QUÍMICA CUÁNTICA

Resume

This course is developed for post-graduate students who aim to achieve a solid understanding of physical and mathematical aspects of elementary quantum chemistry during their Ph.D. studies. The treated topics are: historical background of quantum mechanics, construction of quantum mechanical operators, extended mathematical developments for solving differential Schrödinger equations of simple quantum mechanical systems, development of approximation methods. Theoretical aspects and applications are treated during the course. The aim of this course is that the students are able to solve non-standards one-particle problems employing advanced mathematic techniques in combination with symbolic algebra packages.

Contents

Historical Background of Quantum Mechanics

- Wave-particle dualism
- Experiments
- Uncertainty principle
- Construction of quantum mechanical operators

The Schrödinger Equation

- The time-dependent Schrödinger equation
- The time-independent Schrödinger equation

Simple Quantum Mechanical Systems

- Particle in a box (one-, two- , three-dimensional case)
- Tunneling effect
- Eigenfunctions and eigenvalues
- Degeneracy of energy levels
- Average values
- Harmonic oscillator
- Vibration of molecules
- Rigid and free rotor
- Hydrogen atom
- The bound-state hydrogen-atom wave functions
- Hydrogenlike orbitals
- Zeeman effect
- Applications to simple quantum mechanical systems

Angular Momentum

- Angular momentum of one-particle systems
- The ladder-operator method for angular momentum

Approximation Methods

- The variation method and its extension
- Perturbation theory (non degenerate and degenerate case)
- Applications of the variational methods

Suggested basic literature

- Quantum Chemistry, Ira N. Levine, Prentice Hall, 2000
- Elementary Quantum Chemistry, Frank L. Pilar, Dover Publications Inc., 2001
- Quantum Chemistry, Donald A. McQuarrie, University Science Books, 1983