CHAPTER OVERVIEW

2: Molecular Orbital Theory

Learning Objectives

- Be able to construct molecular orbital diagrams for homonuclear diatomic, heteronuclear diatomic, homonuclear triatomic, and heteronuclear triatomic molecules.
- Understand and be able to articulate how molecular orbitals form – conceptually, visually, graphically, and (semi)mathematically.
- Interrelate bond order, bond length, and bond strength for diatomic and triatomic molecules, including neutral and ionized forms.
- Use molecular orbital theory to predict molecular geometry for simple triatomic systems
- Rationalize molecular structure for several specific systems in terms of orbital overlap and bonding.
- Understand the origin of aromaticity and anti-aromaticity in molecules with π-bonding.

Valence bond (VB) theory gave us a qualitative picture of chemical bonding, which was useful for predicting the shapes of molecules, bond strengths, etc. It fails to describe some bonding situations accurately because it ignores the wave nature of the electrons. Molecular orbital (MO) theory has the potential to be more quantitative. With it we can also get a picture of where the electrons are in the molecule, as shown in the image at the right. This can help us understand patterns of bonding and reactivity that are otherwise difficult to explain.