Wrocław University of Science and Technology
Doctoral School

COURSE CARD

1. Basic information

Course name in English:	Introduction to Modern Theoretical Chemistry	
Course name in Polish:	Wprowadzenie do współczesnej chemii teoretycznej	
Number of hours:	30	
Type of course:	Elective course	
Form of course:	mixed forms (combination of lecture, seminar and 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 (excitation energy transfer, internal conversion and inter-system crossings).
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	**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	lecture
2	**Approximate methods of solving the Schrödinger equation I.** Variation calculus and its applications to model problems. Rayleigh-Ritz method. Molecular orbitals theory.	2	lecture
3	**Approximate methods for solving the Schrödinger equation II.** A time-independent perturbation theory. Perturbation in two-state and multi-state systems. Perturbation theory for degenerate reference states.	2	lecture
4	**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	lecture
5	**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. The self-consistent field method. The Hartree-Fock-Roothan method.	2	lecture
6	**Selected electronic structure calculation packages.** Setting up the calculations. Calculations of the electronic structure of atoms and molecules using the Hartree-Fock method. Interpretation of the results of calculations.	2	laboratory
7	**Electronic correlation I.** Limitations of the Hartree-Fock method. Definition and methods for determining the electron correlation. The configuration interaction method.	2	lecture
8	**Electronic correlation II.** The many-body perturbation theory. The coupled clusters method.	2	lecture
9	**The density functional theory.** One-particle density matrix and pair-density matrix. The Hohenberg-Kohn theorems. The Kohn-Sham method.	2	lecture

10	**Accuracy of computational chemistry methods.** Selection of the basis set. Comparison of the accuracy of selected ab initio methods and density functional theory methods. Validation of electronic structure calculation methods.	2	laboratory
11	**Optimization of equilibrium geometry of molecules and analysis of normal-mode vibrations.** Discussion of gradient geometry optimization algorithms. Calculations of the harmonic vibrational frequencies spectra. Analysis of normal coordinates. Prediction and interpretation of infrared spectra.	2	laboratory
12	**The interaction of matter with electromagnetic radiation.** The fate of molecules in electronically excited states. Photochemical and photophysical processes in molecular systems. Jabłoński diagram. Fermi's golden rule. Selection rules.	2	lecture
13	**Prediction and interpretation of absorption and fluorescence spectra.** Interpretation of the character of electronically excited states. Natural transition orbitals. Exploration of the potential energy surfaces in electronically excited states.	2	laboratory
14	**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.	2	lecture
15	**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

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] Engel, T., Reid, P., Quantum Chemistry and Spectroscopy, 3rd ed. ed. Pearson, Boston, 2013.
[3] D. O. Hayward, "Quantum Mechanics for Chemists", RSC, 2002

SECONDARY LITERATURE:

[1] L. Piela, "Ideas of Quantum Chemistry" 3rd Edition, Elsevier, 2019
[2] Olivucci, M. (Ed.), Computational Photochemistry, 1st ed., Theoretical and computational chemistry. Elsevier, Amsterdam ; Boston, 2005.

9. Other remarks

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

An interdisciplinary course covering several disciplines, rooted in theoretical chemistry and physics. Course in the mixed lecture / hands-on exercises form given in English