Gyanmanjari Innovative University

Syllabus
Gyanmanjari Science College
Semester-7 (B.Sc)

Subject: Computational Chemistry-BSCCM17401

Type of course: Major

Prerequisite: Students should have basic knowledge of physical chemistry, including thermodynamics, chemical bonding, and reaction mechanisms. Understanding of basic mathematics (algebra) and physics concepts like electrostatics is required. Familiarity with basic computer operations is also helpful.

Rationale: Computational chemistry helps in studying molecular structure, energy, and reactions using computer-based methods. It saves time and resources compared to experiments and is widely used in drug design, material science, and research. This subject develops skills to analyze complex chemical systems using modern computational techniques.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks					Total Marks
				SEE		CCE			
CI	T	P	C	Theory	Practical	MSE	LWA/V	ALA	
3	0	2	4	75	25	30	20	50	200

Legends: CI-Class Room Instructions; T – Tutorial; P - Practical; C – Credit; SEE - Semester End Evaluation; MSE- Mid Semester Examination; LWA - Lab Work Assessment; V – Viva voce; CCE-Continuous and Comprehensive Evaluation; ALA- Active Learning Activities.

3 Credits * 25 Marks = 75 Marks (each credit carries 25 Marks) Theory
1 Credits * 25 Marks = 25 Marks (each credit carries 25 Marks) Practical
SEE 100 Marks will be converted in to 50 Marks
CCE 100 Marks will be converted in to 50 Marks
It is compulsory to pass in each individual component.

GYANMANJARI INNOVATIVE UNIVERSITY BHAVNAGAR

Course Content:

Unit No	Course Content	Hrs	% Weightage
1	**Introduction to Computational Chemistry** Introduction,Models vs Real System & Approximations , Fundamental Principles,Energy & Stability of Molecules ,Electrostatics ,Atomic . Units ,Thermodynamics (Enthalpy, Entropy, Gibbs Free Energy) ,Basic Quantum Mechanics ,Statistical Mechanics	11	2%
2	**Molecular Modeling and Geometry Optimization** Predicting Molecular Geometry, Specifying Molecular Geometry, Building the Geometry, Coordinate Space for Optimization.Introduction of population analysis, Mulliken population analysis, electrostatic charges and its benefits, charges from structure only, methods and examples.	11	25%
3	**Molecular Properties and Analysis** Zero-point energies and thermodynamics corrections, Other Chemical Properties(base parameter for computing properties:From energy and geometry,electron density with QSPR technique, Serching database importance,statistical process for Rt, electronic spatial extent and molecular volume, electron affinity and ionization potential, hyperfine coupling, , optical activity,boiling point and melting point, surface tension, vapor pressure, visualization) Methods for Computing Properties; Multipole Moments.Software concerns.	11	25%
4	**Applications of Computational Chemistry:** Reaction Coordinates & Reaction Path,Least with MEPinCoordinates,ReactionRates,ArheniusEquation,Relative rate,HST for Prediction rate with equation,Importance,LSER in solvation,Continuum methods:Solvent Accessible surface area, Poisson–Boltzmann Method.	12	25%

Continuous Assessment:

Sr. No	Active Learning Activities	Marks
1	**Real vs Model Comparison Task** Students take a simple molecule (like H_2O or CH_4) and compare its real structure with a computational model (from software/image). They discuss differences, assumptions, and limitations in a short group presentation and upload them on the GMIU web portal	10
2	**Simulation Demo + Analysis** Show a simple MD or Monte Carlo simulation video/software. Students observe molecular motion and write a short analysis comparing MD vs Monte Carlo based on behavior and results and upload them on the GMIU web portal	10
3	**Temperature Effect on Reaction Rate (Simulation/Graph Based)** Students observe a graph or simulation showing reaction rate at different temperatures and upload them on the GMIU web portal	10
4	**Conformation Study using Model/Software:** The faculty assigns a molecular model, and students represent it using either a physical model or a software-generated image and upload them on the GMIU web portal	10
5	**Attendance**	10
	Total	50

List of Practical:

Sr. No	Descriptions	Unit No	Hrs
1	Introduction to Molecular Visualization - Free tools use Avogadro	1	3
2	Conformational Analysis -Analyze conformers of butane Plot energy vs dihedral angle	1	6
3	Mini Project - Stability of isomers,Thermodynamic feasibility of reactions, Quantum model vs real system comparison.-Report writing	2	3
4	Energy and Stability of Molecules -Free tools use Avogadro	2	4
5	Introduction to Ball-and-Spring Model -Understand molecular mechanics representation -Free tools use Avogadro	3	3

6	Simple Molecular Dynamics Simulation -Perform basic MD simulation (if plugin available) Observe vibrations and movement(Visualization) -Free tools use Avogadro	3	4
7	Radial Distribution Function (Basic Idea) -Study structure of liquids -alculate distance between particles,Plot distribution vs distance	4	3
8	Geometry Optimization -Find the most stable structure Free tools- Gaussian / ORCA	4	4
		Total	30

Suggested Specification table with Marks (Theory):75

Distribution of Theory Marks (Revised Bloom's Taxonomy)						
Level	Remembrance (R)	Understanding (U)	Application (A)	Analyze (N)	Evaluate (E)	Create (C)
Weightage	20%	20%	40%	20%	00	00

Note: This specification table shall be treated as a general guideline for students and teachers. The actual distribution of marks in the question paper may vary slightly from above table.

Course Outcome:

After learning the course the students should be able to:	
CO1	Understand the fundamental principles and theoretical basis of computational chemistry.
CO2	Apply molecular modeling and simulation methods to determine molecular structures and energies.
CO3	Analyze molecular properties and interpret computational results for chemical systems.
CO4	Explain the applications of computational chemistry in reaction mechanisms and real-world chemical systems.

Instructional Method:

The course delivery method will depend upon the requirement of content and the needs of students. The teacher, in addition to conventional teaching methods by black board, may also use any tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.
From the content 10% topics are suggested for flipped mode instruction.
Students will use supplementary resources such as online videos, NPTEL/SWAYAM videos, e-courses, Virtual Laboratory
The internal evaluation will be done on the basis of Active Learning Assignment
Practical/Viva examination will be conducted at the end of semester for evaluation of performance of students in laboratory.

Reference Books:

[1] Essentials of Computational Chemistry: Theories and Models" – Christopher J. Cramer
[2] Introduction to Computational Chemistry – Frank Jensen
[3] Molecular Modelling: Principles and Applications – Andrew R. Leach
[4] Exploring Chemistry with Electronic Structure Methods – James B. Foresman
[5] A Chemist's Guide to Density Functional Theory – Wolfram Koch