Course code: CHY 1005	Introduction to Computational Chemistry	Course Type	LTP
		Credits	4
Pre-requisite	Chemistry of 12th standard or equivalent		

Course Objectives:

- To know the fundamental principles of Computational Chemistry required to solve engineering problems.
- Practical implementation of fundamental theory concepts.
- To enable the students to understand the role of computers in chemistry.
- To study the applications of chemistry in various engineering and technological process.

Expected Course Outcome:

CO1: Utilize computers to understand the role of computer simulations to understand and solve basic problems in chemistry.

CO2: Use the computational tools and methodology to represent chemical systems.

CO3: Use computational and theoretical chemistry concepts to understand chemistry behind every day and industrial processes.

CO4: Develop the basics understanding of scientific simulation and modeling.

Unit	Contents	Lect.	CO
1	**Introduction** Overview of the course, history and promises of computational chemistry, tools for computational chemistry, units, errors in computed quantities	2	1
2	**Quantum Chemistry** Historical development, Bohr's atomic model, de Broglie wavelength, Heisenberg uncertainty principle, Schrodinger equation, Wave function, particle in a box, Hydrogen atom, radial and angular solution to hydrogen atom, applications and limitations	9	1, 2
3	**Thermodynamics** Intensive and extensive variables, state and path functions, Laws of Thermodynamics (First law and enthalpy; second law and entropy, spontaneity, and equilibrium; third law and absolute entropy) free energy, Gibbs and Maxwell's relations, Ideal and real gases	8	2
4	**Potential Energy Surfaces** Chemical bonds and intermolecular interactions, Types of intermolecular interactions (charge distribution of isolated molecules, electrostatic interaction, induction interaction, London or dispersion forces, hydrogen bonding, repulsive interaction, relative contribution of different terms), representing the potential energy surfaces (pair additivity, rare gas),	9	1, 2, 3

	intramolecular interactions (bond stretching, angle bending, torsional and improper terms)		
5	**Molecular Dynamics** Introduction to ensembles, force fields, integration of Newton's laws of motion, force calculation, energy minimization, periodic boundary conditions, choice of input configuration, velocities, and time-step, applications, and calculation of simple thermodynamic variables.	10	1, 2, 3, 4
6	**Guest lectures**	2	1, 3
	Total Lectures:	**40**	
	Hands-on Sessions:		
1.	Molecular visualization in Gaussview		
2.	Energy minimization of diatomic molecules using Avogadro		
3.	Generation and visualization of molecular orbitals in Avogadro		
4.	Geometry optimization of polyatomic molecules		
5.	Conformational search using potential energy surface		
6.	Conformational search using WebMO		
7.	Molecular modeling of Ar gas		
8.	Visualization of large systems in VMD		
9.	Short MD simulations using QwikMd in VMD		
10.	Calculation of structural and thermodynamic properties from MD simulations		

Text Book(s)	
1.	*Atkins' Physical Chemistry*, Peter Atkins and Julio De Paula, Oxford University Press, 2011.
2.	"Molecular Modelling: Principles and Applications" A. Leach
3.	"Understanding Molecular Simulation: From Algorithms to Applications" Berend Smit and Daan Frenkel

Recommendation by the Board of Studies on	**17.10.2020**
Approval by Academic council on:	
Compiled by:	Dr. Madhulika Gupta; Dr. Saurav Prasad; Dr. Sumit Mittal