Course No.	Course Name	L-T-P-Credits
CY 534	**Advanced Quantum Chemistry**	**3-0-0: 03**
Prerequisite: CY 407 (Quantum Chemistry)		

Course Objectives: The main objective of the course is to explain quantum chemistry beyond H atom by explaining many body problems, Quantum mechanics of many electron atom and poly atomic molecules, matrix formulation of quantum chemistry, and different quantum chemistry methods in electronic structure calculation

Course Outcomes: After successful completion of the course, students will be able to:

1. Have a conceptual understanding of the laws of quantum mechanics necessary for the description of atoms and molecules and their chemical reaction.
2. Understand different approaches of solving complex many body problems
3. Have a basic idea of electronic structure calculations methods and appropriate basis set for a molecular system.
4. Choose the appropriate method (in terms of applicability, accuracy, and economy) for the calculation of a given chemical problem
5. Perform, understand, and interpret the results of the calculations and bring them in a publication ready form

SYLLABUS

Module	Contents	Hours
I	**Many-body problem** Pauli exclusion principle, anti-symmetric wavefunction and Slater Determinants, Variation and Perturbation methods, Born-Oppenheimer approximation, Hartree and Hartree-Fock equations, explicit formulation, Roothaan equations and introduction of basis sets STO and GTO, calculation of integrals, semi-empirical methods, Restricted versus unrestricted Hartree-Fock methods.	13
II	**Quantum Chemistry with Matrix Formulation** Transformation, representations, projection operators, equations of motion. Operator formalism: Virial theorem, exactly solvable systems, Tunnelling effect: square barrier, WKB approximation, electron and proton transfer.	11
III	**Electron correlation problem** Electron correlation problem, Configuration interaction (CI) methods, singles and doubles CI, Size-consistency and size-extensivity, N dependence, Many-body methods , perturbation theory (MP-versions), diagrammatic representations and linked cluster theorem, coupled-cluster method. Brief overview of density functional theory.	12

Essential Readings:

1. A. Szabo, N. S. Ostlund, "Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory", Dover, New Edition 1996.
2. I. N. Levine, "Quantum Chemistry", Prentice Hall, 7th Edition, 2016.
3. D. A. McQuarrie, "Quantum Mechanics", Viva Student Edition, 2016.
4. F. L. Pilar, "Elementary Quantum Chemistry", Dover, 2nd Edition, 2011.

Supplementary Readings:

1. F. Jensen, "Introduction to Computational Chemistry", Wiley, 2nd Revised edition, 2007
2. C. J. Cramer, "Essentials of Computational Chemistry: Theories and Models", Wiley, 2nd Edition, 2004.