



## Subject card

|                                             |                                                                                                                                                                                                                                              |                                                          |                                                                                                                                                                                                                                                                          |                                     |                                                                                                                                                                                                               |                                                                                                                      |     |
|---------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|-----|
| Subject name and code                       | Applied physical chemistry, PG_00066089                                                                                                                                                                                                      |                                                          |                                                                                                                                                                                                                                                                          |                                     |                                                                                                                                                                                                               |                                                                                                                      |     |
| Field of study                              | Chemia fizyczna stosowana                                                                                                                                                                                                                    |                                                          |                                                                                                                                                                                                                                                                          |                                     |                                                                                                                                                                                                               |                                                                                                                      |     |
| Date of commencement of studies             | February 2026                                                                                                                                                                                                                                |                                                          | Academic year of realisation of subject                                                                                                                                                                                                                                  |                                     |                                                                                                                                                                                                               | 2025/2026                                                                                                            |     |
| Education level                             | second-cycle studies                                                                                                                                                                                                                         |                                                          | Subject group                                                                                                                                                                                                                                                            |                                     |                                                                                                                                                                                                               | Obligatory subject group in the field of study<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                           | 1                                                                                                                                                                                                                                            |                                                          | ECTS credits                                                                                                                                                                                                                                                             |                                     |                                                                                                                                                                                                               | 3.0                                                                                                                  |     |
| Learning profile                            | general academic profile                                                                                                                                                                                                                     |                                                          | Assessment form                                                                                                                                                                                                                                                          |                                     |                                                                                                                                                                                                               | assessment                                                                                                           |     |
| Conducting unit                             | Department of Physical Chemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology                                                                                                                                     |                                                          |                                                                                                                                                                                                                                                                          |                                     |                                                                                                                                                                                                               |                                                                                                                      |     |
| Name and surname of lecturer (lecturers)    | Subject supervisor                                                                                                                                                                                                                           |                                                          | dr hab. Aneta Panuszko                                                                                                                                                                                                                                                   |                                     |                                                                                                                                                                                                               |                                                                                                                      |     |
|                                             | Teachers                                                                                                                                                                                                                                     |                                                          |                                                                                                                                                                                                                                                                          |                                     |                                                                                                                                                                                                               |                                                                                                                      |     |
| Lesson types                                | Lesson type                                                                                                                                                                                                                                  | Lecture                                                  | Tutorial                                                                                                                                                                                                                                                                 | Laboratory                          | Project                                                                                                                                                                                                       | Seminar                                                                                                              | SUM |
|                                             | Number of study hours                                                                                                                                                                                                                        | 0.0                                                      | 0.0                                                                                                                                                                                                                                                                      | 30.0                                | 15.0                                                                                                                                                                                                          | 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                                                       |                                                                                                                                                                                                                                                                          | 5.0                                 |                                                                                                                                                                                                               | 25.0                                                                                                                 | 75  |
| Subject objectives                          | The aim of the course is to familiarize the student with various techniques, both experimental and theoretical, used to study the physicochemical properties of solutions and complex systems.                                               |                                                          |                                                                                                                                                                                                                                                                          |                                     |                                                                                                                                                                                                               |                                                                                                                      |     |
| Learning outcomes                           | Course outcome                                                                                                                                                                                                                               |                                                          | Subject outcome                                                                                                                                                                                                                                                          |                                     | Method of verification                                                                                                                                                                                        |                                                                                                                      |     |
|                                             | [K7_K02] is able to cooperate and work in a group, taking on different roles                                                                                                                                                                 |                                                          | The student effectively collaborates in a team, assuming various roles to accomplish common tasks and projects. The student takes responsibility for specific tasks and engages in communication and problem-solving within the group.                                   |                                     | [SK5] Ocena umiejętności rozwiązywania problemów występujących w praktyce<br>[SK1] Ocena umiejętności pracy w grupie<br>[SK4] Ocena umiejętności komunikacji, w tym poprawności językowej                     |                                                                                                                      |     |
|                                             | [K7_U02] prepares detailed documentation of the results of independently conducted experiments and analyzes the obtained results, uses professional vocabulary with understanding and prepares and communicates information                  |                                                          | The student develops and interprets the results of independently conducted physicochemical experiments. The student presents the results in the form of a report.                                                                                                        |                                     | [SU1] Ocena realizacji zadania<br>[SU4] Ocena umiejętności korzystania z metod i narzędzi<br>[SU5] Ocena umiejętności zaprezentowania wyników realizacji zadania                                              |                                                                                                                      |     |
|                                             | [K7_W03] recognizes and describes phenomena in the field of physics, including elements of quantum mechanics, solid state physics and nuclear physics, necessary to predict the course of physical phenomena and to solve technical problems |                                                          | The student builds simple simulation systems and conducts their simulations using molecular dynamics methods. The student analyzes the results obtained through molecular dynamics methods and draws conclusions based on them.                                          |                                     | [SW3] Ocena wiedzy zawartej w opracowaniu tekstowym i projektowym<br>[SW1] Ocena wiedzy faktograficznej                                                                                                       |                                                                                                                      |     |
|                                             | [K7_U04] develops and transmits technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation                    |                                                          | The student develops and delivers technical reports in the form of text documents and spreadsheets. The student creates charts and diagrams for result analysis. The student prepares a multimedia presentation and presents the results in the form of a public speech. |                                     | [SU3] Ocena umiejętności wykorzystania wiedzy uzyskanej w ramach przedmiotu<br>[SU4] Ocena umiejętności korzystania z metod i narzędzi<br>[SU5] Ocena umiejętności zaprezentowania wyników realizacji zadania |                                                                                                                      |     |

|                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                               |
|----------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------|
| Subject contents                                               | Course content – laboratory                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                               |
|                                                                | The subject of the course covers the following issues:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                               |
|                                                                | <ol style="list-style-type: none"><li>1. Infrared spectroscopy in the study of intermolecular interactions: methods of developing spectra, selected chemometric methods in the analysis of spectral series in solving chemical problems. Analysis of the structure and energy of water hydrogen bonds around a solute: isotope dilution technique, difference spectra method, OD band spectral parameters, Badger-Bauer rule, empirical function correlating the oxygen-oxygen intermolecular distance with the position of the band.</li><li>2. Intermolecular interactions in electrolyte solutions containing solvents with different donor properties and spatial structure and in aqueous solutions of non-electrolytes using precise measurements of density and sound speed: determining the limit values of apparent volumes and molar compressibility, division of standard partial volumes and molar compressibility of electrolytes into ionic shares , determination of solvation numbers of ions based on adiabatic compressibility and standard partial molar volume, coefficient of thermal expansion, Hepler's relation, standard partial volumes and molar compressivities of solute transfer, McMillan and Mayer equation.</li><li>3. Heterogeneous redox reactions - calculation of the absolute value of the standard hydrogen electrode potential using the thermodynamic cycle. Standard potential of reduction reactions - determination, application and correlations with parameters reflecting the electronic structure of the molecule.</li><li>4. Basics of molecular modeling methods: models of intermolecular interactions, taking into account constraints; problem of boundaries of simulation systems, periodic boundary conditions; molecular dynamics, numerical solution of equations of particle motion; different simulation conditions (NVT, NpT); results analysis methods: liquid structure, radial distribution functions, time correlation functions, diffusion.</li></ol> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                               |
| Prerequisites and co-requisites                                | Mathematics, Physics, Physical Chemistry,                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                               |
| Assessment methods and criteria                                | Subject passing criteria                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Passing threshold                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Percentage of the final grade |
|                                                                | tests + reports (laboratory)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 60.0%                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 50.0%                         |
|                                                                | reports (project)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 60.0%                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 50.0%                         |
| Recommended reading                                            | Basic literature                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | <ol style="list-style-type: none"><li>1. H. Mark, J. Workman, Jr. , "Chemometrics in spectroscopy", 2007, Elsevier</li><li>2. J. Stangret, <i>Zeszyty Naukowe Politechniki Gdańskiej</i>, Chemia XLV (578), 2000.</li><li>3. Organic Electrochemistry: Revised and Expanded (pp.229-259), Edition: 5th, Chapter: 6, Publisher: CRC Press, Taylor and Francis Group, Editors: Ole Hammerich, Bernd Speiser</li><li>4. M.J. Abraham, D. van der Spoel, E. Lindahl, B. Hess, and the GROMACS Development Team. GROMACS 2023.4 Manual</li></ol> |                               |
|                                                                | Supplementary literature                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <ol style="list-style-type: none"><li>1. M. Śmiechowski, J. Stangret, Vibrational spectroscopy of semiheavy water (hdo) as a probe of solute hydration, <i>Pure Appl. Chem.</i> 82 (10) (2010) 18691887.</li></ol>                                                                                                                                                                                                                                                                                                                          |                               |
|                                                                | eResources addresses                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                               |
| Example issues/<br>example questions/<br>tasks being completed | <ol style="list-style-type: none"><li>1. What are the purposes of chemometric analysis methods for spectral data?</li><li>2. Discuss the Badger-Bauer rule with a simple example.</li><li>3. What fractions make up the standard partial molar volume of an electrolyte?</li><li>4. Carrying out a computer simulation of argon gas under conditions of constant pressure and constant volume.</li></ol>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                               |
| Practical activities within the subject                        | Not applicable                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                               |

Document generated electronically. Does not require a seal or signature.