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| 1.  | Title of the Course   | Quantum Chemistry and Chemical Bonding |
| 2.  | Course Number   | CY5101                                 |
| 3.  | Status of the Course  | Core                                   |
| 4.  | Structure of Credits  | 3-0-0-3                                |
| 5.  | Offered To  | PG                                     |
| 6.  | New Course/Modification to  | New                                    |
| 7.  | To be Offered by  | Department of Chemistry                |
| 8.  | To take effect from   | July 2020                              |
| 9.  | Prerequisite  | Nil                                    |
| 10. | Whether approved by the Department  | Yes                                    |
| 11. | <b>Course Objective:</b> 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.   |  |
| 12. | <b>Course Content:</b> 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: H <sub>2</sub> <sup>+</sup> and H <sub>2</sub> 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. |  |
| 13. | <b>Text book(s):</b><br>1. Atkins P W and de Paula J, <i>Atkin's Physical Chemistry</i> , Oxford University Press (2010).<br>2. Levine I N, <i>Quantum Chemistry</i> , Prentice Hall (2016).  |  |
| 14. | <b>Reference(s):</b><br>1. Atkins P W and Friedman R S, <i>Molecular Quantum Mechanics</i> , Oxford University Press (2010).<br>2. Griffiths J D and Schroeter D F, <i>Introduction to Quantum Mechanics</i> , Cambridge University Press (2018).<br>3. McQuarrie D A and Simon J D, <i>Physical Chemistry: A Molecular Approach</i> , University Science Books (1997).<br>4. Zettili N, <i>Quantum Mechanics: Concepts and Applications</i> , Wiley (2009).  |  |