

。 GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Introduction to Biological Modelling Systems, PG_00049378								
Field of study	Biomedical Engineering, Biomedical Engineering, Biomedical Engineering								
Date of commencement of studies	October 2022		Academic year of realisation of subject			2024/2025			
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								
Name and surname	Subject supervisor		dr hab. inż. Marta Łabuda						
of lecturer (lecturers)	Teachers								
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Projec	t	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		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_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			
	[K6_U07] can apply methods of process and function support, specific to the field of study [K6_U05] can plan and conduct		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. The student can self perform			[SU4] Assessment of ability to use methods and tools [SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools			
	experiments related to the field of study, including computer simulations and measurements; interpret obtained results and draw conclusions		simulations by using given tools for modeling of molecular systems.			[SU2] Assessment of ability to analyse information			

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.						
Assessment methods	Subject passing criteria	Passing threshold	Percentage of the final grade				
and criteria	Lecture-writting exam	50.0%	40.0%				
	Labs-raports	50.0%	60.0%				
Recommended reading	Basic literature	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					
	Supplementary literature	User manual : www.molpro.net					
		Graphical user interfaces, for example: Gabedit (main page of the developer)					
		Instructions how to use the computational packages					
	eResources addresses	Adresy na platformie eNauczanie:					
Example issues/ example questions/ tasks being completed							
Work placement	Not applicable						

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