KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
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FUNDUSZ SPOŁECZNY

Course title	ECTS code
Molecular mechanics & dynamics, coarse-grain modeling	13.3.1291

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. Cezary Czaplewski, profesor uczelni; prof. dr hab. Tomasz Puzyn; dr hab. Artur Giełdoń; dr hab. Adam Sieradzan, profesor uczelni; dr Jakub Brzeski; mgr Annemarie Danielsson

Forms of classes, the realization and number of hours

Forms of classes

Laboratory classes, Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours, Laboratory classes: 45 hours

ECTS credits

6
Lecture 30 h
Laboratory classes - 45 h
student's own work – 30 h
tutorial classes – 45 h
TOTAL: 150 h – 6 ECTS

The academic cycle

2023/2024 summer semester

Type of course

obligatory

Language of instruction

English

Teaching methods

- Practical laboratory work – computational chemistry experiments and case studies, analysis of obtained results and discussion
- multimedia-based lecture

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

Final evaluation

- Graded credit
- Examination

Assessment methods

Lecture – exam with multiple-choice questions
Laboratory 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

Lab classes: the arithmetic mean of partial grades received during the semester for written reports on laboratory 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.
Lectures: passing the final exam in the form of a multiple-choice question test (a score of 50% or more required to pass the exam).

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements
lack

B. Prerequisites
ability to use the LINUX operating system, basics of organic chemistry

Aims of education

Practical introduction to the techniques and tools of computational chemistry used in molecular modeling.
Teaching students how to choose the right methods of computational chemistry depending on the system under study

Course contents

Visualization of chemical molecules and macromolecules. Molecular mechanics, determining the structure and conformational changes of chemical molecules. Empirical force fields and their application in conformational analysis. Introduction to computer simulation methods: Monte Carlo and molecular dynamics (MD). Parameterization of empirical force fields used in molecular mechanics and molecular dynamics. Application of ab initio and semi-empirical methods in parametrization of empirical forcefields. Modeling of macromolecules: DNA, RNA, proteins, and their complexes. Protein structure prediction. Molecular docking. Protein-peptide, and protein-protein docking. CASP and CAPRI initiatives. Coarse-grain modeling of macromolecules.

Bibliography of literature

Molecular Modelling: Principles and Applications, Andrew Leach, Prentice Hall 2001
Ideas of quantum chemistry, Lucjan Piela, Elsevier 2006

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

K_W05: has extended knowledge in the field of the specialisation studied

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

K_W08: demonstrates in-depth knowledge of theoretical computational and IT methods used to solve problems in chemistry

K_U02: critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors

K_U04: applies acquired knowledge of chemistry and related scientific disciplines

K_K01: knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so

Knowledge

Student defines and describes basic molecular modeling methods. Distinguishes between methods of quantum chemistry and methods of molecular mechanics as well as deterministic and stochastic methods of computer simulations. Characterizes approximations used in quantum chemistry methods and empirical force fields.

Skills

The student classifies molecular modeling methods used to determine the structure, spectral characteristics, properties of chemical compounds in different states of concentration and selects the appropriate method of computational chemistry to support experimental work. He conducts calculations and computer simulations using selected computational chemistry programs, analyzes the results of computer simulations, compares the results of calculations with experimental data.

Social competence

The student develops the skills of accurate and logical thinking and inference. Learns the principles of working safely, responsibly, and efficiently using the workstations connected to the Internet. Develops the responsibility for his/her personal account on the workstation. Develops the ability to work in a team.

Contact

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