UNIWERSYTET GDAŃSKI

Course title Wykład monograficzny - Oprogramowanie w chemii obliczeniowej/Monographic lecture - Computational chemistry software	**ECTS code** 13.3.0443

Name of unit administrating study
Faculty of Chemistry

Studies

Field of study	Type	Form	
Chemistry	Master	Full-time studies	

Teaching staff
dr hab. Cezary Czaplewski, prof. UG

Forms of classes, the realization and number of hours

A. Forms of classes, in accordance with the UG Rector's regulations
lecture

B. The realization of activities
In-class learning

Number of hours
lecture 30 h

ECTS credits

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

The academic cycle
Second year, summer semester

Type of course
obligatory

Language of instruction
Polish

Teaching methods
Lecture with multimedia presentation

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

A. Final evaluation, in accordance with the UG study regulations
Course completion (with a grade)

B. Assessment methods
Knowledge of available software for quantum chemistry calculations and molecular mechanics and dynamics simulations.

C. The basic criteria for evaluation or exam requirements

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

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

A. Literature required to pass the course

B. 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

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.

Social competence

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