


KAPITAŁ LUDZKI
 NARODOWA STRATEGIA SPÓJNOŚCI

 Projekt współfinansowany przez
 Unię Europejską w ramach
 Europejskiego Funduszu
 Społecznego

UNIA EUROPEJSKA
 EUROPEJSKI
 FUNDUSZ SPOŁECZNY


Course title		ECTS code	
Insights into reaction mechanisms and kinetics via quantum chemistry methods		13.3.1311	
Name of unit administrating study			
null			
Studies			
faculty	field of study	type	drugiego stopnia
Wydział Chemii	Chemia	form	stacjonarne
		specjalty	Digital Chemistry
		specialization	wszystkie
Teaching staff			
dr hab. Iwona Anusiewicz, profesor uczelni; prof. dr hab. Piotr Skurski			
Forms of classes, the realization and number of hours		ECTS credits	
Forms of classes		2	
Laboratory classes		laboratory classes - 30 h	
The realization of activities		student's own work – 10 h	
classroom instruction		tutorial classes – 10 h	
Number of hours		Total: 50 h - 2 ECTS	
Laboratory classes: 30 hours			
The academic cycle			
2024/2025 winter semester			
Type of course		Language of instruction	
an elective course		English	
Teaching methods		Form and method of assessment and basic criteria for evaluation or examination requirements	
Laboratory classes – in-class learning, computer hands-on exercises, multimedia presentation, discussions		Final evaluation	
		Graded credit	
		Assessment methods	
		Laboratory classes – based on the reports containing the solutions of the assigned tasks.	
		The basic criteria for evaluation	
		Assessment criteria in accordance with the University of Gdańsk Study Regulations Laboratory classes: grades based on the quality of the solutions of the assigned exercises (a score of 50% or more required to pass the test).	
Method of verifying required learning outcomes			
Written test (K_W05, K_W07, K_W08).			
- Discussion with the students (K_U02, K_U04).			
- Observation of the student's behavior during classes and during consultations. (K_K01).			
Required courses and introductory requirements			
A. Formal requirements			
none			
B. Prerequisites			
basic knowledge in chemistry			
Aims of education			
Acquiring the knowledge of the fundamental terms related to the mechanisms of chemical reactions.			
Acquiring the ability to evaluate the activation barriers and thermodynamic barriers of chemical reactions.			

Acquiring the ability to use theoretical methods for prediction of the rate constants of chemical reactions.	
Course contents	
The course covers the explanation of fundamental terms related to the mechanisms of chemical reactions, including the formulas required to calculate the reaction rate constant. The students will be taught how to obtain an overall picture of the reaction mechanism, distinguish between concerted and stepwise mechanisms, finding initial complexes of reagents, locating transition states (saddle points) and intermediate products, estimating the heights of kinetic (activation) barriers, evaluating the heights of thermodynamic barriers, and calculating the rate constants. These abilities will be taught by studying the real examples of various reaction mechanisms with the use of computational quantum chemistry tools.	
Bibliography of literature	
Literature required to pass the course	
Energetic Principles of Chemical Reactions, J. Simons, Jones and Bartlett Publishers, Inc., 1983.	
An Introduction to Theoretical Chemistry, J. Simons, Cambridge University Press, 2003	
Extracurricular readings	
Geometrical Derivative of Energy Surfaces and Molecular Properties, P. Jorgensen, J. Simons, D. Reidel Publishing Company, 1985	
The learning outcomes (for the field of study and specialization)	Knowledge
	Skills
	Social competence
K_W05: has extended knowledge in the field of the mechanisms of chemical reactions	Student defines and describes basic terms related to the mechanisms of chemical reactions, understands the role of activation barriers on the reaction rate constant, and knows how to choose the proper theoretical methods and how to perform the study of a given reaction mechanism.
K_W07: selects suitable computational tools to the extent necessary to study various types of reaction mechanisms	
K_W08: demonstrates in-depth knowledge of various reaction mechanisms and their role in chemistry	
K_U02: critically assesses the results of performed theoretical calculations and discusses them in the context of predicted kinetics of chemical reactions	
K_U04: applies acquired knowledge of the reaction mechanisms, general chemistry and related scientific disciplines	
K_U05: presents the results of research in the form of an independently written paper containing a description and justification of the purpose of the work, adopted methodology, results and their significance in comparison to other similar research	
K_K01: knows the limitations of her/his own knowledge; understands the need for further education	
Contact	
iwona.anusiewicz@ug.edu.pl	