KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI
Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego
UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

| Course title | ECTS code |
|---|---|
| Advanced nanoinformatics | 13.3.1314 |

**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**

prof. dr hab. Tomasz Puzyn; dr Agnieszka Gajewicz-Skrętna; 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
Laboratory classes - 30 h
Student's own work – 15 h
Tutorial classes – 5 h
Total: 45 h - 2 ECTS
TOTAL: 50 h – 2 ECTS

**The academic cycle**

2024/2025 winter semester

**Type of course**

an elective course

**Language of instruction**

English

**Teaching methods**

During the auditorium classes students will conduct hands on exercises in the computational laboratory, based on the instructions prepared by the teacher.

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

**Final evaluation**

Graded credit

**Assessment methods**

auditorium classes – colloquia and written reports, final assignment completion in the form of written report and/or oral presentation

**The basic criteria for evaluation**

according to "Rules and regulations for studies at the University of Gdansk"

**Method of verifying required learning outcomes**

**Required courses and introductory requirements**

**A. Formal requirements**

Introduction to Python programming
- Introduction to R programming
- Quantum chemistry in practice
- Exploratory analysis of multidimensional chemical space
- Machine learning in chemistry

Molecular descriptors

**B. Prerequisites**

Introduction to Python programming
- Introduction to R programming
- Quantum chemistry in practice
- Exploratory analysis of multidimensional chemical space
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Molecular descriptors

## Aims of education

familiarizing the students with the current status, challenges and recent efforts in application of computational approaches in nanomaterials' characterization, analysis and modelling
presenting the benefits of using nanoinformatics for modelling activity and toxicity, properties, interactions and fate of nanomaterials (NMs)

## Course contents

The course covers practical issues in nanoinformatics which includes:
introduction to nanotechnology, nanoscience and nanomaterials areas,
introduction to nanoinformatics and statistical modelling (data collection, curation, metadata and ontologies in nanoinformatics; nanodescriptors; unsupervised techniques for similarity analysis, profiling, and grouping; supervised techniques for filling data gaps),
application of computational models/tools/software packages to compute/model activity and toxicity, properties, (bio)interactions and fate of NMs,
application of the combination of modeling approaches for selected case study nanoparticles (e.g., carbon nanostructures, metal oxide nanoparticles),
group discussions on selected computational nanoscience papers, published in top journals.

## Bibliography of literature

Literature required to pass the course
The EU – US Nanoinformatics 2030 Roadmap: https://www.nanosafetycluster.eu/outputs/eu-us-roadmap-nanoinformatics-2030/
Extracurricular readings
Nanoscience and Advancing Computational Methods in Chemistry: Research Progress (Eds.) Eduardo A. Castro and A.K. Haghi, 2012

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

K_W06:
applies mathematics to the extent necessary to understand, describe and model chemical processes of extended complexity
K_W08:
demonstrates in-depth knowledge of theoretical computational and IT methods used to solve problems in chemistry
K_W09:
classifies specialist IT tools used in statistical evaluation of experiment results
K_U02
critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors
K_U03
finds necessary information in specialist literature, databases and other sources, lists basic scientific journals in chemistry
K_K02
works in a team taking on various roles in it
K_K06
raises her/his professional and personal competences by using information provided in various sources

## Knowledge

At the completion of this course, the student is expected to be able to:
know and understand the basic nanoinformatics concepts,
know theoretical basics of computational methods used in the nanoinformatics,
provide examples of computational models/tools/software packages for nanoinformatics,
describe the most important challenges for the application of computational approaches in nanomaterials' characterization, analysis and modelling,
describe the benefits and advantages of using nanoinformatics.

## Skills

At the completion of this course, the student is expected to be able to critically interpret the results obtained with specific nanoinformatics approaches.

## Social competence

At the completion of this course, the student is expected to be able to:
understand that the nanoinformatics is important in the process of designing new advanced materials as well as in supporting risk assessment of nanomaterials,
understand the need of deeper learning of the nanoinformatics,
develop interpersonal skills such as communication, cooperation in group (taking different roles), and problem-solving abilities,
understand the social aspects of practical use of knowledge and abilities as well as connected with them responsibility.

## Contact

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