Course Type	Course Code	Name of Course	L	T	P	Credit
DC	NCYC510	Quantum Chemistry	3	1	0	4

Course Objective
• Background of origin of Quantum Mechanics • Distinctive features of Quantum Mechanics with respect to Classical Mechanics and its application in Chemistry
Learning Outcomes
• Understanding the fundamentals as well to have an insight of the microscopic world (sub-atomic particles, atoms and molecules) • Rationalization of experimentally observed phenomena, which could not be explained by Classical Mechanics • Application to solve atomic and molecular energetics and structure

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	Operator algebra, Wave Particle Duality, Standing waves, Path integrals and Schrödinger equation, Postulates, Separating variables and particle in 1D box, Time dependent states and expectation values, Particle in a 3D box, Finite well, delta and step function, Tunneling, Schrödinger equation for Harmonic Oscillator, Series solution, orthogonality of Eigenfunctions, Theorem of Hermitian operator.	15L+5T	Students will learn fundamental operator algebra and use the same to construct Schrodinger equations for different motions of particles, namely translational, rotational, and vibrational.
2	Hydrogen atom (separating centre of mass, polar coordinates, separation of variables, theta and phi functions, finding R(r)), Atomic orbitals, Hermitian operators, Generalized uncertainty principle, Angular momentum and spin, Spin Statistics Theorem, Boson and Fermion	14L+4T	Students will get the idea of orbital and use that to solve for many electron atoms
3	Perturbation theory, Variation method, He atom and Pauli's principle, Hydrogen molecular ion-Linear variation method, MO and VB theory, MO of diatoms, Hückel theory, Introduction to many electron atoms	13L+5T	Students will learn to utilize their understanding of approximation methods to solve many electron systems.
Total		**42L+14T**	

Text Books:

1. Quantum Chemistry, I. N. Levine. 7th Edition, Pearson, 2014.

Reference Books:

1. Molecular Quantum Mechanics, P. W. Atkins and Ronald S. Friedman, 4th Edition, Oxford University Press, 2010.
2. Quantum Chemistry, R. K. Prasad, 4th Edition, New Age International Publication, 2010.