**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:** CIQ100167W* delete as applicable

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

## 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 – 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<br>N2. Multimedia presentation<br>N3. Implementation of tasks / projects in the computer lab<br>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)**

Robert W. Góra, robert.gora@pwr.edu.pl

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

**PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES**

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## 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 |

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