UNIWERSYTET IM. ADAMA MICKIEWICZA W POZNANIU

Theoretical chemistry

Educational subject description sheet

Basic information

Study programme Chemistry **Speciality** - **Organizational unit** Faculty of Chemistry **Study level** Second-cycle programme **Study form** Full-time **Education profile** General academic	**Didactic cycle** 2023/24 **Subject code** 02CHSS.22P.00983.23 **Lecture languages** English **Course type** Obligatory **Block** Basic subjects

Subject coordinator	Iwona Gulaczyk
Lecturer	Iwona Gulaczyk, Jerzy Stanek

Period	**Activities and hours**	**Number of ECTS points**
Semester 2	• Lecture: 15, Exam • Classes: 45, Graded credit	5

Goals

Code	Goal
C1	Introduction to basic concepts, calculation methods and modelling techniques of quantum chemistry.
C2	Development of skills in interpretation of quantum chemistry calculations.
C3	Development of skills in numerical and graphical modification of input and output data in the ab initio calculation.

Entry requirements

No prerequisites required.

Subject learning outcomes

Code	Outcomes in terms of	Learning outcomes	Examination methods
Knowledge – Student:			
W1	understands and explains the postulates of quantum mechanics.	CHS_K2_W01, CHS_K2_W02, CHS_K2_W06	Written exam, "Open book" exam, Written colloquium, Test
W2	knows and understands how to solve exactly the basic models of quantum mechanics, how to characterize the solutions, indicates the applications of models.	CHS_K2_W01, CHS_K2_W02, CHS_K2_W06	Written exam, "Open book" exam, Written colloquium, Test
W3	knows how to extract, modify and present the results of quantum mechanical calculations.	CHS_K2_W01, CHS_K2_W02, CHS_K2_W09	Written exam, "Open book" exam, Written colloquium, Test
W4	understands how to present in graphical form the results of ab initio calculations, also those referring to the reaction path.	CHS_K2_W01, CHS_K2_W02, CHS_K2_W07	Written exam, "Open book" exam, Written colloquium, Test
W5	knows how to use the bibliographic sources.	CHS_K2_W01, CHS_K2_W08	Written exam, "Open book" exam, Written colloquium, Test
Skills – Student:			
U1	is able to explain the postulates of quantum mechanics.	CHS_K2_U01, CHS_K2_U05	Written exam, "Open book" exam, Written colloquium, Test
U2	is able to explain how to solve exactly the basic models of quantum mechanics, how to characterize the solutions, indicates the applications of models.	CHS_K2_U01, CHS_K2_U02, CHS_K2_U05, CHS_K2_U08	Written exam, "Open book" exam, Written colloquium, Test
U3	is able to explain the interactions on atomic and molecular level and describes the resulting chemical properties.	CHS_K2_U02, CHS_K2_U05, CHS_K2_U08	Written exam, "Open book" exam, Written colloquium, Test
U4	is able to apply the basic approximate quantum calculations to complex atomic and molecular systems.	CHS_K2_U02, CHS_K2_U05, CHS_K2_U08, CHS_K2_U09	Written exam, "Open book" exam, Written colloquium, Test
U5	is able to extract, modify and present the results of quantum mechanical calculations.	CHS_K2_U01, CHS_K2_U05, CHS_K2_U07, CHS_K2_U08, CHS_K2_U09, CHS_K2_U10, CHS_K2_U12	Written exam, "Open book" exam, Written colloquium, Test
U6	is able to present in graphical form the results of ab initio calculations, also those referring to the reaction path.	CHS_K2_U01, CHS_K2_U05, CHS_K2_U07, CHS_K2_U08, CHS_K2_U10, CHS_K2_U14, CHS_K2_U15	Written exam, "Open book" exam, Written colloquium, Test

Code	Outcomes in terms of	Learning outcomes	Examination methods
U7	is able to use the bibliographic sources.	CHS_K2_U09, CHS_K2_U10, CHS_K2_U11, CHS_K2_U13	Written exam, "Open book" exam, Written colloquium, Test
U8	is able to apply the safety and ergonomics rules in the computer laboratory.	CHS_K2_U15	Written exam, "Open book" exam, Written colloquium, Test
Social competences – Student:			
K1	is ready to critical presentation in graphical form the results of ab initio calculations, also those referring to the reaction path.	CHS_K2_K01, CHS_K2_K02, CHS_K2_K03, CHS_K2_K04	Written exam, "Open book" exam, Written colloquium, Test

Study content

No.	Course content	Subject learning outcomes	Activities
1.	Industrial safety In the computer laboratory.	U8	Lecture, Classes
2.	Introduction to quantum mechanics (black body radiation, photoelectric effect, wave-particle duality). Postulates of the quantum mechanics.	W1, W2, U1, U2	Lecture, Classes
3.	Exact solution of the Schrödinger equation: tunnelling effect, particle in a box. Analysis and visualization of the solutions for a hydrogen atom.	W1, W2, U1, U2	Lecture, Classes
4.	Approximate variational method of solving the Schrödinger equation. One-electron approximation. Hartree-Fock method. Electron correlation. Molecular orbitals, functional basis.	U2, U4	Lecture, Classes
5.	The Gaussian package: possible applications, graphical interface GaussView. Practical quantum mechanical calculations using the Gaussian package. Multielectron atom, Mendeleev periodic table.	W3, W4, U4, U5, U6, K1	Lecture, Classes
6.	Separation of electrons and nuclei in molecules. Chemical Bond. Potential energy surface. Force constants. Force field. Energy levels in molecules. Molecular geometry optimization. Excited states, the CI method.	W3, W4, U4, U5, U6, K1	Lecture, Classes
7.	Graphical presentation of the ab initio calculation.	W3, W4, U4, U5, U6, K1	Lecture, Classes
8.	Calculation of the two-dimensional potential function for a molecule.	W3, W4, W5, U3, U4, U5, U6, U7, K1	Lecture, Classes
9.	Modelling the reaction energy path, activation energy for a complex molecular system.	W3, W4, U4, U5, U6, K1	Lecture, Classes

Additional information

Activities	Teaching and learning methods and activities
Lecture	Lecture with a multimedia presentation of selected issues, Discussion, Problem-based learning

Activities	Teaching and learning methods and activities
Classes	Solving tasks (e.g. computational, artistic, practical), Classes method, Laboratory method, Workshop method, Work in groups

Activities	Credit conditions
Lecture	The exam will be in written form. Minimum 25 points must be obtained to pass the exam (maximum is 50). The final mark will base on points obtained on a written exam as well as on points collected on laboratories. Grading scale with applied percentage distribution: • excellent (5.0): achievement of the student's expected learning outcomes at a minimum of 90.0%. • very good (4.5): achievement by the student of the desired learning outcomes ranging from 80.0% - 89.9%. • good (4.0): achievement of student learning outcomes 70.0% - 79.9%. • average (3.5): achievement of student learning outcomes 60.0% - 69.9%. • satisfactory (3.0): attainment of the student learning outcomes within 50.0% - 59.9%. • unsatisfactory (2.0): failure of the student to achieve the expected learning outcomes below 50.0%.
Classes	Before starting the laboratory student should be familiar with the principles of occupational health and safety in the laboratory. This knowledge will be checked before first laboratory (formative assessment). Before each laboratory the knowledge and skills concerning the current topic will be checked. To start the experiments a student should obtain at least 2 points (the scale is from 0 to 3). Additional 1 point can be obtained for excellent performance of experiment (mainly assessment of student's skills) and 1 point for correctness of report, including aesthetics. At the last laboratory, beside of weekly test of knowledge and skills, students will solve the test, which cover the main topics raised on laboratories. The questions will be given in the form of problems to be solved. The maximum points that can be obtained is 8. Grading scale with applied percentage distribution: • excellent (5.0): achievement of the student's expected learning outcomes at a minimum of 90.0%. • very good (4.5): achievement by the student of the desired learning outcomes ranging from 80.0% - 89.9%. • good (4.0): achievement of student learning outcomes 70.0% - 79.9%. • average (3.5): achievement of student learning outcomes 60.0% - 69.9%. • satisfactory (3.0): attainment of the student learning outcomes within 50.0% - 59.9%. • unsatisfactory (2.0): failure of the student to achieve the expected learning outcomes below 50.0%.

Literature

Obligatory

1. Atkins, Peter W., and Friedman, Ronald S., Molecular Quantum Mechanics; 4th Edition; Oxford University Press; 2005
2. Piela, Lucjan, Ideas of quantum chemistry, 2nd Edition, Elsevier, 2013

Optional

1. Levine, Ira N., Quantum Chemistry; 7th Edition; Pearson/Prentice Hall; 2013.

Calculation of ECTS points

Activities	Activity hours*
Lecture	15
Classes	45

Preparation for classes	15
Preparation for the exam	30
Reading the indicated literature	15
Report preparation	30
Student workload	**Hours** 150
Number of ECTS points	**ECTS** 5

* academic hour = 45 minutes

Efekty uczenia się dla kierunku

Kod	Treść
CHS_K2_K01	The graduate is ready to identify and evaluate cognitive and practical problems in the field of chemical research
CHS_K2_K02	The graduate is ready to evaluate the collected information critically
CHS_K2_K03	The graduate is ready to propose alternative solutions aimed at responsible decision-making, taking into account economic and social factors
CHS_K2_K04	The graduate is ready to appreciating, promoting and adhering to professional ethics in their own and others' activities
CHS_K2_U01	The graduate can use chemical terminology consistent with IUPAC recommendations
CHS_K2_U02	The graduate can analyze the physicochemical properties of substances based on the selection of appropriate methods and tools
CHS_K2_U05	The graduate can use mathematical methods in calculations for complex chemical and physicochemical systems and to evaluate the obtained results critically
CHS_K2_U07	The graduate can prepare a final report on conducted research projects and conduct a critical analysis of experiments
CHS_K2_U08	The graduate can find and use information obtained from databases and literature resources in order to plan and carry out a research project
CHS_K2_U09	The graduate can use information and communication techniques in order to deepen his knowledge and communication in specialist circles of recipients
CHS_K2_U10	The graduate can use English at the B2 + level of the European System for the Description of Language Education in the field of chemistry and the discipline in which conducts research
CHS_K2_U11	The graduate can present a complex chemical or physicochemical problem and propose a solution
CHS_K2_U12	The graduate can draw conclusion properly and evaluate critically on the basis of data from self-conducted chemical or physicochemical experiments and literature resources
CHS_K2_U13	The graduate can deepens his specialistic knowledge to the extent necessary to solve and interpret the undertaken problem correctly
CHS_K2_U14	The graduate can express in an accessible way the acquired knowledge, conduct a debate and present the results of scientific projects in chemistry
CHS_K2_U15	The graduate can work in a group, performing various roles, including a leader
CHS_K2_W01	The graduate knows and understands selected advanced issues in the field of chemistry
CHS_K2_W02	The graduate knows and understands concepts and relationships allowing for a quantitative description of complex physico-chemical phenomena
CHS_K2_W06	The graduate knows and understands the use of chemicals of key importance for the progress of science
CHS_K2_W07	The graduate knows and understands classifies advanced laboratory, analytical and instrumental techniques used in chemistry
CHS_K2_W08	The graduate knows and understands advanced chemical technology processes
CHS_K2_W09	The graduate knows and understands the ethical, legal and economic conditions applicable in the field of chemical sciences