UNIWERSYTET IM. ADAMA MICKIEWICZA W POZNANIU

Quantum chemistry

Educational subject description sheet

Basic information

Study programme Chemia (General Chemistry) **Speciality** - **Organizational unit** Faculty of Chemistry **Study level** First-cycle programme **Study form** Full-time **Education profile** General academic	**Didactic cycle** 2023/24 **Subject code** 02CENS.18P.01829.23 **Lecture languages** English **Course type** Obligatory **Block** Basic subjects

Subject coordinator	Jacek Komasa
Lecturer	Jacek Komasa

Period	**Activities and hours**	**Number of ECTS points**
Semester 4	• Lecture: 30, Graded credit • Classes: 45, Graded credit	6

Goals

Code	Goal
C1	Transfer of knowledge in the field of the basics of quantum chemistry; computational methods and modelling in quantum chemistry.
C2	Developing the ability to select appropriate models of quantum chemistry to study specific quantum processes; developing the ability to apply computational methods to solve problems in quantum chemistry.
C3	Preparation for the proper interpretation of experimental and theoretical results.
C4	Developing the ability to use computer tools for calculations and modelling in quantum chemistry.
C5	Developing communication and teamwork skills; transfer of knowledge in the field of safety and hygiene in the laboratory.

Entry requirements

Knowledge of mathematics in complex numbers, differential and integral calculus (verified on a written test).

Subject learning outcomes

Code	Outcomes in terms of	Learning outcomes	Examination methods
Knowledge – Student:			
W1	understands and explains the essence of the postulates of quantum mechanics.	CEN_K1_W01, CEN_K1_W02	Written colloquium, Oral colloquium, Test
W2	explains how to strictly solve basic models in quantum mechanics, how to characterize solutions and shows their applications.	CEN_K1_W01, CEN_K1_W02, CEN_K1_W03	Written colloquium, Oral colloquium, Test
W3	applies the most important approximate computational methods to solve complex atomic and molecular systems.	CEN_K1_W03	Project
W4	selects and applies appropriate computational and modelling techniques to study specific properties of atomic and molecular systems.	CEN_K1_W03, CEN_K1_W04, CEN_K1_W08	Project
W5	correctly interprets the results of theoretical calculations and experiments.	CEN_K1_W01, CEN_K1_W02, CEN_K1_W03, CEN_K1_W04, CEN_K1_W05, CEN_K1_W06, CEN_K1_W08	Project
Skills – Student:			
U1	explains how to strictly solve basic models in quantum mechanics, how to characterize solutions and shows their applications.	CEN_K1_U01, CEN_K1_U02, CEN_K1_U03, CEN_K1_U08, CEN_K1_U12, CEN_K1_U21	Written colloquium, Oral colloquium, Test

Code	Outcomes in terms of	Learning outcomes	Examination methods
U2	applies the most important approximate computational methods to solve complex atomic and molecular systems.	CEN_K1_U01, CEN_K1_U02, CEN_K1_U03, CEN_K1_U12, CEN_K1_U21	Written colloquium, Oral colloquium, Test, Project
U3	selects and applies appropriate computational techniques and modelling to study specific properties of atomic and molecular systems.	CEN_K1_U01, CEN_K1_U02, CEN_K1_U03, CEN_K1_U08, CEN_K1_U09, CEN_K1_U11, CEN_K1_U12, CEN_K1_U21	Project
U4	correctly interprets the results of theoretical calculations.	CEN_K1_U01, CEN_K1_U02, CEN_K1_U03, CEN_K1_U08, CEN_K1_U09, CEN_K1_U10, CEN_K1_U11, CEN_K1_U12, CEN_K1_U21	Project
U5	uses literature sources, also in English.	CEN_K1_U19, CEN_K1_U21, CEN_K1_U22	Project
U6	objectively assesses the contribution of own and others' work in the analysis of the jointly obtained theoretical results.	CEN_K1_U19	Project
Social competences – Student:			
K1	selects and applies appropriate computational techniques and modelling to study specific properties of atomic and molecular systems.	CEN_K1_K01, CEN_K1_K02	Project
K2	correctly interprets the results of theoretical calculations.	CEN_K1_K01, CEN_K1_K02, CEN_K1_K06	Project
K3	uses literature sources, also in English.	CEN_K1_K02, CEN_K1_K06	Project
K4	objectively assesses the contribution of own and others' work in the analysis of the jointly obtained theoretical results.	CEN_K1_K01, CEN_K1_K02, CEN_K1_K05, CEN_K1_K06	Project

Study content

No.	Course content	Subject learning outcomes	Activities
1.	Introduction to quantum mechanics (photoelectric effect, wave-particle duality, definitions), postulates of quantum mechanics.	W1	Lecture, Classes

No.	Course content	Subject learning outcomes	Activities
2.	Exact solutions of the Schrödinger equation: free particle, tunnelling, infinite potential well, harmonic oscillator, analysis and visualization of solutions to the Schrödinger equation for the rigid rotator and the hydrogen atom.	W1, W2, U1	Lecture, Classes
3.	Approximate methods of solving the Schrödinger equation: variation method, perturbation theory, one-electron approximation, Hartree-Fock method, electron correlation, molecular orbitals, one-electron basis sets.	W1, W2, W3, U2, U3, U4, K2	Lecture, Classes
4.	Gaussian computing package: its capabilities and applications, GaussView - the graphical interface, practical quantum-chemical calculations.	W3, W4, W5, U2, U3, U4, K1, K2	Lecture, Classes
5.	Separation of the movement of nuclei and electrons in molecules, chemical bonds, potential energy surface, force constants, energy levels, excited states, configuration interaction method.	W3, W4, W5, U2, U3, U4, K1, K2	Lecture, Classes
6.	Modelling of physicochemical properties of molecules in the gas phase, electronic structure, electron density distribution, population analysis, multipole moments, prediction of reactivity of molecules.	W3, W4, W5, U3, U4, K1, K2	Lecture, Classes
7.	Reaction path modelling, the activation energy for complex molecular systems.	W3, W4, W5, U3, U4, K1, K2	Lecture, Classes
8.	Application of quantum chemical methods to the prediction of spectroscopic properties of molecules – nuclear magnetic resonance spectroscopy (NMR), spectroscopy in the infrared (IR), visible and ultraviolet (UV-Vis) range of frequencies.	W3, W4, W5, U2, U3, U5, K1, K2, K3	Lecture, Classes
9.	Numerical processing of ab-initio calculation results, graphical presentation of results, electron density contours, differential densities, projection of properties on density surface, animation of chemical reaction.	W4, W5, U3, U4, U5, U6, K2, K3, K4	Lecture, Classes

Additional information

Activities	Teaching and learning methods and activities
Lecture	Lecture with a multimedia presentation of selected issues
Classes	Solving tasks (e.g. computational, artistic, practical), Work in groups

Activities	Credit conditions
Lecture	Passing a written test exam with the possibility of oral resit. Grading scale with the applied percentage distribution of achievable points: • very good (bdb; 5.0): achievement of the expected learning outcomes by the student at a minimum level of 92.0% • good plus (db+; 4.5): achievement of the expected learning outcomes by the student within the range of 84.0% - 91.9% • good (db; 4.0): achievement of the expected learning outcomes by the student within the range of 76.0% - 83.9% • satisfactory plus (dst+; 3.5): achievement of the expected learning outcomes by the student within the range of 68.0% - 75.9% • satisfactory (dst; 3.0): achievement of the expected learning outcomes by the student within the range of 60.0% - 67.9% • unsatisfactory (ndst; 2.0): failure to achieve the expected learning outcomes, resulting in a score below 60.0%
Classes	Attendance for at least 90% of classes. Completion of all tests. Completion of an individual project. Grading scale with the applied percentage distribution of achievable points: • very good (bdb; 5.0): achievement of the expected learning outcomes by the student at a minimum level of 92.0% • good plus (db+; 4.5): achievement of the expected learning outcomes by the student within the range of 84.0% - 91.9% • good (db; 4.0): achievement of the expected learning outcomes by the student within the range of 76.0% - 83.9% • satisfactory plus (dst+; 3.5): achievement of the expected learning outcomes by the student within the range of 68.0% - 75.9% • satisfactory (dst; 3.0): achievement of the expected learning outcomes by the student within the range of 60.0% - 67.9% • unsatisfactory (ndst; 2.0): failure to achieve the expected learning outcomes, resulting in a score below 60.0%

Literature

Obligatory

1. L. Piela, Ideas of Quantum Chemistry

Calculation of ECTS points

Activities	Activity hours*
Lecture	30
Classes	45
Preparation for classes	20
Reading the indicated literature	10
Preparation of a project	30
Preparation for the assessment	15
Preparation for the exam	30

Student workload	**Hours** 180
Number of ECTS points	**ECTS** 6

* academic hour = 45 minutes

Efekty uczenia się dla kierunku

Kod	Treść
CEN_K1_K01	The graduate is ready to the development of new chemical technologies
CEN_K1_K02	The graduate is ready to understand the importance of presenting selected developments in chemistry in an accessible manner
CEN_K1_K05	The graduate is ready to understand and appreciate the importance of professional ethics in his/her own actions and those of others
CEN_K1_K06	The graduate is ready to formulate precise questions to deepen his/her own understanding of a topic or to find missing pieces of reasoning
CEN_K1_U01	The graduate can use basic chemical terminology according to IUPAC and PTChem recommendations
CEN_K1_U02	The graduate can present the knowledge acquired in an accessible manner
CEN_K1_U03	The graduate can identify and justify the properties of a substance on the basis of its structure
CEN_K1_U08	The graduate can apply mathematical methods in chemical and physicochemical calculations
CEN_K1_U09	The graduate can select and apply statistical methods to describe chemical and physicochemical processes and analyse data
CEN_K1_U10	The graduate can interpret and analyse quantitative descriptions of basic physical and chemical phenomena
CEN_K1_U11	The graduate can use specialised computer software to visualise and describe chemical processes
CEN_K1_U12	The graduate can perform basic model calculations for chemical molecules or processes
CEN_K1_U19	The graduate can analyse and develop test results and prepare a final report on the chemical and physico-chemical experiments carried out
CEN_K1_U21	The graduate can independently obtain information from both Polish and foreign literature, physicochemical tables and other available sources
CEN_K1_U22	The graduate can prepare a summary of the analyses of the literature data carried out
CEN_K1_W01	The graduate knows and understands basic chemical laws and issues
CEN_K1_W02	The graduate knows and understands basic physics and their relationship to chemical laws
CEN_K1_W03	The graduate knows and understands techniques of higher mathematics for the formal description of basic physical and chemical processes
CEN_K1_W04	The graduate knows and understands fundamental knowledge of natural sciences
CEN_K1_W05	The graduate knows and understands the mechanisms of basic chemical reactions
CEN_K1_W06	The graduate knows and understands structure of molecules and crystals
CEN_K1_W08	The graduate knows and understands the chemical properties of substances according to their structure/composition