GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Spectroscopic research methods, PG_00031955		
Field of study	Technical Physics		
Date of commencement of studies	February 2023	Academic year of realisation of subject	2023/2024
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		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Tomasz Wąsowicz	
	Teachers	dr inż. Marcin Dampc dr inż. Ireneusz Linert dr hab. Tomasz Wąsowicz	

Lesson types and methods of instruction

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	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
[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
[K7_U03] Has enhanced laboratory work experience.	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.	[SU4] Assessment of ability to use methods and tools [SU1] Assessment of task fulfilment
[K7_W07] Has extended knowledge of the methodology of physics laboratory work, based on experience in laboratory work. Knows the health and safety rules, sufficient for independent work at the research or measuring position.	The student will ba able to perform experiments in the field of spectroscopic methods, will be able to analyse the measurement results, will get experienced in lab work. He knows the safety rules in force at scientific laboratory. Introductions to subequent laboratory exercices include instructions on work safety.	[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge

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 (UPS, XPS); 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 (physics of materials), quantum mechanics and nonorganic chemistry.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Solving tasks and problems as part of homework	50.0%	10.0%
Performance of laboratory exercises and laboratory reports preparation	100.0%	40.0%
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	Adresy na platformie eNauczanie: Metody badań spektroskopowych MBS sem zim 2023/24 - Moodle ID: 29719 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=29719

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

	(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