



Subject card

Subject name and code	Modelling of physical phenomena, PG_00031936						
Field of study	Technical Physics						
Date of commencement of studies	February 2023	Academic year of realisation of subject				2023/2024	
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 Information -> Faculty of Applied Physics and Mathematics						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Julien Guthmuller				
	Teachers		prof. dr hab. Julien Guthmuller				
Lesson types and methods of instruction	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_U06] Can apply obtained knowledge of physics to exact sciences, natural and technical sciences.		The knowledge acquired by the students can be applied in the fields of solid state physics, nanotechnology, chemistry and biology.			[SU4] Assessment of ability to use methods and tools [SU3] Assessment of ability to use knowledge gained from the subject	
	[K7_U05] Can plan and conduct theoretical calculations, experimental research and computer simulations, critically analyze their results, draw conclusions and form reasoned opinions.		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_W04] Has enhanced knowledge of mathematical, numerical and simulation methods applied 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	

Subject contents	<p>- Born-Oppenheimer approximation and definition of the potential energy surface. Calculation of potential energy curves, dipole moments and bond lengths for diatomic molecules.</p> <p>- Hartree-Fock approximation and Roothaan equations. Optimization of molecular geometries, calculation of ionization energies, electron affinities and molecular orbitals.</p> <p>- Post-Hartree-Fock methods and atomic basis sets. Accurate calculation of ionization energies with the Coupled-Cluster methods. Investigation of the basis set convergence.</p> <p>- Vibrational energies in the harmonic approximation. Calculation of vibrational frequencies, normal modes, infrared spectra and Raman spectra for polyatomic molecules.</p> <p>- Density functional theory and time-dependent density functional theory. Calculation of excited state properties, absorption spectra, fluorescence energies and solvent effects.</p>		
Prerequisites and co-requisites	Not applied.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	test	55.0%	40.0%
	projects	55.0%	60.0%
Recommended reading	Basic literature	<p>Piela L., Idee chemii kwantowej, PWN 2005</p> <p>Jensen F., Introduction to Computational Chemistry, John Wiley & Sons Ltd. 2011</p> <p>Szabo A. and Ostlund N. S., Modern Quantum Chemistry, Dover Publications, Inc.</p> <p>https://orcaforum.cec.mpg.de/</p>	
	Supplementary literature	Not applied.	
	eResources addresses	Adresy na platformie eNauczanie:	
Example issues/ example questions/ tasks being completed	not applied		
Work placement	Not applicable		