GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	MOLECULAR SIMULATIONS, PG_00070148		
Field of study	InfoBioChem		
Date of commencement of studies	February 2026	Academic year of realisation of subject	2026/2027
Education level	second-cycle studies	Subject group	Obligatory subject group in the field of study Subject group related to scientific research in the field of study
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish Literature and additional materials available in English only
Semester of study	2	ECTS credits	2.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Jacek Czub	
	Teachers	prof. dr hab. inż. Jacek Czub	

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	0.0	30.0	0.0	45

E-learning hours included: 0.0

eNauczanie source address: https://enauczanie.pg.edu.pl/2025/course/view.php?id=6206

Learning activity and number of study hours

Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours	Self-study	SUM
Number of study hours	45	2.0	3.0	50

Subject objectives

The course provides students with a broad overview of the applications of molecular simulations in scientific research, together with an in-depth practical introduction to selected aspects of molecular simulation workflows. The theoretical component covers the physical foundations of molecular simulations, commonly employed approximations, specialized applications, and current best practices, enabling students to critically evaluate and design research projects involving molecular simulations, with particular emphasis on the formulation of research hypotheses and their validation. The practical component introduces best practices in simulation studies, familiarizes students with the most widely used molecular simulation software, and illustrates the multi-stage organization of simulation projects - from selecting an appropriate methodology, defining the molecular system, and performing simulations, to analyzing the resulting data and drawing scientifically sound conclusions.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_W01] knows and understands the methods, techniques, and tools used to solve bioinformatics tasks, including molecular modeling.	understands the concept of multiscale modeling, recognizes the limitations of molecular simulation methods and the approaches used to overcome them, and possesses a basic intuition for interpreting typical simulation results.	[SW1] Assessment of factual knowledge
[K7_K03] is ready to formulate questions precisely to deepen one's understanding of a topic or identify missing elements of reasoning	is able to formulate a research hypothesis that falls within the domain of applicability of molecular simulation methods, select an appropriate computational approach to test it, and justify this choice.	[SK3] Assessment of ability to organize work [SK1] Assessment of group work skills
[K7_U05] is able to select computer modeling methods and apply them to solve problems related to the operation and regulation of complex systems.	is able to carry out the complete workflow of a molecular simulation study, from defining the simulation system and configuring the software, through performing the simulation, to analyzing the resulting data and validating the research hypothesis.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task [SU3] Assessment of ability to use knowledge gained from the subject

Subject contents

Course content – lecture

- Fundamentals of molecular simulations: motivation and principal algorithms
- Representations of biomacromolecules
- Force fields and their components
- Analysis of a basic molecular simulation
- Fundamentals of statistical mechanics
- Enhanced sampling methods
- Modeling experimental data
- Quantum-classical (QM/MM) simulations
- Coarse-grained simulations
- Strategies for overcoming the limitations of classical simulations
- Technical aspects of molecular simulations
- Integration of molecular simulations with bioinformatics
- Documentation and accessibility of simulation data
- Future directions in molecular simulations

Course content – project

- Preparation and execution of a standard molecular dynamics simulation of a short biopolymer, followed by analysis of its behavior using different force fields
- Formulation of a research hypothesis and selection of an appropriate advanced simulation method for its validation
- Selection of a biomolecular system suitable for testing the proposed hypothesis
- Configuration of simulation software appropriate for the chosen methodology and molecular system
- Preparation, execution, and analysis of simulations using open-source software
- Analysis and interpretation of simulation results, formulation of conclusions, and validation or rejection of the research hypothesis
- Preparation and presentation of a short report summarizing the computational study

Prerequisites and co-requisites

Knowledge of basic physics (electrostatic interactions, harmonic model), fundamental biochemistry (composition and structure of biomolecules), basic knowledge of the Python programming language

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Project: Assessment of a Practical Project	50.0%	50.0%
Lecture: final test	50.0%	50.0%

Recommended reading

Basic literature	Daniel M. Zuckerman, "Statistical Physics of Biomolecules. An Introduction" GROMACS Reference Manual (Documentation, Chapter 5)
Supplementary literature	Christopher J. Cramer, "Essentials of Computational Chemistry" Ivet Bahar, Robert L. Jernigan, Ken A. Dill, "Protein Actions. Principles and Modeling"

	eResources addresses	Supplementary https://www.youtube.com/watch?v=TDzzvKoDOuQ&list=PLuIpgNT2hMwRQKFy4okoNQKiJwM8li3Sz - Molecular Biophysics - a series of lectures by Erik Lindahl on the fundamental concepts in biomolecular simulation https://phasespaceinvaders.buzzsprout.com/ - Phase Space Invaders - podcast/series of interviews with top principal investigators on the history and development of their research programs, and the perspectives for the field
Example issues/ example questions/ tasks being completed	• Interpret the provided graphs to determine what happens in the simulated system. • Propose a simulation methodology to study the following processes: • protein adsorption on a metal catode • shift in the light absorption spectrum due to a change in the environment • lowering of the binding constant due to a mutation in a protein domain • Determine which structural element first causes the simulation to destabilize as the time step increases. • Study the effect of high salt concentrations on the pKa of a polyelectrolite. • Determine the lowest concentration of component A at which the mixture undergoes clear phase separation.	
Practical activites within the subject	Not applicable	

Document generated electronically. Does not require a seal or signature.