KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

Course title	ECTS code
Introduction to digital chemistry	13.3.1368

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 Agnieszka Gajewicz-Skrętna; dr inż. Karolina Jagiełło; prof. dr hab. Tomasz Puzyn; prof. dr hab. Piotr Skurski; dr Alicja Mikołajczyk; dr hab. Adam Sieradzan, profesor uczelni; prof. dr hab. Cezary Czaplewski, profesor uczelni; dr hab. Artur Giełdoń; dr Marcin Czapla

Forms of classes, the realization and number of hours

Forms of classes

Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 10 hours

ECTS credits

1
Lecture - 10 h
Student's own work: 7 h
Tutorial classes: 8 h
TOTAL: 25 h – 1 ECTS

The academic cycle

2023/2024 winter semester

Type of course

obligatory

Language of instruction

English

Teaching methods

multimedia-based lecture

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

Final evaluation

Graded credit

Assessment methods

written test in a form of a set of questions

The basic criteria for evaluation

Assessment criteria in accordance with the University of Gdańsk Study Regulations

a score of 51% or more required to pass the test

Method of verifying required learning outcomes

The method of verifying the acquisition of knowledge: passing the final test in a form of a set of questions and argumentation during the discussion.
The method of verifying the acquisition of skills: the student solves problems in writing (test) or oral (oral answer) in the field of digital chemistry.
The method of verifying the acquisition of social competences:
observation of the student's behavior during classes and during consultations

Required courses and introductory requirements

A. Formal requirements
none

B. Prerequisites
basic knowledge in chemistry and physics

Aims of education

The ability to describe the importance of digital chemistry across academia and industry. The ability to describe computational methods used to collect, analyze, and utilize a large quantity of chemometrics data, understand its complexity and the use of the digital chemistry in the designing process of advanced chemicals and materials with desired properties.

Course contents

Review of the most important aspects of digital chemistry, including the latest progress in advanced materials science, advances in big-data, molecular modelling, artificial intelligence, and machine learning methods used across academia and industry for design and synthesis of advanced materials.

Bibliography of literature

Literature required to pass the course
J. D. Lee – Concise inorganic chemistry
L. Jones, P. Atkins – Chemical principle
S. D. Brown, R. Tauler, B. Walczak (ed): Comprehensive chemometrics: Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009
R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 2005
Molecular Modelling: Principles and Applications, Andrew Leach, Prentice Hall 2001 Ideas of quantum chemistry, Lucjan Piela, Elsevier 2006
• R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 200

Extracurricular readings
L. Pauling – General chemistry
J. Leszczynski, A. Kaczmarek-Kedziera, T. Puzyn, M. G. Papadopulos, H. Reis, M. Shukla (ed): Handbook of Computational Chemistry (2nd Edition). Springer 2016. Volume 5: Chemoinformatics, Puzyn T (ed.).
T. Puzyn, J. Leszczynski, M. T. D. Cronin (ed): Recent Advances in QSAR Studies: Methods and Applications. Springer 2010. ISBN: 978-1-4020-9782-9.
K. Roy, S. Kar, R. Narayan Das (ed): A Primer on QSAR/QSPR Modeling - Fundamental Concepts. Springer 2015. ISBN: 978-3-319-17281-1.

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

K_W04: applies the acquired knowledge to an in-depth description of the properties of chemical connections, methods of their synthesis, and analysis

K_W07: selects experimental and theoretical techniques to the extent necessary to understand the description and modeling of extended complexity chemical processes

K_W09: classifies specialist IT tools used in statistical evaluation of experiment results

K_W11: demonstrates in-depth knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field

K_U03: finds necessary information in specialist literature, databases, and other sources, lists basic scientific journals in chemistry

K_U04: applies acquired knowledge of chemistry and related scientific disciplines

K_U06: presents the results of scientific discoveries in chemistry and related disciplines in an understandable way

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

Knowledge

The student knows the most important aspects of digital chemistry, including the latest progress in advanced materials science, molecular modelling methods, advances in big data, artificial intelligence, and machine learning methods used across academia and industry for the design and synthesis of advanced materials.
The student can name and describe the types of data-driven approaches used across academia and industry for design and synthesis of advanced materials.

Skills

The student can describe basic information about digital chemistry, i.e., describe advances in big data, the application of the computational modelling allowing predictive insights into the behavior and safety of complex molecules and systems, and most relevant chemoinformatic methods (including big-data, artificial intelligence, and machine learning techniques) used across academia and industry in the design process of advanced materials.

Social competence

At the end of the lecture, every student:
understand the application of digital chemistry across academia, and industry
is convinced that digital chemistry is being revolutionized by advances in artificial intelligence, machine learning, materials modeling, and big data
is convinced that digital chemistry is one of the most important field in the development of advanced materials with desire properties and safety

Contact

agnieszka.gajewicz@ug.edu.pl