GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Bachelor of Engineering
Level: UG
Branch: Biotechnology
Subject Code: BE05004061
Subject Name: Biophysics

w. e. f. Academic Year:	2024-2025
Semester:	5
Category of the Course:	Professional Elective Course - 2

Prerequisite:	None
Rationale:	The subject *Biophysics* explores the physical principles underlying biological systems and processes. It integrates concepts from physics, chemistry, and biology to explain molecular structures, energy transfer, and dynamics in living organisms. By combining experimental and computational techniques, students learn to analyze biomolecular interactions, enzyme behavior, and structural stability.

Course Outcomes:

Sr. No.	CO statement	Marks% weightage
CO-1	Define ergocity in a system and concept of ensembles	20
CO-2	Understand forces involved in biological systems	15
CO-3	Illustrate difference between quantum and molecular mechanics	15
CO-4	Identify Stochastic and deterministic simulation techniques	15
CO-5	Apply Molecular Dynamics Simulations for biological systems	15

Teaching and Examination Scheme:

Teaching / Learning Scheme (in Hours per semester)					Total Credits	Assessment Pattern and Marks					Total Marks
						Theory		Tutorial / Practical			
L	T	P	PBL	Total no of hours per semester		ESE (E)	PA / CA (M)	PA/ CA (I)	PBL (I)	ESE (V)	
45	0	30	15	90	3	70	30	20	30	50	200

Content:

Sr. No.	Content	Total Hrs
1	**Introduction to Statistical Mechanics:** Concept of Macro-state and Microstate- Thermodynamic Ensembles- Boltzman distribution- Introduction to Quantum Mechanics and Molecular Mechanics. Integration of Newton's laws of Motion. Intermolecular forces in biological systems. Stabilizing forces in proteins, lipids and nucleic acids.	**20**

2	**Basic concepts of molecular structure:** bond length, bond angle, torsion angle and non-covalent interactions – Molecular structure and internal energy – Energy minimization of small molecules – Types of energy minimization- Empirical representation of molecular energies –Use of force fields and the molecular mechanics method –Discussion of global energy minimum –Molecular visualization tools.	**15**
3	**Simulation Techniques:** Stochastic and Deterministic simulations Molecular Dynamics and Monte Carlo simulation- Definition & Types Model Building- Velocity Verlet and Leap-frog algorithms, Periodic Boundary conditions, generating *ab initio* and template-based models Applications of Molecular Dynamics Simulations.	**20**
	TOTAL	**45**

Suggested Specification table with Marks (Theory): (For B.E. only)

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
20	**20**	**20**	**20**	**10**	**10**

R: Remembrance; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create and above Levels (Revised Bloom's Taxonomy)

The syllabus of Advanced Power Electronics directly contributes to

SDG 3	The syllabus contributes to understanding biomolecular interactions, drug-target binding, enzyme kinetics, and molecular simulations that support drug discovery, disease diagnosis, and healthcare advancements.
SDG 4	Biophysics promotes interdisciplinary scientific learning by integrating biology, physics, chemistry, and computational modeling to strengthen analytical and research skills.
SDG 9	The subject supports innovation in computational biology, molecular simulations, protein modeling, and bioinstrumentation for scientific and industrial applications.
SDG 3	Molecular docking and simulation techniques contribute to rational drug design, biomarker discovery, and improved understanding of biological systems.
SDG 12	Computational simulation approaches reduce laboratory resource consumption by enabling in silico analysis and predictive modeling before experimental validation.

Reference Books:

1. Peter Atkins and Julio De Paula, Atkins' Physical Chemistry, Oxford University Press, 2018, 11th Edition
2. Andrew R. Leach, Molecular Modelling-Principles and Applications, Pearson Education, 2009, 2nd Edition
3. Frenkel & Smith, Understanding Molecular Simulation, From Algorithms to Applications, Elsevier,

Academic Press, 2002, 2nd Edition

4. Meyer B Jackson, Molecular and Cellular Biophysics, Cambridge University Press, 2010, 1st Edition
5. Alan Hinchliffe, Molecular Modelling for Beginners, Wiley Publishers, 2008, 2nd Edition

List of Experiments / Practical Demonstrations

1. Measurement of absorption spectra of biomolecules using UV-Visible spectrophotometer.
2. Determination of protein concentration using the Beer-Lambert law.
3. Fluorescence spectroscopy of biological samples.
4. Study of enzyme kinetics and reaction rate constants.
5. Measurement of viscosity of biological fluids.
6. Determination of diffusion coefficient of molecules.
7. Analysis of molecular interactions using molecular docking simulations.
8. Demonstration of electrophoresis for biomolecule separation.
9. Structural visualization of proteins using molecular modeling software.
10. Simulation of membrane transport processes.

Major Equipment

1. UV-Visible spectrophotometer.
2. Fluorimeter or fluorescence spectrometer.
3. Electrophoresis apparatus.

Open-Source Software / Learning Websites

1. PyMOL, Chimera, VMD (for molecular visualization).
2. GROMACS, NAMD (for molecular dynamics simulations).
3. AutoDock, SwissDock (for molecular docking).
4. Python and R for data analysis and visualization.

List of suggested activities for Project Based Learning (PBL):

Sr. No.	PBL Category	Name of the Activity	No. of Hours	Evaluation Criteria
1	Industry / Research Laboratory Visit	Visit to biophysics laboratory / molecular modeling research laboratory / spectroscopy or bioinstrumentation facility	Visit = 5 hrs, Report preparation = 5 hrs Total = 10 hrs	Based on report submitted. Report should contain observations on spectroscopy, molecular modeling, biomolecular interaction analysis, and computational biology tools.
2	Video Based Learning	Technical video-based learning related to molecular dynamics, statistical mechanics, molecular docking, spectroscopy, and biophysical simulations (MOOC/NPTEL Video)	Duration of video = 5 hrs, Report preparation = 5 hrs Total = 10 hrs	Report/presentation based on video learning outcomes and understanding of biophysical concepts.

3	Assignment / Technical Writing / Research Writing	Numerical and theory-based assignments related to molecular interactions, enzyme kinetics, molecular simulations, and statistical mechanics	5 assignments of 2 hrs each Total = 10 hrs	Based on assignment submitted, technical depth, calculations, and understanding of concepts.
4	Complex Problem-Solving targeting relevant SDGs / Mini Project	Comparative analysis of protein–ligand interaction using molecular docking or molecular dynamics simulation	15 hrs	Based on scientific problem-solving approach, simulation quality, interpretation of results, and technical feasibility.
5	Research Paper Review / Analysis	Discussion on research paper based on molecular docking, molecular dynamics, enzyme kinetics, protein folding, or computational biophysics (SCOPUS Indexed / reputed Journal)	5 research papers = 20 hrs	Summarize research paper and evaluate critical scientific parameters.
6	Poster / Chart / PowerPoint Presentation	Poster/chart/power point preparation on topics such as Molecular Dynamics, Statistical Mechanics, Protein Folding, Spectroscopy, Molecular Docking	Duration = 6 hrs	Based on poster/chart preparation, scientific understanding, and presentation skills.
7	Micro Project	Working/non-working model or simulation of enzyme kinetics, molecular docking, protein structure visualization, or diffusion process	5 hrs	Based on internal/external evaluation, innovation, scientific relevance, and technical understanding.
8	Group Discussion / Quiz / Simulation	Group discussion on emerging topics such as AI in Molecular Simulation, Protein Engineering, Computational Drug Design, and Biophysical Modeling	Duration = 1 hr each	Based on participation, technical knowledge, communication skills, and scientific depth.
9	Case Study Analysis / Seminar	Real-world case study on protein folding disorders, drug-target interactions, enzyme inhibition, or computational drug discovery	Data collection/study = 5 hrs, Report preparation = 5 hrs Total = 10 hrs	Based on in-depth scientific study, data collection, technical depth, and conclusions.
10	Other	Patent Search and Innovation Gap Identification in molecular simulations, bioinstrumentation, drug discovery, or computational biology	10 hrs (Search + Report)	Based on number of relevant patents analyzed and identification of innovation scope.

Note:

1. Mini Project – 10 Marks , Micro Project – 5 Marks
2. The hours allocated to specific activities should be proportionate to the total no. of PBL hours and marks.

****