School of Interdisciplinary Engineering and Sciences (SINES)
National University of Sciences & Technology (NUST)

Title : Quantum Chemistry
Code : CSE-884
Credit Hours: 3-0

Description: Particular emphasis in quantum chemistry is placed on the understanding of chemical bonding and reactivity, together with the theoretical basis for optical spectroscopy. The course also provides the fundamental quantum chemical background required in molecular modeling, spectroscopy, inorganic, physical and organic chemistry. In chemical reactions, quantum chemistry studies the ground state of individual atoms and molecules, the excited states, and the transition states that occur during chemical reactions. On the calculations quantum chemical studies use semi-empirical and other methods based on quantum mechanical principles, and deal with time dependent problems.

Objectives: Primary focus of Quantum chemistry is the application of quantum mechanics in physical models and experiments of chemical systems. It involves heavy interplay of experimental and theoretical methods. The goal of the course is to provide students with a fundamental understanding of the quantum chemical description of atoms and molecules.

Outcomes: After finishing the course, the student will be able to -apprehend the Born-Oppenheimer approximation - account for approximation methods such as variational theory and perturbation theory, -to use the basics of quantum mechanics and is able to formulate the implications of quantum mechanics for chemical problems.

Course Contents:

1. Background and introduction of quantum theory
2. Basic postulates and theorems of quantum mechanics.
3. Electronic structure of atoms and molecules, and the theory of atomic and molecular spectra
4. Schrödinger's wave equation
5. Operators
6. Hermitian angular momentum
7. Eigen functions, Eigen values and Eigen value equations.
8. Quantum mechanical treatment of some model systems
9. Particle in three dimensional box, harmonic oscillator, rigid rotator
10. Treatment of many-electron atoms: Pauli's principle, Hund's rule, spin-orbit interaction.
11. The Hartree-Fock method, Variational method, Perturbation theory.
12. Molecular symmetry.

Contents with proposed contact hours

Week	Topics
1	Introduction and background of Classical Mechanics and failure of classical mechanics
2	Advent of Quantum Mechanics, Black body radiation, Spectral interpretation, Heat capacity
3	Basic postulates and theorems of quantum mechanics

4	The electronic structure of atoms and molecules, and the theory of atomic and molecular spectra
5	Schrodinger Wave Equation, Operators, Laplacian operatore, Hermitian Operator, Hamiltonian Operators
6	Hermitian angular momentum, Eigen functions, eigen values and eigen value equations.
7	Quantum mechanical treatment of some model systems
8	Potential Energy Surfaces, Long Range Potentials, Molecular Bonding Potentials, Potential Energy surface calculations using HPC
9	**Midterm**
10	Intermolecular Potentials , *Ab-initio* Calculations of Potential Energy Surfaces, Analytical Potential Energy Functions
11	Intermolecular Potentials , *Ab-initio* Calculations of Potential Energy Surfaces,
12	Analytical Potential Energy Functions
13	Particle in box, harmonic oscillator, rigid rotator Complex scattering Processes
14	Hydrogen like atoms, Atomic and molecular orbital coefficients,
15	Treatment of many-electron atoms: Pauli's principle, Hund's rule, spin-orbit interaction
16	The Hartree-Fock method, Variational method, Perturbation theory.
17	Computational methods based on Chemical Bonding: Valence Bond Theory and molecular orbital Theory, band gap theory,.
18	**ESE**

Text Books/Reference Material:

1. Ira N. Levine "*Quantum Chemistry"* (7th Edition) 2012. Publisher: Prentice Hall, USA.
2. John. P. Lowe (2005) "*Quantum Chemistry"* (Third Edition). Elsevier Academic Press, UK.
3. Donald A. McQuarrie (2017). (2nd Edition), "*Quantum Chemistry".* Publisher: University Science Books. Dulles, Virginia, U.S.A.
4. Hayward, D.O (2002). "*Quantum Mechanics for Chemists"* Royal Society of Chemistry, UK
5. Pavel N. D'yachkov, 2019, Quantum Chemistry of Nanotubes: Electronic Cylindrical Waves 1st Edition

Nature of Assessments:

Homework/ Assignments: 10%
Quizzes: 10%
MSE: 30%
Final Exam: 50%