SECTION OVERVIEW

7.1: Molecular Orbitals and Band Structure

Learning Objectives

- Explain the physical basis of the Hubbard and Mott models of metal-insulator transitions.
- Understand why good superconductors derive from bad metals.
- Know the structures and the periodic trends in band gaps and colors of semiconductors.
- Obtain the band gap of an intrinsic semiconductor from the temperature dependence of the conductivity.
- Predict the doping type when impurities or defects are introduced into a semiconductor.
- Correlate the band picture and Fermi level with n- or p-type doping.
- Understand the physical principles of operation of diodes, LEDs, solar cells, and FETs.
- Explain the differences in structures and electronic properties of crystalline and amorphous semiconductors.

The band model (like MO theory) is based on a *one-electron* model. This was an approximation we made at the very beginning of our discussion of MO theory: we used hydrogen-like (one-electron) solutions to the Schrödinger equation to give us the shapes of s, p, d, and f atomic orbitals. In a one-electron atom, these orbitals are degenerate within a given shell, and the energy differences between, e.g., 2s and 2p orbitals arise only when we consider the energy of an electron in the field of other electrons in the atom. Moving from atoms to molecules, we made linear combinations to generate one-electron molecular orbitals (and, in solids, one-electron energy bands). But as in multi-electron atoms, life is not so simple for real molecules and solids that contain many electrons. Electrons repel each other, and so their movement in molecules and in solids is ***correlated***.

7.1.1: Prelude to Electronic Properties of Materials - Superconductors and Semiconductors

7.1.2: Metal-Insulator Transitions

7.1.3: Periodic Trends- Metals, Semiconductors, and Insulators

7.1.4: Semiconductors- Band Gaps, Colors, Conductivity and Doping

7.1.5: Semiconductor p-n Junctions

7.1.6: Diodes, LEDs and Solar Cells

7.1.7: Amorphous Semiconductors

7.1.8: Discussion Questions

7.1.9: Problems

7.1.10: References