Course Type	Course Code	Name of Course	L	T	P	Credit
DE	NCYD506	Computational Chemistry	3	0	0	3

Course Objective

- The course is aimed at developing elementary programming skills in C++ to enable them write short programs for performing scientific calculations. Introducing the basics of theoretical and numerical methods for computer simulation of model systems. Introducing various simulation techniques using standard softwares based on time and length scales of various phenomena.

Learning Outcomes

- At the end of the course, the learners should be able to:
- Write short simple programs in C++ and be able to compile and execute them in a host of machines. Using TeraChem software the students should be able to do basic electronic structure calculations. Use standard software tools such as NAMD, AMBER to perform molecular dynamics simulation of various phenomena. The student should be also able to interpret the simulated data (with its limitations) and correlate with experimental observations.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	Programming languages (C++) : C++ basics, loop and decision making, functions, classes and objects, pointer and references, overloading and type conversions; inheritance and polymorphism;	10L	Brief introduction of programming languages, learning how to write C++ programs to help perform and understand quantum chemical and molecular mechanics calculations.
2	Review of postulates of quantum chemistry, The Born-Oppenheimer approximation, variational method and principle, Hartree-Fock method, restricted and unrestricted references, selfconsistent- field (SCF) procedure, Geometry optimization, basis set, semiempirical methods, geometry optimization, vibrational frequency analysis, Density-functional theory.	8L	Discussion on various methods and algorithms to solve Schrodinger equations and how to perform quantum chemical calculations for small model systems
3	Molecular Mechanics / Force Field Methods: Introduction to molecular mechanics; review of basic Concepts; comparison of popular force fields; performance of molecular mechanics, Lagrangian, Hamiltonian, and Newtonian equations of motions, integration algorithms, Periodic boundary conditions, force calculations, methods for long range interactions calculation.	12L	In-depth understanding of the nature of molecular interactions and force calculation. Discussion of various algorithms involved in performing different types of molecular mechanics calculations.

4	Modelling of macromolecules: all atom and ab-initio molecular dynamics, Coarse-Graining and Multiscale Simulations for Nanoscale Systems, Quantum mechanics/molecular mechanics (QM/MM) approaches, study of self-organized assemblies, biomolecules like peptides, proteins, membranes and ion channels. Dynamical and structural studies of molecules using molecular dynamics simulations.	12L	A comprehensive discussion about different types of molecular dynamics methods. Hand-on experience in molecular mechanics simulations and data analysis of bio-molecules/polymer/nanosystems using various open-source softwares.
Total		**42**	

Text Books:

1. Programming: Principles and Practice Using C++, B. Stroustroup, Addison Wesley, 2014.
2. Understanding Molecular Simulations: From Algorithms to Applications, D. Frenkel and B. Smit, Academic Press, 2002.
3. Molecular Modelling:Principles and Applications, Andrew R. Leach, 2nd Edition, Pearson, 2001.

Reference Books:

1. Introduction to Computational Chemistry, F. Jensen, Wiley Publishers, 2007.Let Us C++, Y. P. Kanetkar, BPB Publications, 2003.
2. Introduction to Computational Chemistry, Frank Jensen, 3rd Edition, Wiley, 2017
3. Essentials of Computational Chemistry: Theories and Models, Christopher J. Cramer, 2nd Edition, Wiley, 2004.