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: NCQ100167W

* delete as applicable

	Lecture	Foreign language course	Seminar	Mixed forms
Number of hours of organized classes in university (ZZU)	30	-	-	
Grading	Exam	-	-	
Number of ECTS points	**3**			

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.

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PROGRAM CONTENTS

Form of classes – lecture (Lec)		Number of hours
Lec1	**Introduction to molecular quantum mechanics.** Discussion of postulates of non-relativistic quantum mechanics. Definition of a wave function and its probabilistic interpretation. Definition of operators representing mechanical observables and elements of operator algebras. Time-dependent and time-independent Schrödinger's equation.	2
Lec2	**Approximate methods of solving the Schrödinger equation I.** Variation calculus and its applications to model problems. Rayleigh-Ritz method.	2
Lec3	**Approximate methods of solving the Schrödinger equation II.** Molecular orbitals theory. Hückel's method and its illustrative applications.	2
Lec4	**Approximate methods for solving the Schrödinger equation III.** A time-independent perturbation theory. Perturbation in two-state and multi-state systems. Perturbation theory for degenerate reference states.	2
Lec5	**Wave functions for many-electron systems.** Symmetry of the wave function. A determinantal wave function. The Slater-Condon rules. General expressions for matrix elements between Slater's determinants.	2
Lec6	**The Hartree-Fock method.** The self-consistent field method. The Hartree-Fock-Roothan method. The charge density and matrix elements of the Fock operator.	2
Lec7	**Molecular Hamiltonian.** Separation of the electronic and nuclear degrees of freedom. The adiabatic approximation and the Born-Oppenheimer approximation. The harmonic approximation. Normal modes analysis and interpretation of absorption spectra in the infrared range.	2
Lec8	**Molecular orbitals.** Elements of point group theory. Symmetry and nomenclature of molecular orbitals. Molecular orbitals diagrams for diatomic and polyatomic molecules. Walsh diagrams.	2
Lec9	**Electronic correlation I.** Limitations of the Hartree-Fock method. Definition and methods for determining the electron correlation. The configuration interaction method.	2
Lec10	**Electronic correlation II.** The Møller-Plesset perturbation theory. Elements of the coupled clusters method.	2
Lec11	**The density functional theory.** One-particle density matrix and pair-density matrix. The Hohenberg-Kohn theorems. The Kohn-Sham method.	2
Lec12	**The interaction of matter with electromagnetic radiation.** The fate of molecules in electronically excited states. Photochemical and photophysical processes in molecular systems. Jabłoński diagram.	2
Lec13	**Absorption and fluorescence spectra in the UV and visible range.** Fermi's golden rule. Selection rules. Fine structure of absorption and fluorescence spectra.	2
Lec14	**Processes of nonradiative deactivation of excited states.** Internal conversion. Conical intersections. Intersystem crossings. Excitation energy transfer - Förster's and Dexter's mechanisms. Natural and artificial light-harvesting systems. Photosynthesis.	2
Lec15	**Theoretical and experimental methods for studying photochemical and photophysical properties of molecular systems.** Non-adiabatic dynamics. Transient absorption spectra and their interpretation.	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
Knowledge	P8U_W	exam
Knowledge	P8S_WG	exam
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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