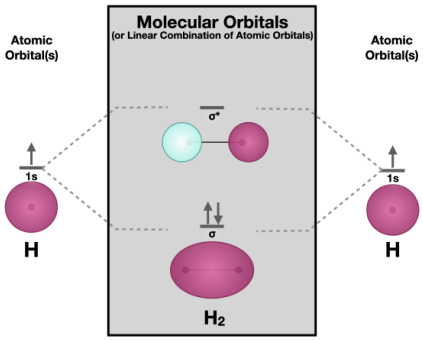
CHAPTER OVERVIEW

Unit 5: Molecular Orbitals

Molecular Orbital Theory



Molecular Orbital (MO) Theory is a sophisticated bonding model. It is generally considered to be more powerful than *Lewis* and *Valence Bond Theories* for predicting molecular properties; however, this power comes at the price of complexity. In its full development, MO Theory requires complex mathematics, though the ideas behind it are simple. Atomic orbitals (AOs) that are localized on individual atoms combine to make molecular orbitals (MOs) that are distributed over the molecule. The simplest example is the molecule dihydrogen (H_2), in which two independent hydrogen 1s orbitals combine to form the σ bonding MO and the σ antibonding MO of the dihydrogen molecule (see figure). The MO's are also called Linear Combinations of Atomic Orbitals (LCAO).

5.1: Valence Bond Theory

5.1.1: The Shapes of Molecules (VSEPR Theory) and Orbital Hybridization

5.2: Linear Combination of Atomic Orbitals

5.2.1: Formation of Molecular Orbitals from Atomic Orbitals

5.2.2: Molecular Orbitals from s Orbitals

5.2.3: Molecular Orbitals from p Orbitals

5.2.4: Molecular orbitals from d orbitals

5.2.5: Nonbonding Orbitals and Other Factors

5.3: Diatomic MO Diagrams

5.3.1: Homonuclear Diatomic Molecules

5.3.1.1: Molecular Orbitals

5.3.1.2: Orbital Mixing

5.3.1.3: Diatomic Molecules of the First and Second Periods

5.3.1.4: Photoelectron Spectroscopy

5.3.2: Heteronuclear Diatomic Molecules

5.3.2.1: Orbital ionization energies

5.3.2.2: Polar bonds

5.3.2.3: Ionic Compounds and Molecular Orbitals

5.4: Polyatomic MO Diagrams

5.4.1: Ligand Group Orbitals and Generator Functions

5.4.2: Polyatomic Molecules

5.4.2.1: Bifluoride anion

5.4.2.2: Carbon Dioxide

5.4.2.3: H_2O

5.4.2.4: NH_3

5.4.3: Why is BeH_2 Linear and H_2O Bent?

5.5: Pi Bonding and Hypervalency

5.5.1: BF_3

5.5.2: Expanded Octets and Molecular Orbitals