KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

Course title	ECTS code
Monographic lecture - Computational chemistry software	13.3.0443

Name of unit administrating study

null

Studies

faculty	field of study		
Wydział Chemii	Chemia	type	drugiego stopnia
		form	stacjonarne
		specialty	chemia biomedyczna, analityka i diagnostyka chemiczna, chemia i technologia środowiska, chemia obliczeniowa
		specialization	wszystkie

Teaching staff

prof. dr hab. Cezary Czaplewski, profesor uczelni; prof. dr hab. Józef Liwo

Forms of classes, the realization and number of hours

Forms of classes

Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours

ECTS credits

3
classes 30 h
tutorial classes 10 h
student's own work 35 h
TOTAL: 75 h - 3 ECTS

The academic cycle

2023/2024 summer semester

Type of course

obligatory

Language of instruction

polish

Teaching methods

multimedia-based lecture

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

Final evaluation

Graded credit

Assessment methods

assignment work – project or presentation

The basic criteria for evaluation

Correctness and attractiveness of the presentation of a selected program in the field of computational chemistry.
Assessment criteria in accordance with the University of Gdansk Studies Regulations

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements
Information technology, Quantum Chemistry, Teoretical Chemistry

B. Prerequisites
Ability to work in the Unix system, knowledge of basics of quantum chemistry, knowledge of terminology and nomenclature used in quantum chemistry, ability to describe the geometry of chemical molecules, the basics of statistical mechanics and molecular mechanics

Aims of education

Introduction to the available software for quantum chemistry calculations as well as molecular mechanics and molecular dynamics simulations

Course contents

Using UNIX shell scripts. The sed stream editor and awk scripts, their application to the analysis of results obtained from computational chemistry software. Running tasks in high performance computer centers. Queuing systems: PBS, LSF and NQS. Software for ab initio and semi-empirical quantum chemistry calculations: GAMESS, GAUSSIAN, MOPAC, MOLPRO, TURBOMOLE packages. Software for molecular mechanics and

molecular dynamics simulations: AMBER, GROMACS, TINKER, NAMD, ECEPPAK packages. Molecular editors and visualization software: Avogadro, Molden, MolMol, RasMol, Pymol, VMD, Chimera, Sirius. CSDS database of crystallographic structures of small molecules and PDB database of biomolecular structures and their use.

Bibliography of literature

Literature required to pass the course

Extracurricular readings

D.W. Heermann, Podstawy symulacji komputerowych w fizyce, WNT, 1997
L. Piela, Idee chemii kwantowej, PWN, 2018
A.Leach, Molecular Modelling: Principles and Applications, Prentice Hall, 2001
C.J. Cramer, Essentials of Computational Chemistry, Wiley, 2004

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

Knowledge

The student recognizes and characterizes the available software for quantum chemistry as well as molecular mechanics and molecular dynamics calculations. Distinguishes between programs for quantum chemistry calculations and programs using molecular mechanics methods

Skills

Social competence

Learns the principles of safe, responsible and effective work on supercomputers in data centers.

Contact

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