Teaching Plan (2024-2025)
B.Sc. (H) Chemistry Semester III and V
(01-Aug-24 to 27-Nov-24)
Dr. Radhika Gupta
Department of Chemistry, Shyam Lal College

Dates	Topics To Be Covered	
	B.Sc. (H) Chemistry Semester III DSE-1 Inorganic Materials of Industrial Importance	**B.Sc. (H) Chemistry Semester V DSC-15 Quantum Chemistry and Chemical Bonding**
01-Aug-24 to 10-Aug-24	**Unit 4:** Primary Batteries	**Unit 1:** Introduction to quantum chemistry. Postulates of quantum mechanics
12-Aug-24 to 17-Aug-24	**Unit 4:** Primary and secondary batteries, characteristics of an Ideal Battery	**Unit 1:** Postulates of quantum mechanics, Schrödinger equation and its application to free particle and particle in a box rigorous treatment)
19-Aug-24 to 24-Aug-24	**Unit 4:** Pb- acid battery	**Unit 1:** Quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle, Extension to two and three-dimensional boxes, separation of variables, degeneracy
26-Aug-24 to 31-Aug-24	**Unit 4:** Li-metal batteries, Li-ion batteries, Li-polymer batteries	**Unit 1:** Wave functions, probability distribution functions, nodal properties, Quantum mechanical operators and commutation rules
02-Sep-24 to 07-Sep-24		**Unit 1:** Qualitative treatment of simple harmonic oscillator model of vibrational motion:
09-Sep-24 to 14-Sep-24	**Unit 4:** Solid state electrolyte batteries, fuel cells	**Unit 1:** Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy.
16-Sep-24 to 21-Sep-24		**Unit 1:** Angular momentum. Rigid rotator model of rotation of diatomic molecule. Schrödinger equation in Cartesian and spherical polar coordinates
23-Sep-24 to 05-Oct-24	**Unit 4:** Solar cells and polymer cells	**Unit 1:** Separation of variables. Spherical harmonics. Discussion of solution (Qualitative)
07-Oct-24 to 12-Oct-24	**INTERNAL ASSESSMENT TEST-1**	**Unit 2:** Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar

		coordinates, radial part and quantization of energy **INTERNAL ASSESSMENT TEST-1**
14-Oct-24 to 19-Oct-24	**Unit 5:** Introduction to zero, one and two-dimensional nanomaterial	**Unit 2:** Average and most probable distances of electron from nucleus. Zeeman effect, Introduction of spin quantum number and magnetic spin quantum number
21-Oct-24 to 26-Oct-24	**Unit 5:** Synthesis, properties and applications of fullerenes	**Unit 2:** Setting up of Schrödinger equation for many electron atoms (He, Li), Indistinguishability of electrons and Pauli exclusion principle, Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).
27-Oct-24 to 03-Nov-24	**MID SEMESTER BREAK**	
04-Nov-24 to 09-Nov-24	**INTERNAL ASSESSMENT TEST-2**	**Unit 3:** Setting up of Schrödinger equation, Born-Openheimer approximation, LCAO-MO treatment of H_2^+ and its qualitative extension to H_2 **INTERNAL ASSESSMENT TEST-2**
11-Nov-24 to 16-Nov-24	**Unit 5:** Synthesis, properties and applications of carbon nanotubes, carbon fibres	**Unit 3:** Valence bond (VB) treatment of H_2, Comparison of LCAO-MO and VB wave functions of H_2 and their refinements
18-Nov-24 to 27-Nov-24	**Unit 5:** Synthesis, properties and applications of semiconducting and superconducting oxides.	**Unit 3:** Qualitative description of LCAO-MO of homonuclear and heteronuclear diatomic molecules-HF and LiH

SYLLABUS

B.Sc. (H) Chemistry Semester III

DSE-1 Inorganic Materials of Industrial Importance

DISCIPLINE SPECIFIC ELECTIVE COURSE - 2 (DSE-2): Inorganic materials of industrial importance

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Inorganic Materials of Industrial Importance (DSE-2)	**04**	**03**	**0**	**01**	Passed Class 12th with Physics, Chemistry	**NIL**

Unit 4: Batteries (9 Hours)

Primary and secondary batteries, characteristics of an Ideal Battery, principle, working, applications and comparison of the following batteries: Pb- acid battery, Li-metal batteries, Li-ion batteries, Li-polymer batteries, solid state electrolyte batteries, fuel cells, solar cells and polymer cells.

Unit 5: Nano dimensional materials (6 Hours)

Introduction to zero, one and two-dimensional nanomaterial: Synthesis, properties and applications of fullerenes, carbon nanotubes, carbon fibres, semiconducting and superconducting oxides.

B.Sc. (H) Chemistry Semester V

DSC-15 Quantum Chemistry and Chemical Bonding

DISCIPLINE SPECIFIC CORE COURSE-15 (DSC-15): Quantum Chemistry and Organic Chemistry IV Covalent bonding

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Quantum Chemistry and Covalent bonding (DSC-15, Physical Chemistry V)	**04**	**03**	**--**	**01**	**Class 12th with Physics, Chemistry, Mathematics**	

SYLLABUS OF DSC-15

Unit-1: Quantum Chemistry **(Hours: 22)**

Postulates of quantum mechanics, quantum mechanical operators and commutation rules, Schrödinger equation and its application to free particle and particle in a box rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wave functions, probability distribution functions, nodal properties, Extension to two and three- dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum. Rigid rotator model of rotation of diatomic molecule. Schrödinger equation in Cartesian and spherical polar coordinates (derivation not required). Separation of variables. Spherical harmonics. Discussion of solution (Qualitative).

Unit-2: Hydrogen atom **(Hours: 08)**

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part and quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Zeeman effect, Introduction of spin quantum number and magnetic spin quantum number Setting up of Schrödinger equation for many electron atoms (He, Li), Indistinguishability of electrons and Pauli exclusion principle, Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

Unit-3: Covalent bonding **(Hours: 15)**

Setting up of Schrödinger equation, Born-Openheimer approximation, LCAO-MO treatment of H_2^+ and its qualitative extension to H_2, Valence bond (VB) treatment of H_2, Comparison of LCAO-MO and VB wave functions of H_2 and their refinements, Qualitative description of LCAO-MO of homonuclear and heteronuclear diatomic molecules-HF and LiH.