KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

Course title	ECTS code
Chemical bonding via quantum chemistry tools	13.3.1320

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 hab. Iwona Anusiewicz, profesor uczelni

Forms of classes, the realization and number of hours

Forms of classes

Auditorium classes

The realization of activities

classroom instruction

Number of hours

Auditorium classes: 30 hours

ECTS credits

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

The academic cycle

2024/2025 summer semester

Type of course

an elective course

Language of instruction

English

Teaching methods

auditorium classes – computer exercises, solving chemistry problems using computational software tools, discussions.

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

Final evaluation

Graded credit

Assessment methods

auditorium classes – the final grade is based on partial grades received during the semester for written reports and/or presentation of assignments..

The basic criteria for evaluation

Assessment criteria in accordance with the University of Gdańsk Study Regulations
Auditorium classes: the arithmetic mean of partial grades received during the semester for written reports on exercises and presentation of the final assignment; the main criteria for evaluation of reports are the correct answers to the questions in the exercise instructions.

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements
none

B. Prerequisites
basic knowledge in chemistry

Aims of education

Explaining how to identify via quantum chemical calculations types of various chemical bonding.
Teaching students about the applications of computational methods to chemical bonding analysis

Course contents

Various types of chemical bonding: covalent bonding, ionic bonding, intermolecular forces; theoretical methods used for identification of chemical bonding in molecular structure; determination of physical properties (bond lengths, bond energy, charge distribution, polarizability, dipole moments) related to different types of chemical bonding/molecular interactions; molecular orbitals- visualization and interpretations; natural bond orbital calculation and analysis; visualization of NBO plots. The calculation and interpretation of Wiberg bond orders.

Bibliography of literature

Literature required to pass the course
Atkins' Molecules, P. Atkins, Cambridge University Press, 2003
Extracurricular readings
Handbook of Computational Chemistry, ed. J. Leszczyński, Springer, Science+Business Media B.V. 2012

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

K_W01: uses in-depth knowledge of spectroscopic methods of chemical compound analysis

K_W05: has extended knowledge in the field of chemical bonding

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

K_W08: demonstrates in-depth knowledge of various types of chemical bonding and their role in molecular structure stability

K_U02: critically assesses the results of performed theoretical calculations and discusses them in the context of predicted properties of inter- and intramolecular structure

K_U04: applies acquired knowledge of the chemical bonding, general chemistry and related scientific disciplines

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

Knowledge

Student defines and describes basic types of chemical bonding and explains the stability of molecular systems by characterizing the most important interactions responsible for binding.

Skills

Student has the ability of estimating the stability of various molecular systems, develops the ability of choosing a proper quantum chemistry method to investigate the type of chemical bonding, and the ability of visualizing and interpreting the results of the performed theoretical calculations.

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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