GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Modeling in Chemistry, PG_00036532		
Field of study	Chemistry		
Date of commencement of studies	October 2021	Academic year of realisation of subject	2023/2024
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	3	Language of instruction	Polish
Semester of study	5	ECTS credits	2.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Inorganic Chemistry -> Faculty of Chemistry		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Andrzej Okuniewski	
	Teachers	dr inż. Andrzej Okuniewski	

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	15.0	0.0	0.0	0.0	0.0	15

E-learning hours included: 0.0

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	15	5.0	30.0	50

Subject objectives

The aim of the course is to familiarize students with modeling in chemistry with particular emphasis on methods of computational chemistry (molecular modeling and graphics), structural research and databases (both for small molecule compounds and for complex biological systems).

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U08] is capable to design and carry out the experiment which is necessary to confirm a given hypothesis and sees wider context, often beyond-technical, of the analysed phenomena	knows how to choose a computational method and its selected parameters appropriate to the model problem in order to obtain reliable results in the shortest possible time	[SU2] Assessment of ability to analyse information
[K6_W05] knows and understands the chemical processes and algorithms of mathematical models which are necessary for the design of technological processes, knows chemical structure of contemporary materials and its relation to their properties, enabling the selection of the materials for sustainable development technology and material-efficient and energy-efficient methods	understands the principle of molecular modeling methods (from simple methods using force fields to complex ab-initio and semi-empirical methods); has knowledge in the field of modeling of nanomaterials and biological systems	[SW1] Assessment of factual knowledge
[K6_K07] is aware of his social role as a graduate of a Technical University, especially in presenting information and opinion to the public about the risks and opportunities posed by chemical sciences; undertakes actions to communicate such information in a comprehensible manner	is aware of the rapid development in field of molecular modeling; can explain in an accessible way what molecular modeling is	[SK2] Assessment of progress of work

Subject contents

History of structural chemistry. Structural studies. Structural databases. Popular chemical file formats. Basics of molecular modeling. Force fields. Molecular mechanics. Molecular dynamics. Monte Carlo simulations. Conformational analysis. Biological systems simulations. Modeling software and equipment. Molecular graphics.

<table>
<tr><td>Prerequisites and co-requisites</td><td colspan="3">The student must have mastered the following courses at the undergraduate level: mathematics, physics, general chemistry, theoretical chemistry.</td></tr>
<tr><td>Assessment methods and criteria</td><td colspan="3"><table><tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr><tr><td>Final test</td><td>60.0%</td><td>100.0%</td></tr></table></td></tr>
<tr><td rowspan="3">Recommended reading</td><td>Basic literature</td><td colspan="2">A. R. Leach: Molecular Modelling: Principles and Applications. Pearson , 2001.</td></tr>
<tr><td>Supplementary literature</td><td colspan="2">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.</td></tr>
<tr><td>eResources addresses</td><td colspan="2">Adresy na platformie eNauczanie:</td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td colspan="3">https://chem.pg.edu.pl/kchn/ch-modelowanie-w-chemii</td></tr>
<tr><td>Work placement</td><td colspan="3">Not applicable</td></tr>
</table>

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