GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Modelling of physical phenomena, PG_00031936		
Field of study	Technical Physics		
Date of commencement of studies	February 2027	Academic year of realisation of subject	2027/2028
Education level	second-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	1	Language of instruction	English
Semester of study	2	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Theoretical Physics and Quantum Computing -> Faculty of Applied Physics and Mathematics -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. Julien Guthmuller	
	Teachers		

Lesson types							
	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	30.0	0.0	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	5.0	25.0	75

Subject objectives	Introduce the students to the basic theoretical and computational methods to perform quantum simulations of molecular systems properties. The students will gain knowledge in the quantum chemistry techniques and will apply them in practice to diatomic and polyatomic molecules. The students will learn how to analyze their results and how to assess them by comparison with experimental data.

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[K7_W04] possesses advanced knowledge of mathematical, numerical and simulation methods used in the description and modelling of physical phenomena.	The students will learn the theories, approximations and algorithms required to simulate atomic and molecular phenomena.	[SW1] Assessment of factual knowledge
	[K7_U03] is capable of conducting advanced laboratory work in physics and related disciplines, selecting and adapting appropriate methods and tools, and critically evaluating existing technical solutions.	The students will learn to solve problems, work in groups and complete laboratory projects.	[SU1] Assessment of task fulfilment
	[K7_U05] is able, individually or as part of a team (including in a leadership role), to plan and conduct advanced theoretical calculations, experimental studies and computer simulations aimed at solving complex and non-standard scientific and engineering problems, and to critically analyse results and formulate well-founded conclusions	The students will learn the use of computer programs to describe molecular properties. The students will learn how to analyze their results and how to assess them by comparison with experimental data.	[SU4] Assessment of ability to use methods and tools [SU2] Assessment of ability to analyse information [SU1] Assessment of task fulfilment
	[K7_U02] demonstrates advanced programming skills in a selected language and the ability to use specialised software packages.	The students will learn how to select the appropriate physical parameters to run a quantum calculations and how to prepare the input files in the suitable format. The students will learn how to use visualization graphical tools to prepare the input data and analyze the output results.	[SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools

Subject contents

Course content – lecture

- Born-Oppenheimer approximation and definition of the potential energy surface. Calculation of potential energy curves, dipole moments and bond lengths for diatomic molecules.

- Hartree-Fock approximation and Roothaan equations. Optimization of molecular geometries, calculation of ionization energies, electron affinities and molecular orbitals.

- Post-Hartree-Fock methods and atomic basis sets. Accurate calculation of ionization energies with the Coupled-Cluster methods. Investigation of the basis set convergence.

- Vibrational energies in the harmonic approximation. Calculation of vibrational frequencies, normal modes, infrared spectra and Raman spectra for polyatomic molecules.

- Density functional theory and time-dependent density functional theory. Calculation of excited state properties, absorption spectra, fluorescence energies and solvent effects.

Course content – laboratory

Project 1: Optimization of molecular geometries, calculation of ionization energies, electron affinities and molecular orbitals.

Project 2: Calculation of vibrational frequencies, normal modes, infrared spectra and Raman spectra for polyatomic molecules.

Project 3: Calculation of excited state properties, absorption spectra, fluorescence energies and solvent effects.

Prerequisites and co-requisites

Not applied.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
test	50.0%	40.0%
projects	50.0%	60.0%

Recommended reading	Basic literature	Piela L., Idee chemii kwantowej, PWN 2005 Jensen F., Introduction to Computational Chemistry, John Wiley & Sons Ltd. 2011 Szabo A. and Ostlund N. S., Modern Quantum Chemistry, Dover Publications, Inc. https://orcaforum.cec.mpg.de/
	Supplementary literature	Not applied.
	eResources addresses	
Example issues/ example questions/ tasks being completed	not applied	
Practical activites within the subject	Not applicable	

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