


**KAPITAŁ LUDZKI**  
 NARODOWA STRATEGIA SPÓJNOŚCI

 Projekt współfinansowany przez  
 Unię Europejską w ramach  
 Europejskiego Funduszu  
 Społecznego

**UNIA EUROPEJSKA**  
 EUROPEJSKI  
 FUNDUSZ SPOŁECZNY


<b>Course title</b>		<b>ECTS code</b>	
Quantum chemistry in practice		13.3.1290	
<b>Name of unit administrating study</b>			
null			
<b>Studies</b>			
<b>faculty</b>	<b>field of study</b>	<b>type</b>	drugiego stopnia
Wydział Chemii	Chemia	<b>form</b>	stacjonarne
		<b>specjalty</b>	Digital Chemistry
		<b>specialization</b>	wszystkie
<b>Teaching staff</b>			
prof. dr hab. Piotr Skurski; dr Marcin Czapla; dr hab. Iwona Anusiewicz, profesor uczelni; dr Sylwia Freza			
<b>Forms of classes, the realization and number of hours</b>		<b>ECTS credits</b>	
<b>Forms of classes</b>		6	
Laboratory classes, Lecture		lectures - 30 h	
<b>The realization of activities</b>		laboratory classes – 45 h	
classroom instruction		student's own work – 45 h	
<b>Number of hours</b>		tutorial classes: 30 h	
Lecture: 30 hours, Laboratory classes: 45 hours		TOTAL: 150 h – 6 ECTS	
<b>The academic cycle</b>			
2023/2024 winter semester			
<b>Type of course</b>		<b>Language of instruction</b>	
obligatory		English	
<b>Teaching methods</b>		<b>Form and method of assessment and basic criteria for evaluation or examination requirements</b>	
<ul style="list-style-type: none"> <li>- Laboratory classes – computer hands-on exercises, discussions.</li> <li>- discussion</li> <li>- multimedia-based lecture</li> </ul>		<b>Final evaluation</b>	
		<ul style="list-style-type: none"> <li>- Graded credit</li> <li>- Examination</li> </ul>	
		<b>Assessment methods</b>	
		<ul style="list-style-type: none"> <li>- written exam (test)</li> <li>- Laboratory classes – based on the reports containing the solutions of the assigned tasks.</li> </ul>	
		<b>The basic criteria for evaluation</b>	
		Assessment criteria in accordance with the University of Gdańsk Study Regulations	
		Lectures: passing the final exam in a form of a set of open questions (a score of 50% or more required to pass the exam).	
		Laboratory classes: grades based on the quality of the solutions of the assigned exercises.	
		Laboratory classes – credit obtained for participation in the classes and solving all assignments	
<b>Method of verifying required learning outcomes</b>			
Test exam, quality of the solutions of the assigned exercises			
<b>Required courses and introductory requirements</b>			
<b>A. Formal requirements</b>			
none			
<b>B. Prerequisites</b>			

basic knowledge in chemistry and physics	
<b>Aims of education</b>	
Acquainting students with the possibilities of using quantum chemistry methods and quantum chemistry software to solve chemical problems	
<b>Course contents</b>	
Basic knowledge concerning various types of chemical problems that might be solved using quantum chemistry methods and software, the use of software designed to evaluating physicochemical properties of molecules, defining the problem that is to be solved, the ability to perform desired calculations using computers, the ability to properly interpret the results and formulate conclusions, preparing input data files for QM software, graphical interpretation of the results, determining the equilibrium structures of molecules, simulating IR, NMR, and UV spectra, evaluating physicochemical parameters (energy, Gibbs free energy, entropy, heat capacity, dipole and quadrupole moments, polarizability and hyperpolarizability), determining stationary points on the potential energy surface.	
<b>Bibliography of literature</b>	
Literature required to pass the course	
An Introduction to Theoretical Chemistry, Jack Simons, Cambridge University Press, 2003	
Molecular Quantum Mechanics, P. W. Atkins, R. S. Friedman, Oxford University Press Inc., New York (2011)	
Energetic Principles of Chemical Reactions, J. Simons, Jones and Bartlett Publishers, Inc., 1983.	
Extracurricular readings	
Quantum Mechanics in Chemistry, J. Simons, J. Nichols, Oxford University Press (1997)	
Geometrical Derivative of Energy Surfaces and Molecular Properties, P. Jorgensen, J. Simons, D. Reidel Publ. Company, 1985	
<b>The learning outcomes (for the field of study and specialization)</b>	<b>Knowledge</b>
	<b>Skills</b>
<p>K_W05: has extended knowledge in the field of quantum chemistry tools and techniques</p> <p>K_W07: selects suitable computational tools to the extent necessary to study various types of chemical problems</p> <p>K_W08: demonstrates in-depth knowledge of the ability of solving various chemical problems by using quantum chemistry tools</p> <p>K_U02: critically assesses the results of performed theoretical calculations and discusses them in the context of predicted properties of molecules</p> <p>K_U04: applies acquired knowledge of the structure and properties of molecules, general chemistry and related scientific disciplines</p> <p>K_K01: knows the limitations of her/his own knowledge; understands the need for further education</p>	<b>Social competence</b>
	<p>After the course, the students are capable of: recognizing the problems that might be solved using quantum chemistry methods and software, choosing proper quantum chemistry tools (methods and software) for solving certain chemical problems, preparing input data for quantum chemistry software, analyzing output data, interpreting the results, formulating the conclusions.</p> <p>After completing the course, the students are capable of choosing the basis set and quantum chemistry method (to solve chemical problem), perform calculations using the quantum chemistry software packages and computers, prepare presentation demonstrating graphical results.</p> <p>Student develops the skills of accurate and logical thinking and inference. Learns the principles of working safely, responsibly, and efficiently. Develops the ability to work in a team. After the course, the students are expected to understand the necessity of further learning, they are also taught to approach the problems and formulate their opinions with caution and criticism. In addition, the students are expected to remain open-minded for new ideas.</p>
<b>Contact</b>	
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