Molecular Orbital Theory

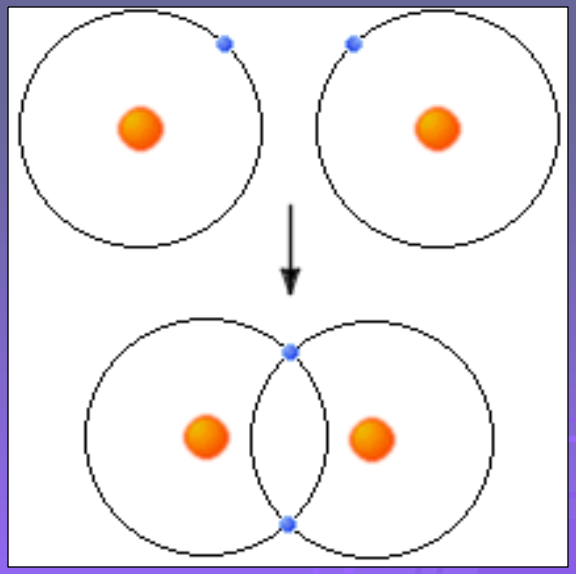
- The goal of molecular orbital theory is to describe molecules in a similar way to how we describe atoms, that is, in terms of orbitals, orbital diagrams, and electron configurations
- Describes the properties based on the bonding within the molecule

Bonding and Antibonding Orbitals
"what happening within the bond itself"

- Bonding Orbital – lower energy and greater stability, during this time a greater possibility to find the electrons between the nuclei of the atom
- Antibonding Orbital – higher energy and lower stability, low possibility to finding the electrons between the nuclei of the atom

Atomic and Molecular Orbitals (cont'd)

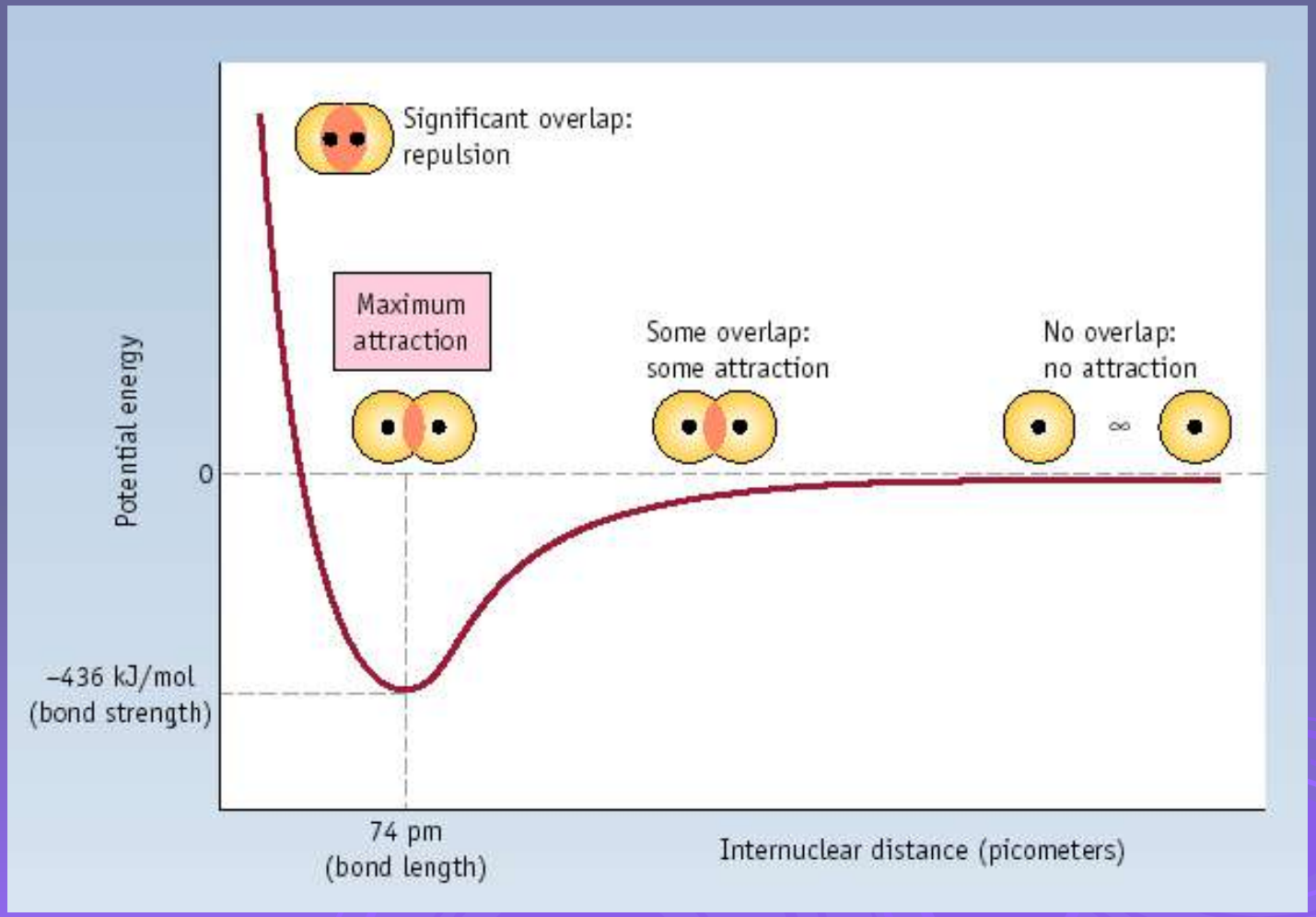
- Orbital Mixing
  - When atoms share electrons to form a bond, their atomic orbitals mix to form molecular bonds. In order for these orbitals to mix they must:
    - Have similar energy levels.
    - Overlap well.
    - Be close together.



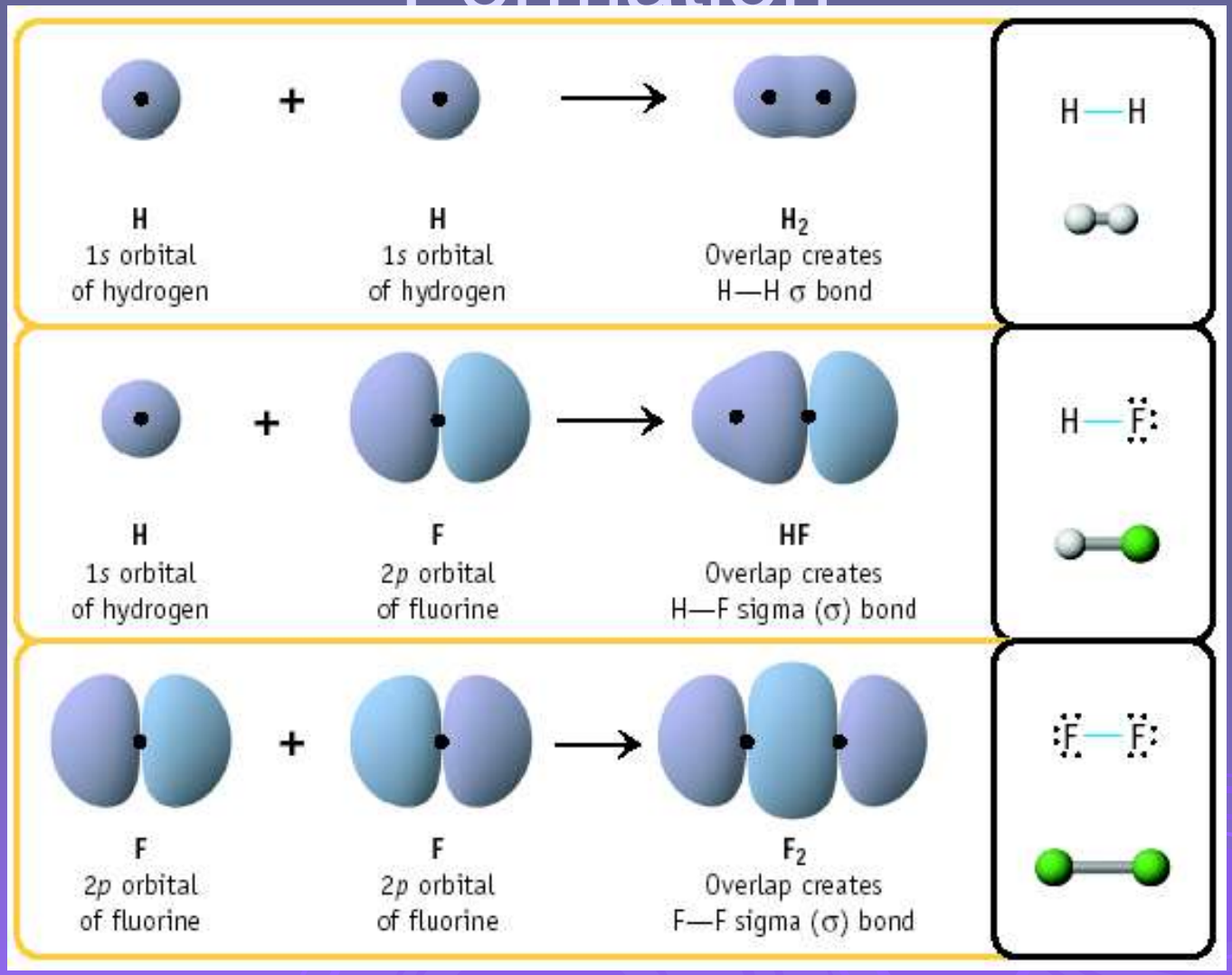
http://library.thinkquest.org/27819/ch2_2.shtml

This is and example of orbital mixing. The two atoms share one electron each from there outer shell. In this case both 1s orbitals overlap and share their valence electrons.

Energy Diagram of Sigma Bond Formation by Orbital Overlap

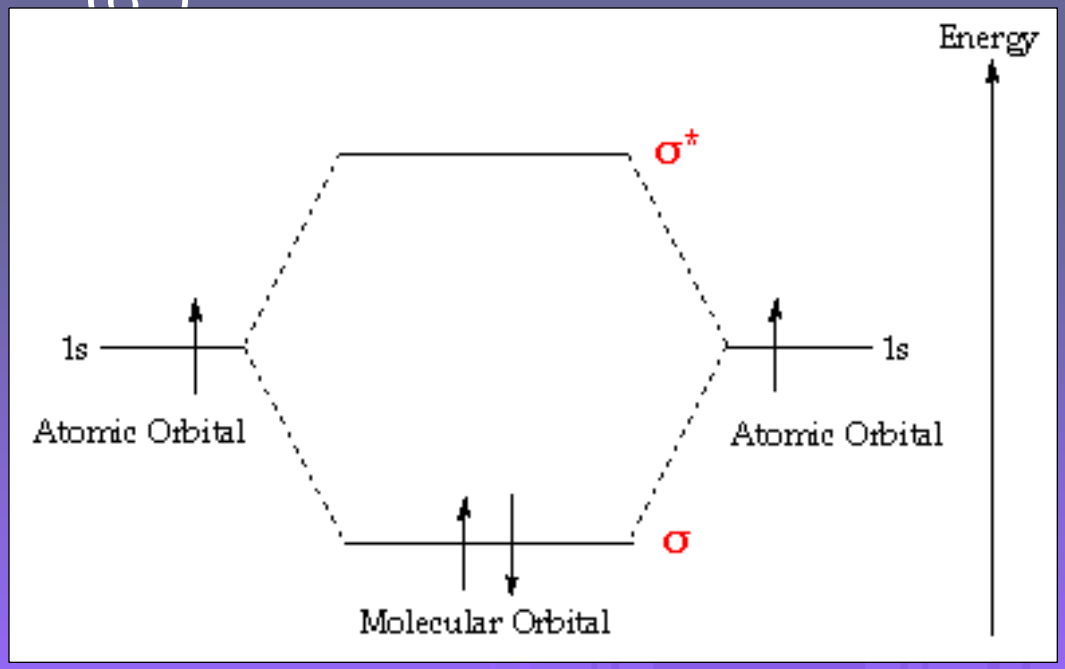


Examples of Sigma Bond Formation



Atomic and Molecular Orbitals

- In atoms, electrons occupy **atomic orbitals**, but in molecules they occupy similar **molecular orbitals** which surround the molecule.
- The two 1s atomic orbitals combine to form two molecular orbitals, one bonding (σ) and one antibonding (σ^*)



http://www.ch.ic.ac.uk/vchemlib/course/mo_theory/main.html

- This is an illustration of molecular orbital diagram of H_2.
- Notice that one electron from each atom is being "shared" to form a covalent bond. This is an example of orbital mixing.

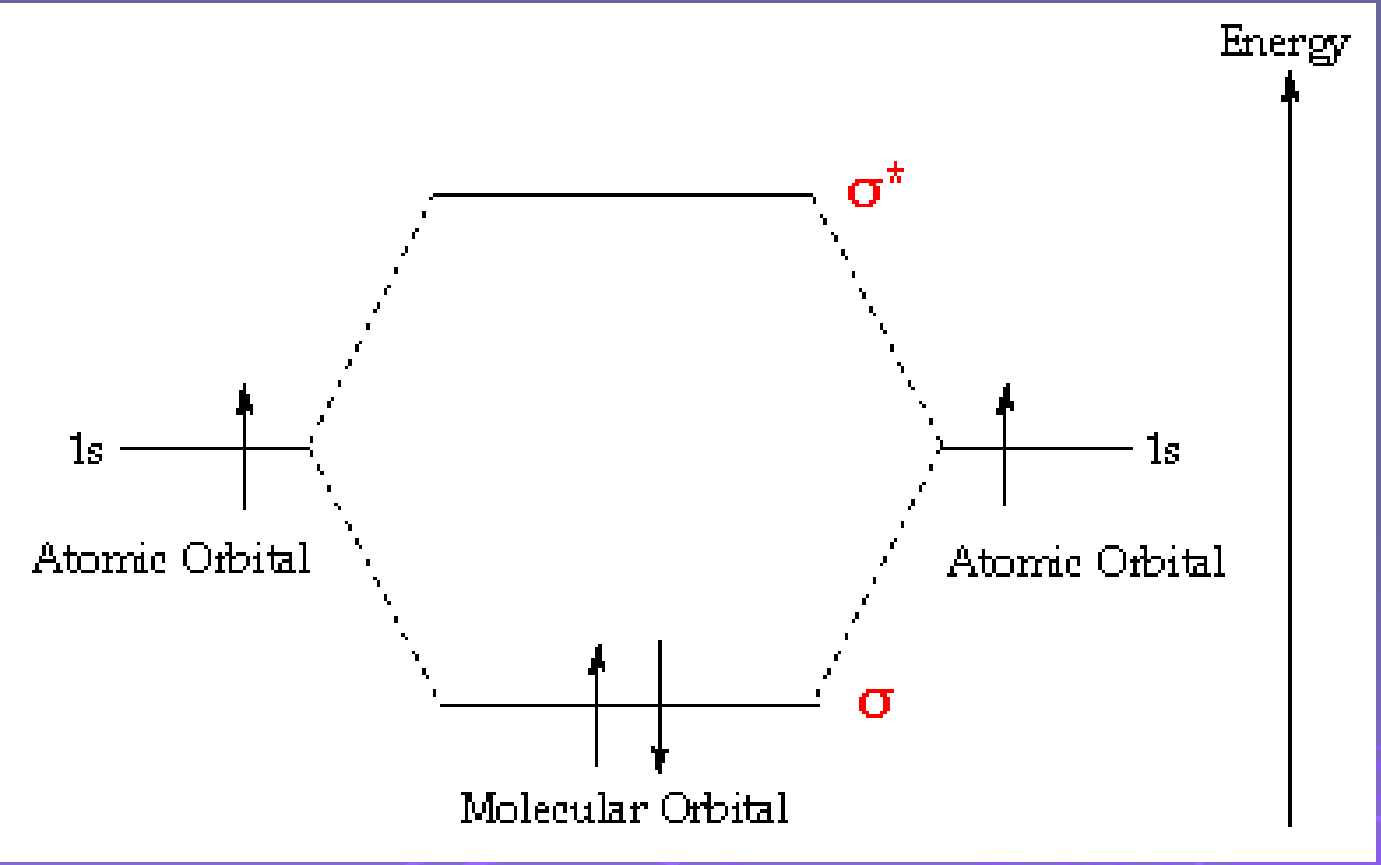
Molecular Orbital Theory

- Each line in the diagram represents an orbital.
- The molecular orbital volume encompasses the whole molecule.
- The electrons fill the molecular orbitals of molecules like electrons fill atomic orbitals in atoms

Molecular Orbital Theory

- Electrons go into the lowest energy orbital available to form lowest potential energy for the molecule.
- The maximum number of electrons in each molecular orbital is two. (Pauli exclusion principle)
- One electron goes into orbitals of equal energy, with parallel spin, before they begin to pair up. (Hund's Rule.)

Molecular Orbital Diagram (H_2)



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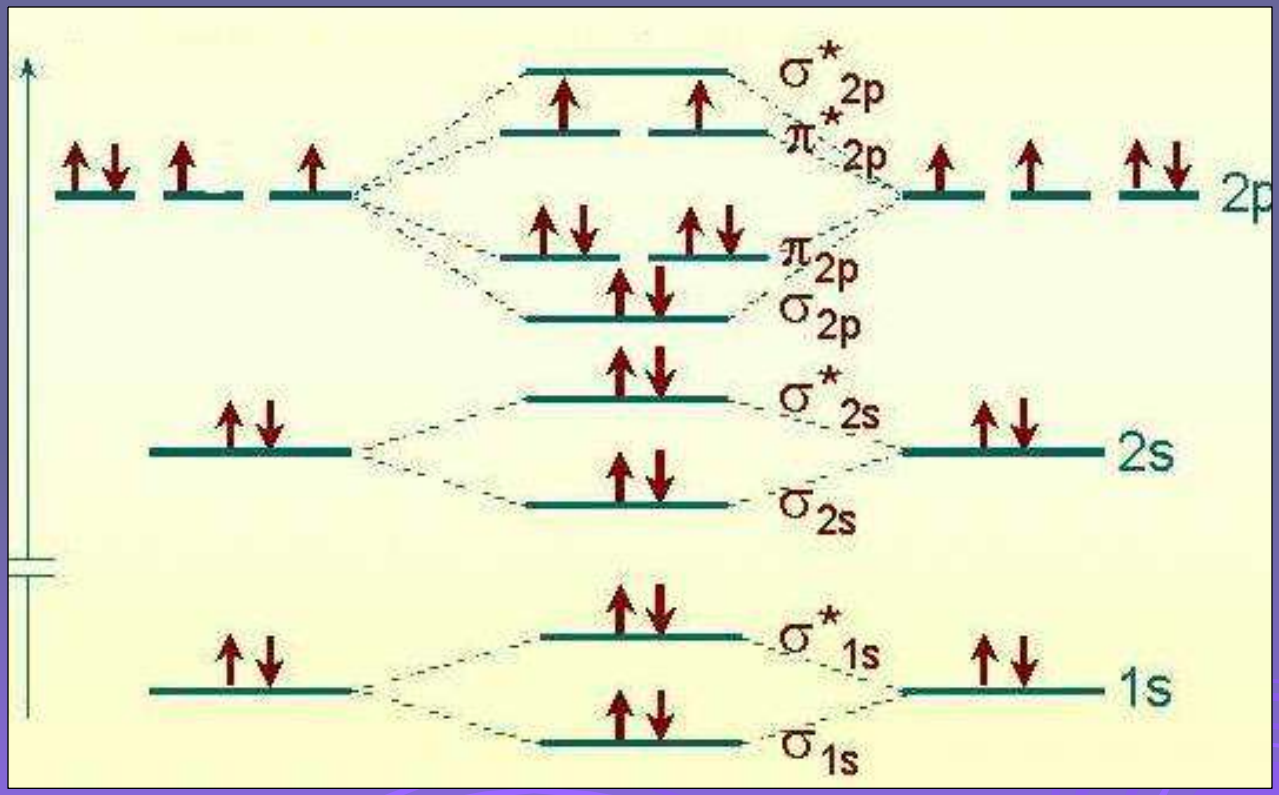
MO Diagram for O_2



http://www.chem.uncc.edu/faculty/murphy/1251/slides/C19b/sld027.htm

Conclusions

- Bonding electrons are localized between atoms (or are lone pairs).
- Atomic orbitals overlap to form bonds.
- Two electrons of opposite spin can occupy the overlapping orbitals.
- Bonding increases the probability of finding electrons in between atoms.
- It is also possible for atoms to form ionic and metallic bonds.