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 2024 | Academic year of realisation of subject | 2024/2025 |
| Education level | second-cycle studies | Subject group | Optional subject group<br>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 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_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. | [SW1] Assessment of factual knowledge<br>[SW3] Assessment of knowledge contained in written work and projects |
| [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. | [SU1] Assessment of task fulfilment<br>[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 |

**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 |
|---|---|---|
| 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 | [1] J.M.Hollas, „Modern Spectroscopy”, John Wiley & Sons, Ltd.<br>[2] J.Sadlej, „Molecular Spectroscopy”, WNT, Warszawa (in Polish)<br>[3] D.L.Pavia i in., „Introduction to Spectroscopy”, Brooks/Cole<br>[4] Z.Kęcki, "Basics of molecular spectroscopy", PWN, Warszawa (in Polish)<br>[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<br>[7] C.D.Wagner i in. „Handbook of photoelectron spectroscopy”, Perkin-Elmer Corporation<br>[8] G.Bunker, „Introduction to XAFS”, Cambridge Univ. Press<br>[9] A.Gołębiewski, „Elements of quantum mechanics and chemistry”, PWN (in Polish) |
| eResources addresses | Adresy na platformie eNauczanie: |

| | |
|---|---|
| Example issues/ example questions/ tasks being completed | 1. What is a spectroscopy? Describe the types of spectroscopy due to the kind of radiation used.<br><br>2. What is a spectrum? Specify and describe the main parameters that characterize the spectral line shape.<br><br>3. List and describe the main causes of spectral lines broadening.<br><br>4. Define: transmittance, absorbance and absorption coefficient.<br><br>5. Formulate and explain Beer-Lambert law and define attenuation length.<br><br>6. Describe term symbol which characterize atomic states under Russell-Saunders coupling (Spin-Orbit coupling) condition.<br><br>7. Discuss the Hund's rules.<br><br>8. Write the selection rules for rotational transitions and define the rotational energy levels in a rigid rotor approximation.<br><br>9. How on the basis of rotation spectrum the molecule bond length can be determined (in a rigid rotor approximation)?<br><br>10. Write the selection rules for vibrational transitions and define the vibrational energy levels in an harmonic oscillator approximation.<br><br>11. Write the selection rules for vibrational transitions and define the vibrational energy levels for real oscillator (anharmonic oscillator).<br><br>12. How on the basis of vibration spectrum, bond energy of molecule can be determined?<br><br>13. Describe the shape of the vibration-rotation spectrum.<br><br>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.<br><br>15. Specify what the complementarity of Raman and IR spectroscopies means.<br><br>16. What is the origin of color of the transition metals complexes?<br><br>17. Explain the main cause of the line broadening observed in UV-Vis spectrum.<br><br>18. What is the auxochrome and how it can change the UV-Vis spectrum?<br><br>19. Explain hyperchromic and hypochromic effect, bathochromic and hypsochromic shift.<br><br>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).<br><br>21. Why photoelectron spectroscopy is a „surface sensitive” technique?<br><br>22. X-ray absorption spectroscopy (XAS): describe the origin of the phenomenon.<br><br>23. What kind of information can provide us X-ray absorption spectrum analysis close to absorption edge |

| | |
|---|---|
| | (XANES, X-ray absorption near edge structure)?<br><br>24. Explain the origin of the absorption coefficient fine structure observed in the extended energy range of X-ray absorption spectrum (EXAFS).<br><br>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 |