| CHEM2042 | PHYSICAL CHEMISTRY-II | L | T | P | S | J | C |
|---|---|---|---|---|---|---|---|
| | | 3 | 0 | 0 | 0 | 0 | 3 |
| Pre-requisite | None | | | | | | |
| Co-requisite | None | | | | | | |
| Preferable Exposure | None | | | | | | |

**Course Description:**

Quantum Chemistry deals with the behavior of matter at atomic and sub-atomic dimensions with particular emphasis on the electronic structure that profoundly influences the feasibility and progress of any chemical reaction. Group theory is concerned with symmetry present in molecules and how symmetry enables the prediction of molecular properties.

**Course Educational Objectives:**

- To introduce the concept of wave-particle duality, fundamental axioms of quantum theory and significance of Schrodinger wave equation.
- To illustrate applications of Schrodinger equation to simple model systems and establish their connection to realistic atomic and molecular systems.
- To demonstrate ideas underlying various approximation methods in dealing with multielectron systems and necessity of making such approximations
- To provide a quantum mechanical perspective of chemical bonding through using various modern theories like Valence Bond Theory and Molecular Orbital Theory
- To introduce molecular symmetry and group theory and provide insights into its applications in chemical problems.

**MODULE 1 INTRODUCTION AND POSTULATES OF QUANTUM MECHANICS 9 Hrs**

Introduction to quantum mechanics, Wave-particle duality and Uncertainty principle, Postulates of quantum mechanics, setting up of operators, observables.
Operator algebra -linear and non-linear operators. Properties of Hermitian operators. Eigenvalue problem. Commutators

**MODULE 2 APPLICATIONS OF QUANTUM MECHANICS 9 Hrs**

Elementary applications of quantum mechanics- unbound motion in one dimension. Tunneling. Bound motion – particle-in-a-box (1D & 3D), Harmonic oscillator and rigid rotor. Selection rules, Angular momentum algebra, Hydrogen atom.
Methods of obtaining approximate solution to the time-independent Schrödinger equation –perturbation theory and variational method.

**MODULE 3 ELECTRONIC STRUCTURE THEORY 9 Hrs**

Many electron atoms, Spin and Pauli exclusion principle, Hund’s rule, Slater determinants, atomic term symbol
The Born-Oppenheimer approximation. Electronic structure theory: MO and VB theories, Applications to H2+ and H2 , H■ckel pi-electron theory.

**MODULE 4 SYMMETRY ELEMENTS AND GROUP THEORY 9 Hrs**

Symmetry elements and operations; Axioms of group theory, matrix representation of symmetry operations; properties of groups and point groups; reducible and irreducible representations, Great Orthogonality Theorem

**MODULE 5 APPLICATION OF SYMMETRY** **9 Hrs**

Construction of character tables; Direct product representations; projection operators and symmetry-adapted linear combinations.

**Texbook(s):**

1. D. A. McQuarrie, Quantum Chemistry, University Science Books,
2. I. N. Levine, Quantum Chemistry. , PHI Learning Private Ltd.,
3. H. Eyring, J. Walter and G. E. Kimball, Quantum Chemistry, John Wiley & Sons.,
4. F. A. Cotton, Chemical Applications of Group Theory., John Wiley & Sons, Inc.,

**Reference(s):**

**Course Outcomes:**

1. Understand the necessity of axioms and wave equation in describing electrons
2. Acquaintance with methodologies for solving Schrodinger equation for simple systems
3. Insights into various approximation methods and necessity of approximations in problem solving
4. Understanding the molecular symmetry and the necessity of the axioms of group theory
5. Insights into the symmetry arguments in solving chemical problems

**Course Articulation Matrix:**

| | POs | | | | | | | | | | | | | | | | PSOs | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **CO** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** | **11** | **12** | **13** | **14** | **15** | **16** | **1** | **2** | **3** | **4** |
| **1** | 2 | 2 | 1 | | 2 | 1 | | | 1 | | | | | | | | 3 | | 2 | |
| **2** | 3 | 3 | 2 | | 3 | 1 | | | 1 | | | | | | | | 2 | | 1 | |
| **3** | 3 | 3 | 2 | | 2 | 2 | | | 1 | | | | | | | | 3 | | 2 | |
| **4** | 2 | 2 | 1 | | 2 | 1 | | | 1 | | | | | | | | 3 | | 2 | |
| **5** | 3 | 3 | 2 | | 2 | 2 | | | 1 | | | | | | | | 3 | | 2 | |

3 – High, 2 – Medium & 1 – Low Correlation

**APPROVED IN MEETINGS HELD ON:**

BOS : 26-06-2023 Academic Council Number: 27 Academic Council : 06-07-2023

**SDG No(s). & Statement(s) :**

9 & Industry, Innovation and Infrastructure : Build resilient infrastructure, promote inclusive and sustainable industrialization and foster innovation.

**SDG Justification(s):**

The acquired knowledge about quantum chemistry and group theory will be helpful to understand molecular properties, reaction pathways and designing new materials for innovation and industry purpose.