UNIWERSYTET GDAŃSKI

Course title	**ECTS code**
Wykład monograficzny - Wprowadzenie do kwantowej chemii komputerowej/Monographic lecture - Introduction into quantum computer chemistry	13.3.0440

Name of unit administrating study
Faculty of Chemistry

Studies

Field of study	Type	Form	
Chemistry	Master	Full-time studies	

Teaching staff
Prof. dr hab. Janusz Rak

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
2020/2021 summer semester

Type of course
obligatory

Language of instruction
Polish

Teaching methods
Lacture with a multimedial 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
oral credit, test

C. The basic criteria for evaluation or exam requirements

Passing with no less than 51% of the maximum score.
Those who do not reach the required threshold take an oral examination.

Required courses and introductory requirements

a. **Formal requirements** Chemia fizyczna, chemia kwantowa
b. **Prerequisites** Abilities to describe a chemical reaction in the context of thermodynamics and kinetics, basic knowledge on molecular spectroscopy.

Aims of education
Acquisition of the ability to:
- choose an appropriate computational chemistry method to a given chemical problem,
- design a computational algorithm assuring possibly swift solution,
- judge the accuracy of numerical data.

Course contents

Born-Oppenheimer approximation, time independent Schrödinger equation, one-electron approximation, Slater determinant, Hartree-Fock (HF) and Hartree-Fock-Roothan (HFR) methods, semiempirical schemes of the HFR method: CNDO, INDO, NDDO; modified NDDO methods: MNDO, AM1, P<3, M5, RM1, PM6, MNDO/d, SAM1, SAM1d. Basis sets. Electron correlation: configuration interaction, Møller–Plesset perturbation theory (MPn), coupled cluster method (CC). Density functional theory (DFT). Application of HFR and electron correlation methods: choice of the basis set, optimization of molecular geometry, determining reaction enthalpy, harmonic vibrational modes (IR spectrum), NMR shifts and electronic absorption spectrum for a molecular system.

Bibliography of literature

A. Literature required to pass the course

Lucjan Piela „Idee chemii kwantowej", PWN 2003.
Frank Jensen „Introduction to Computational Chemistry", Wiley, 2006.
Christopher J. Cramer „Essentials of Computational Chemistry: Theories and Models", Wiley, 2004

B. Extracurricular readings

Attila Szabo, Neil S. Ostlund „Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory", Dover Publi-cations, 1996.

Knowledge

A student:

• has knowledge on concepts, rules and theories functioning in computational chemistry,
• characterizes Hartree-Fock methods and has knowledge on the employed approximations and limitations,
• mentions basis sets used in quantumchemical calculations,
• identifies methods accounting for electron correlation,
• characterizes density functional methods,
• mentions applications of quantumchemistry methods.

Social competence

A student:
• can work independently,
• keeps caution and criticism in expressing opinions