


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	type	drugiego stopnia
Wydział Chemii	Chemia	form	stacjonarne
		specjalty	chemia biomedyczna, chemia i technologia środowiska, analityka i diagnostyka chemiczna, 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		ECTS credits	
Forms of classes		3	
Lecture		classes 30 h	
The realization of activities		tutorial classes 10 h	
classroom instruction		student's own work 35 h	
Number of hours		TOTAL: 75 h - 3 ECTS	
Lecture: 30 hours			
The academic cycle			
2023/2024 summer semester			
Type of course		Language of instruction	
obligatory		polish	
Teaching methods		Form and method of assessment and basic criteria for evaluation or examination requirements	
multimedia-based lecture		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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