Course Specifications

General Information

Course name	
Course number	CHEM3221
Faculty	
Department	
Course type	Major Needs
Course level	3
Credit hours (theoretical)	2
Credit hours (practical)	0
Course Prerequisites	

Course Objectives

1 - Students should be able to: 1. Understand fundamental quantum chemistry principles and problem-solving techniques. 2. Understand how can use Schrodinger equation to solve simple models 3. Develop working knowledge of terminology and tools used by quantum chemists. 4. Learn how quantum mechanics manifests itself in nature and experimental science. 5. Understand advantages and limitations of approximation methods for solving complex problems

2 - The course will be graded on the examinations (three online homework/quizzes/activities/assignments, one med-term examination and one final examination). A score will be assigned on the basis of the results in this examination and the final grade will be made on this basis.

3 - The course will examine the fundamental ideas behind the application of quantum mechanics to chemical systems. Rather than follow an historical approach as is generally done in undergraduate courses, it will treat the ideas of quantum mechanics as a series of postulates that successfully predict experimental results. 1. Introduction to quantum mechanics. Mathematical background, series solutions to differential equations. 2. Description of the postulates of quantum mechanics. 3. “Exact”, i.e. analytical solutions to the Schr?dinger equation for: Particle in a box Potential step Simple harmonic oscillator Spherically symmetric solutions, and hydrogen atom. 4. Use of approximate methods in the solution of the Schr?dinger equation using: Time-independent perturbation theory The variation principle WKB theory. 5. Analysis of angular momentum in quantum mechanics. Commutation and raising and lowering operators Spin angular momentum The addition of angular momentum and the calculation of the resultant eigenfunctions (resulting in the definition of ClebschGordon or Wigner coefficients)

4 - Learning Outcomes: At the end of the course, the student will be able to 1. Describe the concept of energy quantization and wave-particle duality of light and matter 2. Describe the differences between classical and quantum mechanics 3. Construct the Schro?dinger equation for simple systems 4. Normalize a wavefunction and calculate the probability density of a system in a region 5. Construct quantum chemical operators and determine expectation values of observables 6. Describe the solution of the Schro?dinger equation for a free motion in one dimension and confined motion in one and two dimensions and calculate their properties 7. Use the separation of variables technique 8. Describe the solution of the Schro?dinger equation for a harmonic oscillator and calculate it’s properties. 9. Describe the solutions of the Schro?dinger equation for hydrogenic atoms and their properties: quantum numbers, orbital energies, classification in shells

5 - Levine, Ira N. Quantum Chemistry; 6th Edition; Pearson/Prentice Hall

6 - Lectures in class

Course Contents

1	-	ntroduction. Wave Paticle Duality schrodinger equation. ... Simple Applications. Separting Variables and Particle in a Box. ... Tunneling and Harmonic Oscillator. Tunneling -part1. ... The Hydrogen Atom. ... Uncertainty Principle, Angular Momentum. ... Approximation Methods, spin and Pauli\s priinciple. ... Chemical Bonding.