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 - Introduction into quantum computer chemistry	13.3.0440

Name of unit administrating study

Faculty of Chemistry

Studies

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

Teaching staff

prof. dr hab. Janusz Rak

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

- (mid-term / end-term) test
- oral credit, test

The basic criteria for evaluation

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

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements

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

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

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

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.

Skills

Social competence

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

Contact

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