KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

Course title	ECTS code
Quantum chemistry in practice	13.3.1290

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

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

Forms of classes, the realization and number of hours

Forms of classes

Laboratory classes, Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours, Laboratory classes: 45 hours

ECTS credits

6
lectures - 30 h
laboratory classes – 45 h
student's own work – 45 h
tutorial classes: 30 h
TOTAL: 150 h – 6 ECTS

The academic cycle

2022/2023 winter semester

Type of course

obligatory

Language of instruction

english

Teaching methods

- Laboratory classes – computer hands-on exercises, discussions.
- discussion
- multimedia-based lecture

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

Final evaluation

- Graded credit
- Examination

Assessment methods

- written exam with open questions
- 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

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

Method of verifying required learning outcomes

Exam, quality of the solutions of the assigned exercises

Required courses and introductory requirements

A. Formal requirements

none

B. Prerequisites

basic knowledge in chemistry and physics

Aims of education

Acquainting students with the possibilities of using quantum chemistry methods and quantum chemistry software to solve chemical problems

Course contents

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.

Bibliography of literature

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

The learning outcomes (for the field of study and specialization)

K_W05: has extended knowledge in the field of quantum chemistry tools and techniques

K_W07: selects suitable computational tools to the extent necessary to study various types of chemical problems

K_W08: demonstrates in-depth knowledge of the ability of solving various chemical problems by using quantum chemistry tools

K_U02: critically assesses the results of performed theoretical calculations and discusses them in the context of predicted properties of molecules

K_U04: applies acquired knowledge of the structure and properties of molecules, general chemistry and related scientific disciplines

K_K01: knows the limitations of her/his own knowledge; understands the need for further education

Knowledge

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.

Skills

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.

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. 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.

Contact

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