UNIWERSYTET GDAŃSKI

Course title
Modelowanie molekularne / Molecular modelling

ECTS code
13.3.0441

Name of unit administrating study
Faculty of Chemistry

Studies

Field of study	Type	Form	
Chemistry	Masters	Full-time studies	

Teaching staff
Dr hab. Cezary Czaplewski, prof. nadzw.

Forms of classes, the realization and number of hours

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

B. The realization of activities
in-class learning

C. Number of hours
45 h (15 h lecture, 30 h laboratory class)

ECTS credits 7

classes - 45 h
tutorial classes – 15 h
student's own work – 115 h

Total: 175 h - 7 ECTS

The academic cycle
2020/21 winter semester

Type of course
obligatory

Language of instruction
Polish

Teaching methods

Lecture with multimedia presentation
Perfoming experiments

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

A. Final evaluation, in accordance with the UG study regulations
lecture – exam
laboratory classes – course completion (with a grade)

B. Assessment methods
Exam, multiple-choice question test
The final grade is based on partial grades received during the semester.

C. The basic criteria for evaluation or exam requirements

Lab classes: the arithmetic mean of partial grades received during the semester for written reports on laboratory exercises, 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).

Required courses and introductory requirements
Completed course on Information technology and Theoretical chemistry.
Ability to use the UNIX operation system, describe geometry of chemical molecules, knowledge of basics of statistical mechanics

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. Molecular mechanics, determining the structure and conformational changes of chemical molecules. Empirical force fields and their application in conformational analysis. Application of ab initio and semi-empirical methods. Basis sets used in ab initio calculations. The canonical and localized orbitals. Limits of single-electron approximation accuracy, energy of electron correlation. Methods that go beyond the one-electron approximation. Basis set superposition error (BSSE) in calculations of intermolecular interactions. Thermodynamics and kinetics of chemical reactions on the ground of quantum chemistry. Introduction to computer simulation methods: Monte Carlo and molecular dynamics. Parameterization of empirical force fields used in molecular mechanics and molecular dynamics. Modeling of macromolecules - DNA, RNA, proteins.

Bibliography of literature

A. Literature required to pass the course

Podstawy symulacji komputerowych w fizyce, Heermann Dieter W., WNT 1997
Komputery w chemii medycznej z Chemia medyczna. Podstawowe zagadnienia, Graham Baker, Graham L. Patrick, WNT 2003

B. Extracurricular readings

Knowledge

Student defines and describes basic molecular modeling methods and basis sets used in ab initio calculations. 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. Distinguishes between natural and localized orbitals. Defines a basis set superposition error.

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 of working in a team.