A COURSE SYLLABUS – DOCTORAL SCHOOL

REGARDING THE QUALIFICATION CYCLE FROM 2020 TO 2024

REGARDING THE QUALIFICATION CYCLE FROM 2021 TO 2025

GENERAL INFORMATION ABOUT COURSE	
Course title	**Atomic and molecular spectroscopy**
Name of the unit running the course	**Doctoral School at University of Rzeszów**
Type of course *(obligatory, optional)*	Obligatory
Year and semester of studies	2022/2023; sem. IV and VI
Discipline	Physics
Language of Course	English
Name of Course coordinator	Dr hab. Rafał Hakalla, prof. UR
Name of Course lecturer	Dr hab. Rafał Hakalla, prof. UR
Prerequisites	Knowledge and skills in the field of the basics of physics, mathematical methods of physics and quantum mechanics, which are required learning outcomes at the level of second-cycle studies in the field of Physics.

BRIEF DESCRIPTION OF COURSE (100-200 words)

This course introduces students to the key issues for interpreting the spectra of atoms and molecules, and thus to understanding the structure of the studied particles. In order to achieve this goal, experimental results will be presented, as well as a theoretical models which explain them. A synthesis between theory and experiment will also be proposed, i.e. finding the relationship between the measured spectral parameters and the microscopic properties of molecules. Such a synthesis is to lead to the correct interpretation of experimental results and knowledge of the quantum-mechanical structure of the tested objects.

COURSE LEARNING OUTCOMES AND METHODS OF EVALUATING LEARNING OUTCOMES

Learning outcome	The description of the learning outcome defined for the course	Relation to the degree programme outcomes (symbol)	Learning Format (Lectures, classes,…)	Method of assessment of learning outcomes (e.g. test, oral exam, written exam, project,...)
Knowledge (no.)	**(Knows and understands)**			
1	Advanced issues of atomic and molecular spectroscopy to the extent that allows the revision of existing paradigms, both theoretical and experimental.	P8S-WG/1	lectures	project
2	The main development trends of modern atomic and molecular spectroscopy.	P8S-WG/2	lectures	project
3	The research methodology used in atomic and molecular spectroscopy.	P8S-WG/3	lectures, classes	project
Skills (no.)	**(Able to)**			
1	Use knowledge from various	P8S-UW/1	classes	project

	fields of science to creatively identify and solve complex problems in an innovative way or to perform research tasks in the field of atomic and molecular spectroscopy, and in particular: (i) define the purpose and subject of scientific research; (ii) formulate a research hypothesis; (iii) develop methods, techniques, research tools and use them creatively; (iv) draw conclusions based on scientific research.			
2	Critically analyze and evaluate the results of atomic and molecular spectroscopy research, expert activities and other creative works and their contribution to the development of knowledge.	P8S-UW/2	classes	project
3	Communicate on topics related to atomic and molecular spectroscopy to the extent that allows active participation in the international scientific community.	P8S-UK/1	classes	project
4	Disseminate the results of scientific activity in the field of atomic and molecular spectroscopy, also in popular forms.	P8S-UK/2	classes	project
5	Initiate a debate on advanced issues of atomic and molecular spectroscopy.	P8S-UK/3	lectures, classes	project
6	Participate in scientific discourse in the field of advanced issues of atomic and molecular spectroscopy.	P8S-UK/4	lectures, classes	project
7	Speak English at the B2 level of the European Language Education System to the extent that allows participation in the international scientific community related to atomic and molecular spectroscopy.	P8S-UK/5	classes	project
Social competence (no.)	**(Ready to)**			project
1	Critically evaluate their achievements in the field of atomic and molecular spectroscopy.	P8S-KK/1	lectures, classes	project

2	Recognize the importance of knowledge in solving cognitive and practical problems on the example of atomic and molecular spectroscopy.	P8S-KK/3	lectures, classes	project
3	Initiate actions for the public interest.	P8S-KO/2	lectures, classes	project

LEARNING FORMAT – NUMBER OF HOURS

Semester (n0.)	Lectures	Seminars	Lab classes	Internships	others	ECTS
IV and VI	5	10	—	—	—	0

METHODS OF INSTRUCTION

- presentation
- discussion
- solving computational tasks
- troubleshooting

COURSE CONTENT

1. Lectures (5h):

1. Atomic spectroscopy
   1.1. Atoms in a magnetic field: experiments and their semi-classical description.
   1.2. Atoms in a Magnetic Field: An Description in Quantum Mechanics.
   1.3. Atoms in an electric field. General laws of optical transitions.
   1.4. Lasers.

2. Separation of the motion of nuclei and electrons in molecules.
   2.1. The Schrödinger equation for the motion of nuclei.
   2.2. Separation of rotation and vibration.
   2.3. Approximate eigenvalues of the total Hamiltonian.
   2.4. Energy levels of the electron and nucleus spin.
   2.5. Effective Hamiltonian.
   2.6. Adiabatic approximation.
   2.7. Born-Oppenheimer approximation.

3. Macroscopic and microscopic electrical and magnetic properties of molecules.
   3.1. Macroscopic electrical properties of molecules.
   3.2. Polarizability. The induced electric dipole moment of a molecule.
   3.3. Microscopic theory of multipole moments of a molecule.
   3.4. Interaction of electric multipole moments with the external electric field.

4. Electron spectroscopy of two- and multi-atomic molecules.
   4.1. Electronic structure of molecules.
   4.2. Spectroscopic classification of electronic states.
   4.3. Electronic spectra.
   4.4. Intensity of electronic transitions, selection rules.
   4.5. Dissociation and predissociation.
   4.6. Isotope effect in the electronic spectra.
   4.7. Applications of the electronic spectra.

2. Classes (10h):

Solving problems using modern computational methods of atomic and molecular spectroscopy. The tasks will be selected according to the subject of the lectures.

COURSE ASSESSMENT CRITERIA
The final grade for the exercises will be issued on the basis of partial grades: - *very good*: the student has mastered over 90% of the knowledge; knows how to solve accounting tasks; - *good*: the student has mastered over 70% of the knowledge and is able to solve typical accounting tasks; - *satisfactory*: the student knows the basic concepts of the subject and can solve simple calculation problems.

TOTAL PhD STUDENT WORKLOAD REQUIRED TO ACHIEVE THE INTENDED LEARNING OUTCOMES – NUMBER OF HOURS AND ECTS CREDITS	
Activity	Number of hours
Scheduled course contact hours	15
Other contact hours involving the teacher (consultation hours, examinations)	5
Non-contact hours – student`s own work (preparation for classes or examinations, project, etc.)	15
Total number of hours	**35**
Total number of ECTS credits	**0**

INSTRUCTIONAL MATERIALS	
Compulsory literature:	1. P. W. Atkins, *Physical Chemistry*, Oxford University Press, USA, 2018. 2. G. Gauglitz, D. S. Moore, *Handbook of Spectroscopy*, Wiley-VCH Verlag GmBH, 2014. 3. G. Herzberg, *Molecular Spectra and Molecular Structure, vol. I: Spectra of Diatomic Molecules*, (2nd edition), Krieger Publishing Company, Malabar, Florida, 1989. 4. H. Haken, H. Ch. Wolf, *The Physics of atoms and Quanta,* (7th ed.), Springer-Verlag Berlin, Heidelberg, 2004. 5. H. Haken, H. Ch. Wolf, *Molecular Physics and Elements of Quantum Chemistry*, (2nd ed.) Springer-Verlag Berlin, Heidelberg, 2004.
Complementary literature:	1. W. Demtröder, *Atoms, Molecules and Photons An Introduction to Atomic-, Molecular- and Quantum Physics*, Springer Verlag, 2010.