GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Introduction to Biological Modelling Systems, PG_00049378		
Field of study	Biomedical Engineering		
Date of commencement of studies	October 2025	Academic year of realisation of subject	2027/2028
Education level	first-cycle studies	Subject group	Optional subject group 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	6	ECTS credits	4.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Division Of Theoretical Physics And Quantum Informaton -> Institute Of Physics And Applied Computer Science -> Faculty Of Applied Physics And Mathematics -> Wydziały Politechniki Gdańskiej		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Marta Łabuda	
	Teachers		

Lesson types and methods of instruction

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

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	45	4.0	51.0	100

Subject objectives

Introduce the students to the basics of computational and theoretical methods necessary to perform simulations to illustrate the properties of molecules. Students will gain the knowledge on the quantum chemistry methods and techniques allowing to use them in practice in simple atomic systems as well as complex biological systems.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U07] can apply methods of process and function support, specific to the field of study	The student knows the basic concepts and definitions of molecular physics and quantum-mechanical computations. The student knows and distinguishes basic ab initio quantum chemistry methods.	[SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools
[K6_W02] knows and understands, to an advanced extent, selected laws of physics and physical phenomena as well as methods and theories explaining the complex relationships between them, constituting the basic general knowledge in the field of technical sciences related to the field of study	The student knows the basics of theory necessary for performing calculations in atomic and molecular systems.	[SW3] Assessment of knowledge contained in written work and projects

Subject contents

Introduction. Theoretical background of quantum mechanics. Schroedinger equation. An electron and nuclei movements. Adiabatic approximation. Energy of the excitation. Potential energy curves. Introduction to the quantum chemistry methods. The Self-Consistent Field method and LCAO method. Atomic orbital basis sets. Calculation technique. Ab initio methods.Hartree-Fock method, multi-configurational and multi-reference methods. CI, CC and MP2 methods. Application of the methods to diatomic molecules. Quantum chemistry packages: description, structure and characteristics, advantages and disadvantages of the packages. An interpretation and visualisation of the results. Simple dynamics simulation in the chemical reactions. Simulation of the collisions and interactions between atoms in molecules.

Prerequisites and co-requisites

Introduction to spectroscopy, basics of informatics.

<table>
<tr><td>Assessment methods and criteria</td><td colspan="2"><table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Lecture-writting exam</td><td>50.0%</td><td>40.0%</td></tr>
<tr><td>Labs-raports</td><td>50.0%</td><td>60.0%</td></tr>
</table></td></tr>
<tr><td rowspan="3">Recommended reading</td><td>Basic literature</td><td>Review of the subject in the form of the e-booklet

Distance learning materials

Piela L., Idee chemii kwantowej, PWN 2005

Leach A. ,Molecular Modelling: Principles and applications Longman 1996

Szabo A., Ostlund N. S. Modern Quantum Chemistry McMillan, New York 1982

Schlick T. ,Molecular Modeling and Simulation Springer 2002

Jensen F. ,Introduction to Computational Chemistry, Academic Press 2007</td></tr>
<tr><td>Supplementary literature</td><td>User manual : www.molpro.net

Graphical user interfaces, for example: Gabedit (main page of the developer)

Instructions how to use the computational packages</td></tr>
<tr><td>eResources addresses</td><td>Adresy na platformie eNauczanie:</td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td colspan="2"></td></tr>
<tr><td>Work placement</td><td colspan="2">Not applicable</td></tr>
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