Semester	**4**
Programme	**CHEMISTRY**
Course	**SKILL ENHANCEMENT (INORGANIC CHEMISTRY 4)**
Paper Code	**S2CH230421P**
Credits	**4 (PRACTICAL: 4)**
Hours/week	**4 (PRACTICAL: 4)**
Category: Core/MDC/SEC/VEC	**SEC**
Theory/Practical/Composite	**PRACTICAL**
Number of Modules	**2**
Syllabus	1. Quantum mechanical calculations a. Ab initio methods –I (Hartree Fock) b. Ab initio methods - II (Post Hartree Fock) c. Density functional methods d. Softwares for quantum mechanical calculations e. Different forms of inputs for Ab initio calculations f. Computation of single point energies g. Geometry optimization h. Electron densities and electrostatic potentials i. Analysis of output for a quantum chemistry programme j. Molecular frequencies k. H_2, HCl, CH_4 structure optimization, $PES\ of\ H_2$, IR of CO_2 2. Introduction to Molecular Dynamics a. Molecular Dynamics Basics b. Introduction to GROMACS c. Simple calculations on Argon, water etc 3. Introduction to Chromatography
Course Overview	Practical: 1. Students are introduced to Molecular Dynamics 2. Students are introduced to Electronic Structure Theory Calculations using Quantum Chemistry Software 3. Students are introduced to Chromatographic techniques'
Course Outcomes	Upon successful completion of this course, students will be able to: **CO1**: Differentiate between various quantum mechanical calculation methods, including Hartree-Fock, Post-Hartree-Fock, and Density Functional Theory (DFT). **CO2**: Prepare input files for quantum chemistry software and perform geometry optimizations and single-point energy calculations for simple molecules. **CO3**: Analyze computational outputs to interpret molecular properties such as electron densities, electrostatic potentials, and vibrational frequencies (IR). **CO4**: Execute basic Molecular Dynamics simulations using GROMACS, including system setup and analysis for simple atomic and molecular fluids. **CO5**: Apply the principles of Potential Energy Surfaces (PES) and molecular modeling to understand chemical bonding and structural

	stability. **CO6**: Describe the fundamental principles of chromatographic separation techniques and explain their general relevance to chemical analysis.
Program Outcomes	**PO1**: Fundamental Knowledge: Demonstrate a comprehensive understanding of core concepts in chemistry, including organic, inorganic, physical, analytical, and biochemistry. **PO2**: Laboratory Skills: Acquire hands-on experience in laboratory techniques and instrumentation, applying safety protocols and proper methodologies to conduct experiments and analyse results. **PO3**: Problem Solving: Develop critical thinking and problem-solving skills by applying chemical principles to real-world scenarios, including the ability to design experiments and interpret data. **PO4**: Research Competency: Engage in independent and collaborative research projects, employing scientific methods to formulate hypotheses, conduct experiments, and communicate findings effectively. **PO5**: Interdisciplinary Applications: Understand the interdisciplinary nature of chemistry, exploring its applications in fields such as medicine, environmental science, materials science, and nanotechnology. **PO6**: Communication Skills: Effectively communicate scientific information, both verbally and in written form, to diverse audiences, demonstrating the ability to present complex ideas clearly and concisely. **PO7**: Ethics and Sustainability: Recognize the ethical implications and responsibilities of scientific research and practice in chemistry, emphasizing the importance of sustainability and environmental stewardship in chemical practices.

CO #	Course Outcome Summary	Bloom's Taxonomy (K-Level)	Mapped POs
CO1	Quantum Calculation Methods	**K4 (Analyze)**	PO1, PO3
CO2	Software Operation & Optimization	**K3 (Apply)**	PO2, PO4
CO3	Output Analysis (Frequencies/Densities)	**K4 (Analyze)**	PO2, PO3
CO4	Molecular Dynamics Simulations	**K3 (Apply), K4 (Analyze)**	PO2, PO5
CO5	PES & Structural Stability	**K3 (Apply), K4 (Analyze)**	PO1, PO3
CO6	Introduction to Chromatography	**K2 (Understand)**	PO1, PO5

Reading/Reference Lists	1. Molecular Modelling: Principles and Applications, by Andrew Leach 2. Understanding Molecular Simulation: From Algorithms to Applications, Frenkel & Smit 3. Griebel, Knapek, Zumbusch - Numerical Simulation in Molecular Dynamics: Numerics, Algorithms, Parallelization, Applications 4. Tuckerman - Statistical Mechanics: Theory and Molecular Simulation 5. Applications of DFT on Molecular Systems: How Gaussian Works, Ambrish Kumar Srivastava * and Neeraj Misra	
Evaluation	Practical: 100 CA: 95; Attendance: 5	
Paper Structure for Theory Semester Exam		