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 2024	Academic year of realisation of subject	2024/2025
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_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
[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.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools
[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.	[SU3] Assessment of ability to use knowledge gained from the subject [SU4] Assessment of ability to use methods and tools

<table>
<tr><td>Subject contents</td><td>- 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.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td>Not applied.</td></tr>
<tr><td>Assessment methods and criteria</td><td><table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>projects</td><td>55.0%</td><td>60.0%</td></tr>
<tr><td>test</td><td>55.0%</td><td>40.0%</td></tr>
</table></td></tr>
<tr><td>Recommended reading</td><td><table>
<tr><td>Basic literature</td><td>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/</td></tr>
<tr><td>Supplementary literature</td><td>Not applied.</td></tr>
<tr><td>eResources addresses</td><td>Adresy na platformie eNauczanie:</td></tr>
</table></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td>not applied</td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
</table>

Document generated electronically. Does not require a seal or signature.