Wrocław University of Science and Technology
Doctoral School

COURSE CARD

1. Basic information

Course name in English:	Theoretical methods for studies of photochemistry and photophysics of molecular systems	
Course name in Polish:	Teoretyczne metody badania fotochemii i fotofizyki układów molekularnych	
Number of hours:	30	
Type of course:	Elective course	
Form of course:	laboratory	
Code of course:		
Course leader:	*Dr. Robert Góra, PhD, DSc*	
Faculty of the course leader:	W3 Faculty of Chemistry	
Email address of the course leader:	robert.gora@pwr.edu.pl	
Scientific discipline(s) assigned to the course (doctoral students representing the marked disciplines can participate in the course):	Architecture and urban planning	☐
	Automation, electronic, electrical engineering and space technologies	☐
	Information and communication technology	☐
	Biomedical engineering	☐
	Chemical engineering	☐
	Civil engineering, geodesy and transport	☐
	Materials engineering	☒
	Mechanical engineering	☐
	Environmental engineering, mining, and energy	☐
	Mathematics	☐
	Chemical sciences	☒
	Physical sciences	☒
	Management and quality studies	☐

2. Objectives

O1. 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.
O2. 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).
O3. 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.
O4. Individual work on the assigned project.

3. Content

Detailed information about the course content, including topics and form of classes.

No.	Topic	Number of hours	Form of classes
1	**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	laboratory
2	**Elements of the LINUX system I.** Basic information about the operating system. Selected BASH shell commands.	2	laboratory
3	**Elements of the LINUX system II.** Support for selected text editors. Simple BASH shell scripts.	2	laboratory
4	**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	laboratory
5	**Representation of the structure of molecular systems.** Orthogonal coordinates and internal coordinates on the example of Z-matrix.	2	laboratory
6	**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	laboratory
7	**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	laboratory
8	**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	laboratory
9	**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	project
10	**Accuracy of computational chemistry methods.** Selection of the basis functions. Comparison of the accuracy of selected ab initio methods and density	2	laboratory

	functional theory methods. Validation of electronic structure calculation methods.		
11	**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	laboratory
12	**Project II.** Determination of the fine structure of absorption and fluorescence spectra within the linear coupling model in selected systems.	2	project
13	**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	laboratory
14	**Project III.** Determination of nonradiative deactivation channels in model systems.	2	project
15	**Presentations of the results of projects I-III**	2	seminar

4. Prerequisites

List of prerequisites relating to knowledge, skills and other competences for course participants.

1. General chemistry and physics
2. Introductory linear algebra and mathematical analysis
3. Fundamentals of quantum mechanics

5. Learning outcomes

List of learning outcomes at level 8 of the Polish Qualifications Framework assigned to the course (mark the learning outcomes in the last column).

Symbol	Learning outcome	
	KNOWLEDGE. Doctoral student knows and understands:	
SzD_W3	the main trends in the development of the scientific or artistic disciplines covered in the curricula;	☒
SzD_W4	research methodology;	☒
SzD_W5	the rules for the dissemination of scientific results, including in open access mode;	☒
SzD_W6	the fundamental dilemmas of modern civilization;	☐
SzD_W7	the legal and ethical conditions of scientific activity;	☐
SzD_W8	the economic and other relevant conditions of scientific activity;	☐

SzD_W9	basic principles of knowledge transfer to the economic and social spheres and commercialisation of results of scientific activity and know-how related to these results.	☐
	SKILLS. Doctoral student is able to:	
SzD_U2	use knowledge from different fields of science or art to creatively identify, formulate and innovatively solve complex problems or perform research tasks, in particular: - define the purpose and subject of scientific research, formulate a research hypothesis, - develop research methods, techniques and tools, and use them creatively, - draw conclusions on the basis of scientific research; critically analyse and evaluate the results of scientific research, expertise and other creative work and their contribution to knowledge development; transfer the results of scientific activities to the economic and social spheres;	☒
SzD_U3	communicate on specialised topics to the extent that they enable an active participation in the international scientific community;	☒
SzD_U4	disseminate research results, including in popular forms;	☐
SzD_U5	initiate debates and participate in a scientific discourse;	☒
SzD_U6	be able to speak a foreign language at B2 level of the Common European Framework of Reference for Languages to a level that enables them to participate in the international scientific and professional environment;	☐
SzD_U7	plan and implement an individual or collective research or creative activity, including in an international environment;	☐
SzD_U8	independently plan and act for one’s own development and inspire and organize the development of others;	☐
SzD_U9	plan classes or groups of classes and implement them using modern methods and tools.	☐
	SOCIAL COMPETENCES. Doctoral student is ready to:	
SzD_K3	fulfilling the social obligations of researchers and creators, initiate public interest activities, thinking and acting in an entrepreneurial way;	☐
SzD_K4	maintaining and developing the ethos of research and creative environments, including: - carrying out scientific activities in an independent manner, - respecting the principle of public ownership of research results, taking into account the principles of intellectual property protection.	☐

6. Evaluation

Short description of the method(s) used to evaluate the learning outcomes assigned to the course, e.g., exam, test, report, presentation, etc.

A short report on selected topic

7. Teaching methods

Short description of the teaching methods used during the course, e.g., multimedia presentation, discussion, literature studies, developing written documents, own work, etc.

Lecture at a blackboard, multimedia presentation, discussion, own work.

8. Literature

List of primary and secondary literature used to prepare the course and including additional knowledge for participants, e.g., books, textbooks, research papers, standards, web pages, etc.

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] 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.

9. Other remarks

Additional remarks, comments, (e.g., language of the course)

An interdisciplinary course covering several disciplines, rooted in theoretical chemistry and physics.