DOCTORAL SCHOOL OF WROCŁAW UNIVERSITY OF SCIENCE AND TECHNOLOGY

3SUPERVISOR/TEAM/ DECLARING/CONDUCTING COURSE: Robert Góra
DEPARTMENT K17W03D10

COURSE CARD

Course name in Polish: Teoretyczne metody badania fotochemii i fotofizyki układów molekularnych
Course name in English: Theoretical methods for studies of photochemistry and photophysics of molecular systems
Course language ~~Polish~~ / English*
Specialized courses for PhD students receiving education in discipline:* interdisciplinary course in the field of several disciplines: theoretical chemistry and physics
Subject code: NCQ100206C

* delete as applicable

	Lecture	Foreign language course	Seminar	Mixed forms
Number of hours of organized classes in university (ZZU)		-	-	30
Grading		-	-	Report
Number of ECTS points				

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. General chemistry and physics
2. Linear algebra and mathematical analysis
3. Basics of quantum mechanics

COURSE OBJECTIVES

C1. To acquaint students with modern methods of theoretical description of the electronic structure of atoms and molecules and to acquire the ability to apply these methods to determine the electronic structure and properties of molecular systems.
C2. Acquiring the ability to apply methods of theoretical chemistry to prediction and interpretation of selected spectral properties of molecular systems, including one- and two-quantum absorption spectra, emission spectra and non-adiabatic radiationless processes (transfer of excitation energy, internal conversion and inter-system transitions).
C3. Acquiring knowledge about the practical applications of spectroscopic techniques and photochemical and photophysical processes in technology and various branches of the economy and their significance for society.
C4. Individual work on the assigned project.

PROGRAM CONTENTS

Form of classes – mixed forms (mix)		Number of hours
Mix1	**Work organization in a computer lab and a computing center.** Discussing the principles of health and safety at work. Distribution of accounts and basic information about available operating systems.	2
Mix2	**Elements of the LINUX system I.** Basic information about the operating system. Selected BASH shell commands.	2
Mix3	**Elements of the LINUX system II.** Support for selected text editors. Simple BASH shell scripts.	2
Mix4	**Calculations of the electronic structure in the Hückel model for selected molecules.** Eigenvalue problem in matrix form. Diagonalization of the Hamiltonian and interpretation of eigenvalues spectra and eigenvectors.	2
Mix5	**Representation of the structure of molecular systems.** Orthogonal coordinates and internal coordinates on the example of Z-matrix.	2
Mix6	**Selected electronic structure calculation packages.** Preparation of batch files. Calculations of the electronic structure of atoms using the restricted and unrestricted Hartree-Fock method (HF). Structure of output files and interpretation of the results of calculations.	2
Mix7	**Optimization of equilibrium geometry of molecules and analysis of normal-mode vibrations.** Discussion of gradient geometry optimization algorithms. Calculations of the harmonic frequencies spectrum. Analysis of normal coordinates. Prediction and interpretation of infrared spectra.	2
Mix8	**Molecular orbital theory.** Determination of potential energy curves for diatomic molecules in the HF method. Determination and interpretation of molecular orbital and Walsh diagrams.	2
Mix9	**Configuration interaction method.** Calculation of electronic states' spectra using the configuration interaction method with single (CIS) and double excitations (CISD). Size-extensivity and size-consistency of the CI method. **Project I.** Calculations of the electronic states spectra and their interpretation for selected polyatomic molecules.	2
Mix10	**Accuracy of computational chemistry methods.** Selection of the basis functions. Comparison of the accuracy of selected ab initio methods and density functional theory methods. Validation of electronic structure calculation methods.	2
Mix11	**Prediction and interpretation of absorption and fluorescence spectra in the UV-vis range.** Interpretation of the character of electronically excited states. Natural transition orbitals. Exploration of the potential energy surfaces in electronically excited states.	2
Mix12	**Project II.** Determination of the fine structure of absorption and fluorescence spectra within the linear coupling model in selected systems.	2
Mix13	**Search and characteristics of intersection seams of electronic states and their minima.** Theoretical methods of locating minimum energy intersections of electronic states. Conical intersections and intersystem crossings. Determination of transient absorption spectra.	2
Mix14	**Project III.** Determination of nonradiative deactivation channels in model systems.	2
Mix15	**Presentations of the results of projects I-III**	2
	Total hours	30

TEACHING TOOLS USED
N1. Lecture at the blackboard N2. Multimedia presentation N3. Implementation of tasks / projects in the computer lab N4. Personal computers / resources of the computing center / specialized software

ACHIEVED SUBJECT LEARNING OUTCOMES		
Type of learning outcome	Code of learning outcome	Assessment of learning outcome
Skills	P8S_UW	report
Skills	P8S_UO	report
Social competence	P8S_KO	presentation
Social competence	P8S_KR	presentation

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] R. W. Góra, teaching materials for the interdisciplinary course: "Theoretical methods for studies of photochemistry and photophysics of molecular systems", 2019
[2] L. Piela, "Ideas of Quantum Chemistry" 3rd Edition, Elsevier, 2019
[3] K. Pigoń, Z. Ruziewicz, Chemia Fizyczna (cz. 2), PWN, Warszawa, 2005.
[4] D. O. Hayward, "Quantum Mechanics for Chemists", RSC, 2002

SECONDARY LITERATURE:

[1] Engel, T., Reid, P., Quantum Chemistry and Spectroscopy, 3rd ed. ed. Pearson, Boston, 2013.
[2] Olivucci, M. (Ed.), Computational Photochemistry, 1st ed., Theoretical and computational chemistry. Elsevier, Amsterdam ; Boston, 2005.
[3] May, V., Kühn, O., Charge and Energy Transfer Dynamics in Molecular Systems, 3rd ed. Wiley-VCH Verlag GmbH & Co. KGaA, 2011.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)
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