CHAPTER OVERVIEW

10: Theories of Electronic Molecular Structure

Solving the Schrödinger equation for a molecule first requires specifying the Hamiltonian and then finding the wavefunctions that satisfy the equation. Since the wavefunctions involve the coordinates of all the nuclei and electrons that comprise the molecule, the complete molecular Hamiltonian consists of several terms. The nuclear and electronic kinetic energy operators account for the motion of all of the nuclei and electrons. The Coulomb potential energy terms account for the interactions between the nuclei, the electrons, and the nuclei and electrons.