

Introduction to Quantum Chemistry and Molecular Modeling.

This course is intended to introduce the students to concepts of theoretical chemistry and molecular modeling.

A practical approach will be used guiding the student from the fundamental theoretical background to the practical aspects of the models: definition, analysis and interpretation.

The topics discussed in each section are reinforced with varied exercises, references, and further readings.

The contents of the course is structured as follows:

1. Introduction.
2. The molecular Hamiltonian and the solution of the Schroedinger equation.
 - a.- The Hartree-Fock (HF) approximation. Differential equation.
 - b.- The Roothaan-Hall equations. The algebraic equation.
3. The Born-Oppenheimer approximation. Geometry Optimization.
4. Molecular energy and the potential energy surface.
5. Analysis of the WFN: Molecular properties.
6. Molecular geometry. The concept of molecular structure.

$$\hat{H} \Psi = E \Psi$$

1. INTRODUCTION

The internal structure of atoms and molecules: Quantum Mechanics.