

Subject card

Subject name and code	Spectroscopic research methods, PG_00031955								
Field of study	Technical Physics								
Date of commencement of	February 2024	Academic year of			2024/2025				
studies			realisation of subject			2024/2025			
Education level	second-cycle studies		Subject group			Optional 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 -> Wydziały Politechniki Gdańskiej								
Name and surname	Subject supervisor	dr hab. Tomasz Wąsowicz							
of lecturer (lecturers)	Teachers		dr inż. Marcin Dampc						
			dr inż. Ireneusz Linert						
			dr hab. Tomasz Wąsowicz						
Lesson types and methods	Lesson type	Lecture	Tutorial	Laboratory	Projec	:t	Seminar	SUM	
of instruction	Number of study hours	30.0	0.0	15.0	0.0	<u> </u>	0.0	45	
	E-learning hours incli	uded: 0.0		1	<u> </u>		1		
Learning activity and number of study hours	Learning activity	Participation i classes including		Participation in consultation hours		Self-study		SUM	
	Number of study hours	45		8.0		22.0		75	
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 methods and ways to interpret spectra.								
Learning outcomes	Course outcome		Subject outcome			Method of verification			
	experience in laboratory work. Knows the health and safety rules, sufficient for independent work at the research or measuring position.		experiments in the field of spectroscopic methods, will be able to analyse the measurement			[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects			
			The student has theoretical and practical skills in the laboratory work related, among others with the samples preparation for spectroscopic measurements, preparation and use of the spectroscopy equipment and performing the experiment.			[SU1] Assessment of task fulfilment [SU4] Assessment of ability to use methods and tools			
	[K7_W06] Has enhanced knowledge of the experimental methods and techniques applied in physics.		During lectures and lab exercises the student learns about modern spectroscopic techniques and how to use a number of modern measurement systems.			[SW1] Assessment of factual knowledge			

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Subject contents	Lecture: 1. Introduction to spectroscopy; 2. Theoretical description of the electromagnetic radiation and matter (atom, molecule, solid state); 3. Interaction between the electromagnetic radiation and matter; 4. Spectrum: parameters and ways of its registration; 5. Rotational spectroscopy; 6. Vibrational spectroscopy (IR); 7. Rotational-vibrational spectra; 8. Raman spectroscopy; 9. Electron spectroscopy (UV-Vis); 10. Photoelectron spectroscopy (AES); 11. Auger electron spectroscopy (AES); 12. X-ray absorption spectroscopy. 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 solid state physics (phy	sics of materials), quantum mechanic	es and nonorganic chemistry.				
Assessment methods	Subject passing criteria	Passing threshold	Percentage of the final grade				
and criteria	Final test from the theory	50.0%	50.0%				
	Performance of laboratory exercises and laboratory reports preparation	100.0%	40.0%				
	Solving tasks and problems as part of homework	50.0%	10.0%				
Recommended reading	Basic literature	[2] J.Sadlej, "Molecular Spectroscop [3] D.L.Pavia i in., "Introduction to S [4] Z.Kęcki, "Basics of molecular sp Polish)	Hollas, "Modern Spectroscopy", John Wiley & Sons, Ltd. dlej, "Molecular Spectroscopy", WNT, Warszawa (in Polish) Pavia i in., "Introduction to Spectroscopy", Brooks/Cole cki, "Basics of molecular spectroscopy", PWN, Warszawa (in Ilmott, "An Introduction to Synchrotron Radiation: Techniques blications", 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.Golębiewski, "Elements of quantum mechanics and chemistry", PWN (in Polish)					
	eResources addresses	Adresy na platformie eNauczanie: Metody badań spektroskopowych MBS sem zim 2024/25 - Moodle ID: 29719 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=29719 MBS - Laboratorium 2024/2025 - Moodle ID: 774 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=774					

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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. Formulate and explain Beer-Lambert law and define attenuation length.
- 6. Describe term symbol which characterize atomic states under Russell-Saunders coupling (Spin-Orbit coupling) condition.
- 7. Discuss the Hund's rules.
- 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

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	(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"?
Work placement	Not applicable

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