

## Subject card

|                                             |                                                                                                                                                   |                                                          |                                         |                                     |                                                                                                                      |            |     |
|---------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------|-----------------------------------------|-------------------------------------|----------------------------------------------------------------------------------------------------------------------|------------|-----|
| Subject name and code                       | Quantum chemistry, PG_00082078                                                                                                                    |                                                          |                                         |                                     |                                                                                                                      |            |     |
| Field of study                              | Chemistry                                                                                                                                         |                                                          |                                         |                                     |                                                                                                                      |            |     |
| Date of commencement of studies             | October 2025                                                                                                                                      |                                                          | Academic year of realisation of subject |                                     | 2025/2026                                                                                                            |            |     |
| Education level                             | Bachelor's 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                           | 2                                                                                                                                                 |                                                          | ECTS credits                            |                                     | 3.0                                                                                                                  |            |     |
| Learning profile                            | academic                                                                                                                                          |                                                          | Assessment form                         |                                     | exam                                                                                                                 |            |     |
| Conducting unit                             | Laboratory of Quantum Chemistry -> Department of Theoretical Chemistry -> Faculty of Chemistry -> Rector                                          |                                                          |                                         |                                     |                                                                                                                      |            |     |
| Name and surname of lecturer (lecturers)    | Subject supervisor                                                                                                                                |                                                          | dr hab. Sylwia Freza                    |                                     |                                                                                                                      |            |     |
|                                             | Teachers                                                                                                                                          |                                                          |                                         |                                     |                                                                                                                      |            |     |
| Lesson types                                | Lesson type                                                                                                                                       | Lecture                                                  | Tutorial                                | Laboratory                          | Project                                                                                                              | Seminar    | SUM |
|                                             | Number of study hours                                                                                                                             | 30.0                                                     | 0.0                                     | 0.0                                 | 0.0                                                                                                                  | 0.0        | 30  |
|                                             | 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                                                                                                                             | 30                                                       |                                         | 5.0                                 |                                                                                                                      | 40.0       | 75  |
| Subject objectives                          | The aim of the lecture is to present the concepts of quantum chemistry, basic approximations and selected quantum chemical computational methods. |                                                          |                                         |                                     |                                                                                                                      |            |     |

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| Learning outcomes                                              | Course outcome                                                                                                                                                                                                                                                                                                                                                                                                | Subject outcome                                                                                                                                                                                                                  | Method of verification                       |
|                                                                | [CHEML3_K07] Appreciates the need for understandable presentation of selected chemical issues to the public.                                                                                                                                                                                                                                                                                                  | student is careful and critical in expressing opinions, student is open to innovative concepts                                                                                                                                   | [SK1] oral statement/conversation/discussion |
|                                                                | [CHEML3_U09] Is able to learn independently.                                                                                                                                                                                                                                                                                                                                                                  | student solves eigenvalue equations with quantum mechanical operators, student constructs a determinant wavefunction, student plans the appropriate choice of calculation method                                                 | [SU4] test/exam - oral or written            |
|                                                                | [CHEML3_U08] Presents in an understandable way the basic facts about chemistry using a scientific language typical of chemical sciences.                                                                                                                                                                                                                                                                      | student predicts the measurability of physical quantities, classifies the multiplicity of states, discusses the basic approximations used in quantum chemistry                                                                   | [SU4] test/exam - oral or written            |
|                                                                | [CHEML3_U01] Identifies, analyses and solves problems in the field of broadly understood chemistry on the basis of the acquired knowledge.                                                                                                                                                                                                                                                                    | student estimates the probability of finding an electron in a specific area, calculates the electron energy of molecules                                                                                                         | [SU4] test/exam - oral or written            |
|                                                                | [CHEML3_W08] Demonstrates knowledge of basic computational methods to solve problems in chemistry, physics, mathematics.                                                                                                                                                                                                                                                                                      | student lists the basic methods of quantum chemistry, explains simple applications of quantum chemistry, recognizes the symmetry of the wavefunction, describes the postulates of quantum mechanics, explains the tunnel effect, | [SW4] test/exam - oral or written            |
| Subject contents                                               | wave-particle dualism, postulates of quantum mechanics, solution of the Schrödinger equation for a free particle, a particle in a potential box, a rigid rotator, a harmonic oscillator and a hydrogen atom; electron spin; atomic terms; approximate methods of quantum chemistry: perturbation and variational methods, Ritz method, Hartree-Fock method, CI method, MCSCF, CASSCF, coupled cluster method; |                                                                                                                                                                                                                                  |                                              |
| Prerequisites and co-requisites                                | basic knowledge of linear algebra, differential and integral calculations                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                  |                                              |
| Assessment methods and criteria                                | Subject passing criteria                                                                                                                                                                                                                                                                                                                                                                                      | Passing threshold                                                                                                                                                                                                                | Percentage of the final grade                |
|                                                                | exam                                                                                                                                                                                                                                                                                                                                                                                                          | 51.0%                                                                                                                                                                                                                            | 100.0%                                       |
| Recommended reading                                            | Basic literature                                                                                                                                                                                                                                                                                                                                                                                              | 1. Włodzimierz Kołos Chemia kwantowa A<br><br>2. Alojzy Gołębiewski Elementy mechaniki i chemii kwantowej                                                                                                                        |                                              |
|                                                                | Supplementary literature                                                                                                                                                                                                                                                                                                                                                                                      | 1. Lucjan Piela Idee chemii kwantowej<br><br>2. P.W. Atkins Molekularna mechanika kwantowa                                                                                                                                       |                                              |
|                                                                | eResources addresses                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                  |                                              |
| Example issues/<br>example questions/<br>tasks being completed | 1. What is the one-electron approximation? 2. Describe Heisenberg's uncertainty principle. 3. Discuss quantum numbers.                                                                                                                                                                                                                                                                                        |                                                                                                                                                                                                                                  |                                              |
| Work placement                                                 | Not applicable                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                  |                                              |

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