



Subject card

Subject name and code		Spectroscopic research methods, PG_00067892						
Field of study		Technical Physics						
Date of commencement of studies		February 2027	Academic year of realisation of subject			2027/2028		
Education level		second-cycle studies	Subject group			Specialty subject group Subject group related to scientific research in the field of study		
Mode of study		Full-time studies	Mode of delivery			at the university		
Year of study		1	Language of instruction			Polish		
Semester of study		2	ECTS credits			3.0		
Learning profile		general academic profile	Assessment form			assessment		
Conducting unit		Department of Solid State Physics -> Faculty of Applied Physics and Mathematics -> Faculties of Gdańsk University of Technology						
Name and surname of lecturer (lecturers)		Subject supervisor		dr hab. Tomasz Wąsowicz				
		Teachers		dr hab. Tomasz Wąsowicz				
Lesson types		Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
		Number of study hours	30.0	0.0	15.0	0.0	0.0	45
		E-learning hours included: 0.0						
Learning activity and number of study hours		Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours		Self-study	SUM	
		Number of study hours	45	3.0		17.0	65	
Subject objectives		The aim of the course is to discuss the basic theoretical and practical issues of spectroscopy and presentation of the various types of spectroscopic setups, methods and ways to interpret spectra.						
Learning outcomes		Course outcome		Subject outcome		Method of verification		
		[K7_W02] possesses advanced, theoretically grounded knowledge in physics and, to an extent appropriate to professional needs, in related scientific or technical disciplines, including applied computer science, applied physics and photovoltaics.		The student has advanced theoretical knowledge of spectroscopic methods and their application in the analysis of physical phenomena and materials, at a level appropriate for applied physics.		[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects		
		[K7_W06] possesses advanced knowledge of experimental methods and techniques in physics, as well as occupational health and safety principles enabling independent work at research or measurement workstations.		The student has advanced knowledge of experimental methods and techniques used in spectroscopy, as well as safety regulations, enabling independent work at a research workstation.		[SW3] Assessment of knowledge contained in written work and projects		
		[K7_U01] demonstrates the ability for lifelong independent learning, including acquiring and integrating information from literature, databases and other relevant sources, as well as critically analysing and selecting information, including patent resources.		The student is able to independently acquire and integrate information from scientific literature, databases, and patent sources, critically evaluate it, and apply it to solve problems related to spectroscopic methods.		[SU2] Assessment of ability to analyse information [SU3] Assessment of ability to use knowledge gained from the subject [SU1] Assessment of task fulfilment		

Subject contents

Course content – lecture

Lecture:

Concept of the atom

Introduction to spectroscopic measurement

Quantum-mechanical model of atom

Fine structure

Hyperfine structure

Isotope shift of spectral lines

Stark effect

Zeeman effect

Transition probabilities of radiative processes

Types of chemical bonding

Molecular optical spectroscopy in the UV-VIS range

Fundamentals of vibrational spectroscopy

Fundamentals of rotational spectra formation

Vibrationalrotational spectroscopy

Electronic structure of energy levels

Explaining the principle of photodynamic therapy based on the Jablonski diagram

Photon-induced dissociation

X-ray absorption spectroscopy

Scattering spectroscopy

Mass spectrometry

Molecular beams

Laboratory:

1. Study of a trochoidal electron monochromator;
2. Mass spectrometry using quadrupole mass analyser;
3. Electron impact fluorescence spectra of N₂ molecule;
4. Measurement and analysis of emission and absorption spectra of molecules.

Prerequisites and co-requisites	A course in atomic and molecular physics and quantum mechanics.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Performance of laboratory exercises and laboratory reports preparation	100.0%	40.0%
	Solving tasks and problems as part of homework	50.0%	10.0%
	Final test from the theory	50.0%	50.0%
Recommended reading	Basic literature	[1] J.M.Hollas, Modern Spectroscopy, John Wiley & Sons, Ltd. [2] J.Sadlej, Molecular Spectroscopy, WNT, Warszawa (in Polish) [3] D.L.Pavia i in., Introduction to Spectroscopy, Brooks/Cole [4] Z.Kęcki, "Basics of molecular spectroscopy", PWN, Warszawa (in Polish) [5] P.Willmott, An Introduction to Synchrotron Radiation: Techniques and Applications, John Wiley & Sons, Ltd.	
	Supplementary literature	[6] H. Haken, H. Ch. Wolf., "Molecular physics and elements of quantum chemistry", Springer [7] C.D.Wagner i in. Handbook of photoelectron spectroscopy, Perkin-Elmer Corporation [8] G.Bunker, Introduction to XAFS, Cambridge Univ. Press [9] A.Gołębiewski, Elements of quantum mechanics and chemistry, PWN (in Polish)	
	eResources addresses		

Example issues/
example questions/
tasks being completed

1. What is a spectroscopy? Describe the types of spectroscopy due to the kind of radiation used.
2. What is a spectrum? Specify and describe the main parameters that characterize the spectral line shape.
3. List and describe the main causes of spectral lines broadening.
4. Define: transmittance, absorbance and absorption coefficient.
5. Describe term symbol which characterize atomic states under Russell-Saunders coupling (Spin-Orbit coupling) condition.
8. Write the selection rules for rotational transitions and define the rotational energy levels in a rigid rotor approximation.
9. How on the basis of rotation spectrum the molecule bond length can be determined (in a rigid rotor approximation)?
10. Write the selection rules for vibrational transitions and define the vibrational energy levels in an harmonic oscillator approximation.
11. Write the selection rules for vibrational transitions and define the vibrational energy levels for real oscillator (anharmonic oscillator).
12. How on the basis of vibration spectrum, bond energy of molecule can be determined?
13. Describe the shape of the vibration-rotation spectrum.
14. Raman spectroscopy: describe the origin and the idea of the phenomenon (e.g. on the basis of Placek polarizability theory) and shape of Raman spectrum.
15. Specify what the complementarity of Raman and IR spectroscopies means.
16. What is the origin of color of the transition metals complexes?
17. Explain the main cause of the line broadening observed in UV-Vis spectrum.
18. What is the auxochrome and how it can change the UV-Vis spectrum?
19. Explain hyperchromic and hypochromic effect, bathochromic and hypsochromic shift.
20. Photoelectron spectroscopy (PES, ESCA): describe the main idea of the technique and present the phenomena which accompanying the effect of the core electron photoexcitation (secondary effects, multi-electron effects).
21. Why photoelectron spectroscopy is a surface sensitive technique?
22. X-ray absorption spectroscopy (XAS): describe the origin of the phenomenon.
23. What kind of information can provide us X-ray absorption spectrum analysis close to absorption edge (XANES, X-ray absorption near edge structure)?
24. Explain the origin of the absorption coefficient fine structure observed in the extended energy range of X-ray absorption spectrum (EXAFS).

	25. Why EXAFS (Extended X-ray Absorption Fine Structure) analysis is considered as a probe of local structure at the atomic level?
Practical activities within the subject	Not applicable

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