1.	Title of the course	Quantum Chemistry and Chemical Bonding
2.	Course number	CY501L
3.	Structure of credits	3-0-0-3
4.	Offered to	PG
5.	New course/modification to	Modification To CY5101/10
6.	To be offered by	Department of Chemistry
7.	To take effect from	July 2022
8.	Prerequisite	Nil
9.	**Course Objective(s):** To provide requisite foundations in quantum mechanics and its applications in diverse fields in chemistry and materials science, in particularly at understanding bonding in molecules and solids.	
10.	**Course Content:** Uncertainty Principle; Postulates of quantum mechanics; Schrödinger equation: free particle, particle on ring and in box, harmonic oscillator, hydrogen-like atoms, orbitals, angular momentum, electron spin; Wave functions of many-electron atoms: Slater determinant, Pauli exclusion principle, spin-orbit interaction, fine structure, spectral terms; Variational method and its applications; Time-Independent and time-Dependent Perturbation Theory: Stark and Zeeman Spectroscopies and Radiative Phenomena, Fermi's Golden-Rule; Born-Oppenheimer approximation: H2+ and H2 molecules, homo- and hetero-nuclear molecules, correlation diagrams; Valence bond theory and molecular orbital theory, MO diagrams of few molecules; Bonding in pi-electron systems, Hückel treatment for conjugated hydrocarbons, electron densities, bond-order and bonding in solids.	
11.	**Textbook(s):** 1. Atkins P W and de Paula J, *Atkin's Physical Chemistry*, Oxford University Press (2010). 2. Levine I N, *Quantum Chemistry*, Prentice Hall (2016).	
12.	**Reference(s):** 1. Atkins P W and Friedman R S, *Molecular Quantum Mechanics*, Oxford University Press (2010). 2. Griffiths J D and Schroeter D F, *Introduction to Quantum Mechanics*, Cambridge University Press (2018). 3. McQuarrie D A and Simon J D, *Physical Chemistry: A Molecular Approach*, University Science Books (1997). 4. Zettili N, *Quantum Mechanics: Concepts and Applications*, Wiley (2009).	