duality' is a misnomer?

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Nodes determines energy



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