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		
Faculty of Chemistry	Chemistry	type	second tier studies (MA)
		form	full-time
		specialty	all
		specialization	all

Teaching staff

dr hab. Iwona Anusiewicz, profesor uczelni; prof. dr hab. Piotr Skurski

Forms of classes, the realization and number of hours

Forms of classes

Laboratory classes

The realization of activities

classroom instruction

Number of hours

Laboratory classes: 30 hours

ECTS credits

2
laboratory classes - 30 h
student's own work – 10 h
tutorial classes – 10 h
Total: 50 h - 2 ECTS

The academic cycle

2023/2024 winter semester

Type of course

an elective course

Language of instruction

english

Teaching methods

Laboratory classes – in-class learning, computer hands-on exercises, multimedia presentation, discussions

Form and method of assessment and basic criteria for eveluation or examination requirements

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)

K_W05: has extended knowledge in the field of the mechanisms of chemical reactions

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

Knowledge

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.

Skills

Student has the ability of estimating the heights of activation barriers and thermodynamic barriers, locating transition states on the reaction path, finding the structures of the intermediate products and the final products, calculating the reaction rate constant and providing the overall reaction picture

Social competence

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.

Contact

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