KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

Course title	ECTS code
Monographic lecture - Modern quantum chemistry in use	13.3.1309

Name of unit administrating study

null

Studies

faculty	field of study		
Wydział Chemii	Chemia	type	drugiego stopnia
		form	stacjonarne
		specialty	Digital Chemistry
		specialization	wszystkie

Teaching staff

dr Jakub Brzeski; prof. dr hab. Piotr Skurski

Forms of classes, the realization and number of hours

Forms of classes

Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours

ECTS credits

3
lectures - 30 h
student's own work – 30 h
tutorial classes – 15 h
TOTAL: 75 h – 3 ECTS

The academic cycle

2024/2025 winter semester

Type of course

obligatory

Language of instruction

English

Teaching methods

- discussion
- multimedia-based lecture

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

Final evaluation

Graded credit

Assessment methods

- Lectures – written test in a form of a set of questions.
- written exam (test)

The basic criteria for evaluation

Assessment criteria in accordance with the University of Gdańsk Study Regulations
Lectures: passing the final test in a form of a set of questions (a score of 50% or more required to pass the exam).

Method of verifying required learning outcomes

Written test (K_W05, K_W07, K_W08, K_U02).
Discussion with the students (K_U02, K_U04).
Observation of the student's behavior during classes and during consultations. (K_K01, K_K03).

Required courses and introductory requirements

A. Formal requirements

none

B. Prerequisites

basic knowledge in chemistry and physics

Aims of education

Acquiring knowledge about the possibility of using various theoretical methods to solve chemical problems.
Teaching students about the areas of chemistry which may benefit from the use of computational chemistry tools.

Course contents

The course covers most recent advances in chemistry (chemistry of materials in particular) which were achieved by employing modern quantum chemistry tools (such as sophisticated ab initio and DFT methods). The list of covered issues includes: designing novel nanoparticles, determining properties of nanoparticles, designing novel ionic liquids (including tailor-made ionic liquids exhibiting desired physicochemical properties, e.g., viscosity, electric conductivity), designing strong oxidizing systems, designing novel superacids exhibiting desired acid strength, functionalization of known molecules to obtain the system having certain properties, designing non-metal magnets, designing novel semiconductors.

Bibliography of literature

Literature required to pass the course
Molecular Quantum Mechanics, P. W. Atkins, R. S. Friedman, Oxford University Press Inc., New York (2011)
Extracurricular readings
Quantum Mechanics in Chemistry, J. Simons, J. Nichols, Oxford University Press (1997)

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

K_W05: has extended knowledge in the field of computational chemistry

K_W07: selects suitable computational tools to the extent necessary to solve various chemical problems

K_W08: demonstrates in-depth knowledge of types of chemical problems whose solutions could be supported by the use of computational chemistry tools

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

K_U04: applies acquired knowledge of the possibility of designing novel molecules having desired properties, general chemistry and related scientific disciplines

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

K_K03: understands the need for systematic work on various projects of a long-term nature and knows how to set priorities for the implementation of undertaken tasks

Knowledge

Student defines and describes various functionalized molecules that could be designed to serve as convenient component of materials exhibiting desired properties.

Skills

Student develops the ability to recognize the areas and particular problems that can be solved by using modern quantum chemistry tools.

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

jakub.brzeski@ug.edu.pl