

CHEM 3420: Physical Chemistry II — Spring 2009

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Lecture 20: More on MO's: heteronuclear diatomics

References

1. Levine, *Physical Chemistry*, 19.1–19.5

Key Concepts

- Unpaired electrons lead to paramagnetic behavior, where a substance will be attracted to a magnetic field. This behavior is observed in molecular oxygen (O_2) but not in nitrogen (N_2).
- The bond order is defined as one half the difference between the number of bonding and anti-bonding electrons. The bond order correlates well with the bond length and strength.
- For heteronuclear molecules, the combination of atomic orbitals to make molecular orbitals becomes more complex.
 - Atomic orbitals in each atom have different energies, so atomic orbitals with equal n are not necessarily at equivalent energies. For example, in HF the $1s$ of hydrogen combine with the $2p_z$ of fluorine to create a σ molecular orbital.
 - The more electronegative atom will draw the electrons closer, leading to an increased electron density. This translates into the bonding molecular orbital looking more like the atomic orbital of the more electronegative. The anti-bonding molecular orbital resembles the atomic orbital of the less electronegative atom.
- The geometry of more complex molecules cannot be explained by molecular orbital theory alone.