Semester	JAN 2022
Open to semester	6,8,12,22
Course code	**CH3214/CH6214**
Course title	**Quantum Chemistry**
Credits	4 /4
Course Coordinator & participating faculty (if any)	Arun Venkatnathan
Nature of Course	Lectures
Pre-requisites	First year college level mathematics, in particular multi-variable calculus and applied linear algebra
Objectives (goals, type of students for whom useful, outcome etc)	The objective of this course is to understand the laws governing the behavior of molecules and atoms – the theory of quantum mechanics – and thereby to get a feeling for the fundamental theoretical basis of chemistry. The course starts by discussing the fundamental principles of quantum mechanics with an emphasis on the physical implications of this elegant, yet non-intuitive theory. The quantum mechanical concepts will be applied to study properties of simple model systems and the hydrogen atom. The theories of quantum mechanics to describe multi-electron systems will also be discussed. Finally, the course will briefly examine one of the most quintessential concepts of chemistry: the chemical bond. The ideas discussed in this course will be useful to those who wish to pursue further study in the areas of theoretical and computational chemistry, spectroscopy, biochemistry and materials science.
Course contents (details of topics /sections with no. of lectures for each)	1. Principles of Quantum Mechanics A. Postulates of Quantum mechanics B. Theorems of quantum mechanical operators and eigen-functions 2. Translational Motion A. Particle in a 1-D box: Interpretation from wavefunctions. Application to simple chemical system. B. Particle in 2-D and 3-D systems.

	3. Vibrational Motion A. Reduction of a 2 Body problem to a 1 body problem B. Ladder operator approach to Quantum Harmonic Oscillator C. Quantum Harmonic Oscillator: Interpretation of Wave-functions D. Calculation of Vibrational Frequencies, Zero Point Energies and Force constants of molecules. 4. Rotational Motion A. Particle in a ring: Concept of Angular momentum B. Solutions to Generalized angular momentum: A ladder operator approach C. Particle in a Sphere: Rigid Rotor D. Angular Momentum of Rigid Rotor, Spherical Harmonic Wave-functions and Rotational Constants of molecules. 5. Hydrogen Atom A. Hamiltonian of Hydrogen atom B. Interpretation of wave-functions, Orbital shapes and Probability distribution functions. 6. Approximate Methods A. Hamiltonian For Atoms and Molecules B. Time independent Perturbation theory with examples. C. Variational method with examples. 7. Many Electron Systems A. Spin angular momentum B. Spin-Statistics Theorem and Anti-symmetric wave-functions. C. Slater determinants: Multi-electron Wave-functions with examples. D. Born-Oppenheimer approximation 8. Chemical Bonding A. Valence bond theory – Application to H2 B. Molecular orbital theory - Application to H2
Evaluation /assessment	End-Sem Examination-40% Mid-Sem Examination-30% Others-Quizzes - 30 %%

Suggested readings (with full list of authors, publisher, year, edn etc.)	1. Quantum Chemistry by Donald A. McQuarrie 2. Quantum Chemistry by Ira N. Levine