KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

Course title	ECTS code
Computational methods for designing advanced materials	13.3.1321

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; prof. dr hab. Tomasz Puzyn; dr Alicja Mikołajczyk; dr inż. Karolina Jagiełło

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

•Introduction with the use of the multimedia presentation on computational methods used for the design of advanced materials
•In the computational, students will conduct hands-on exercises
•Project-based method (research, implementation, practical project)

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

Final evaluation

Graded credit

Assessment methods

- completion of the final project (written report) related to the design strategy for an imaginary drug,
- observation, how the students discuss the case studies.

The basic criteria for evaluation

Assessment criteria in accordance with the University of Gdańsk Study Regulations

- correctness of the proposed design strategy and written report

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements
none

B. Prerequisites
basic knowledge in chemistry

Aims of education

The aim of the course is ability to design of advanced materials with the use of computational methods.

Course contents

The concept of computational methods used for designing of advanced materials. The review of the latest progress in materials science and computational tools used to design of advanced chemicals and materials with desired properties and safety. Introduction to nanotechnology. Application of advanced materials in nanotechnology, photocatalysis, and nanomedicine. Safe and sustainability design (SSbD) strategy for the

design of advanced materials which present of an optimal combination of specific features, functionality, and safety. The methods used for physic-based and data-based models' development used for describing and predicting the quantitative relationship between structure, properties, and toxicity of designed advanced materials (reverse modeling, Structure-Activity Prediction Networks, SAPNet).

Bibliography of literature

Literature required to pass the course
I. A. Parinov, S.-H. Chang, V. K. Gupta: Advanced Materials. Springer 2017. ISBN: 978-3-319-78918-7
A. Tiwari; N. A.Murugan; R. Ahuja. Advanced Engineering Materials and Modeling. Scrivener Publishing. ISBN-13: 9781119242468
B. Extracurricular readings
S. Thomas, N. Kalarikkal, A.M. Stephan, B. Raneesh, Advanced Nanomaterials, Synthesis, Properties, and Applicationsm, Academic Press, ISBN 9781774633090

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

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

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

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_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_U06: presents the results of scientific discoveries in chemistry and related disciplines in an understandable way

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

K_K04: correctly identifies and resolves dilemmas related to the profession of a chemist

K_K07: can think and act in an entrepreneurial manner

Knowledge

At the end of the course every student:
knows the basic application of advanced materials in technology, medicine, and industry
knows computational methods applied for the design of advanced materials
knows basic software packages to be used as a tool supporting advanced materials design
explains theoretical background (algorithms development) of the essential chemometric methods used in the prediction of safety and efficiency of chemicals at the early stage of its design
explains the theoretical background of the advanced methods for defining: (1) the relationships between the structural properties and toxicity of designed materials, (1) the relationships between the structural properties and functionality of designed materials

Skills

At the end of the course every student:
correctly prepares data (including molecular models and data matrix) for the design of advanced materials
performs chemoinformatic analyses that may support the design of efficient and safe materials and correctly interprets the results
develops regression and classification models, validates the models correctly, and applies the models for prediction of toxicity and/or functionality of designed materials
use computational methods as tools supporting the design of advanced materials with specific properties (i.e., advanced materials which present an optimal combination of specific features, functionality, and safety)

Social competence

At the end of the lecture, every student:
is convinced that the use of a computer and exploratory analysis strengthens the potential of data analysis
can critically evaluate experimental results and understand the necessity of their control
understands the need for deeper learning as a method supporting the design of advanced materials
is convinced that the use of in silico models strengthens the potential of limiting the number of animal tests and increasing the efficiency of the design process

Contact

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