



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 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_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		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.			[SU4] Assessment of ability to use methods and tools [SU1] Assessment of task fulfilment	
	[K6_U05] can plan and conduct experiments related to the field of study, including computer simulations and measurements; interpret obtained results and draw conclusions		The student can self perform simple calculations and computer simulations by using given tools for modeling of molecular systems.			[SU4] Assessment of ability to use methods and tools [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 and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Lecture-writing 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 : <a href="http://www.molpro.net">www.molpro.net</a>  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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