GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	THEORETICAL CHEMISTRY AND MODELLING IN CHEMISTRY, PG_00064390		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2025/2026
Education level	first-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	2	Language of instruction	Polish
Semester of study	4	ECTS credits	4.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Inorganic Chemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Andrzej Okuniewski	
	Teachers	dr inż. Andrzej Okuniewski	

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	30.0	0.0	30.0	0.0	0.0	60

E-learning hours included: 0.0

eNauczanie source addresses:

Moodle ID: 3127 Chemia teoretyczna i modelowanie w chemii 2025/26
https://enauczanie.pg.edu.pl/2025/course/view.php?id=3127

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	60	10.0	30.0	100

Subject objectives

The aim of the course is to familiarize students with the basics of quantum mechanics, theoretical chemistry and molecular modeling methods, and to develop the ability to use computational tools to analyze the structure and properties of chemical systems.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_K01] understands the need for continuous learning, can inspire and organise learning and others, understands the importance of group and team activities	The student works independently and in a team when carrying out molecular modelling tasks, demonstrates responsibility for the results of calculations and is aware of the need to update knowledge of computational methods.	[SK3] Assessment of ability to organize work [SK5] Assessment of ability to solve problems that arise in practice
[K6_U08] applies computer-aided, common methods, chemical apparatus and tools necessary for the solution of simple engineering tasks involving for example technological processes, with a preliminary economic analysis of the engineering activities undertaken	The student applies molecular modeling and quantum chemistry tools to optimize molecular geometry, calculate energy, and simulate chemical processes, interprets calculation results, and evaluates the limitations of the methods used.	[SU3] Assessment of ability to use knowledge gained from the subject [SU4] Assessment of ability to use methods and tools
[K6_U01] gathers information from literature, databases and other sources, interpreting, critically evaluating, summarising, formulating and justifying opinions, independently analyses and produces technical drawings with the use of computer assistance	The student obtains structural data from chemical databases and literature, uses various structural file formats, interprets calculation results and presents them in graphical and descriptive form.	[SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools
[K6_W03] demonstrates knowledge in the area of theoretical chemistry and related engineering disciplines, necessary to predict structures, design and conduct basic process operations using molecular mechanics tools	The student has the knowledge necessary to explain the fundamentals of quantum mechanics, molecular modeling, molecular mechanics, and molecular dynamics. They will understand the importance of potential energy hypersurfaces and be able to describe the relationship between the structure and energy of a system.	[SW3] Assessment of knowledge contained in written work and projects

Subject contents

Course content – lecture

History of structural chemistry. Structural studies. Databases and structural file formats. The concept of molecular modeling, force fields. Molecular mechanics and dynamics. Monte Carlo simulations. Conformational analysis. Simulations of biological systems. Modeling software and hardware. Molecular graphics. History of quantum mechanics. Wave-particle duality. Postulates of quantum mechanics, uncertainty. Functions of many variables, differential equations. A particle in a one-dimensional potential well. The tunneling phenomenon. The harmonic oscillator. A particle on a circle. A particle in a two-dimensional potential well. The rigid rotor. The hydrogen atom and hydrogen-like ions. Multi-electron systems.

Course content – laboratory

Introduction to the HyperChem package. Molecular mechanics and dynamics. Geometry optimization and investigation of the electronic structure of molecules. Determination of reaction intermediates/transition states. Investigation of the mechanism of a selected reaction (teamwork).

Prerequisites and co-requisites

The student should have knowledge of general chemistry, physics and mathematics (differential and integral calculus) and basic computer skills.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Lecture	60.0%	50.0%
Laboratory	60.0%	50.0%

Recommended reading

Basic literature	• D. O. Hayward: Mechanika kwantowa dla chemików. *Wydawnictwo Naukowe PWN*, Warszawa 2007. • A. R. Leach: Molecular Modelling: Principles and Applications. *Pearson*, 2001.
Supplementary literature	• R. F. Nalewajski: Podstawy i metody chemii kwantowej. Wykłady. *Wydawnictwo Naukowe PWN*, Warszawa 2001. • L. Piela: Idee chemii kwantowej. *Wydawnictwo PWN*, Warszawa 2006. • P. W. Atkins: Molekularna mechanika kwantowa: wstęp do chemii kwantowej. *Wydawnictwo PWN*, Warszawa 1974. • H. Buchowski: Elementy termodynamiki statystycznej. *Wydawnictwa Naukowo-Techniczne*, Warszawa 1998.
eResources addresses	

Example issues/ example questions/ tasks being completed

Example topics can be found on the eNauczanie platform.

Practical activites within the subject

Not applicable

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