Approval: 8th Senate Meeting

Course Name: Advanced Quantum Chemistry

Course Number: CY512

Credits: 3-0-0-3

Prerequisites: B.Sc. (with Chemistry) or Teachers Consent

Intended for: UG/PG

Distribution: Core

Semester: Odd/Even

Course Preamble: The main focus of this course is to provide the students with deeper understanding of the quantum properties of molecules. In addition, this course also aims to strengthen the knowledge of the students in some fundamental concepts related to Physical Chemistry, especially how the quantum chemistry could be used to solve structure, chemical bonding and spectroscopic transition of the molecules etc.

Course Outline:

1. **[6 Lectures]**

   Review, Basic concepts and postulates of quantum mechanicsof quantum mechanics: Schrödinger wave equation, Eigenfunction, eigenvalues and operators, Interpretation of wavefunctions.

2. **[6 Lectures]**

   Free particle, Particle-in-a-box, Rigid rotor, Harmonic oscillator, Hydrogen atom.

3. **[10 Lectures]**

   Introduction to Self Consistent Field Theories; Valence Bond and Molecular Orbital theories; Introduction to Molecular spectroscopy: absorption, emission and resonance.

4. **[6 Lectures]**

   Approximate methods of quantum chemistry: variational principle; LCAO approximation; Huckel Theory; Time-independent perturbation theory. Many electron atoms: Orbital approximation, Slater determinant; Hartree-Fockselfconsistent field theory; Slater type orbitals.

5. **[8 Lectures]**

   Angular momentum of many-particle systems. Spin orbital interaction; LS and JJ coupling. Spectroscopic term symbols for atoms. Molecules and Chemical bonding: Born-Oppenheimer approximation, MO and VB theories illustrated with H2-molecule

6. **[6 Lectures]**

   Spectroscopic term symbols for diatomics; Directed valence & hybridization in simple polyatomic molecules. Elementary treatments of scattering and density functional theories

Text Books:

1. Physical Chemistry: A Molecular Approach by Donald A. McQuarrie and John D. Simon, Viva Books, First South Asia Edn. 1998.
2. Physical Chemistry by Peter Atkins and Julio de Paula (Oxford University Press 7thEdn. 2002.

Reference Book:

1. Ira N. Levine, Quantum Chemistry, Prentice-Hall: Englewood Cliffs, NJ, USA (1991).
2. Physical Chemistry By Alberty and Silbey Wiley 4thEdn. 2005.
3. Quantum Chemistry and Spectroscopy by Thomas Engel and Philip Reid Pearson Education 2005.