Semester	**4**
Course	**Skill Enhancement**
Paper Code	S2CH230421P
Paper Title	Inorganic Chemistry 4
No. of Credits	Practical: 4
Theory / Practical / Composite	Practical
Minimum No. of preparatory hours per week a student has to devote	4
Number of Modules	
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

Learning Outcomes	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'	
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		