Zał. nr 5 do ZW 78/2023

Attachment no. 4. to the Program of Studies

FACULTY OF CHEMISTRY

SUBJECT CARD

Name of subject in Polish **Chemia Teoretyczna**
Name of subject in English **Theoretical Chemistry**
Main field of study (if applicable): **Biosciences**
Specialization (if applicable):
Profile: **academic**
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code W03BSS-SM2001W, W03BSS-SM2001C, W03BSS-SM2001L
Group of courses NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30	15	30		
Number of hours of total student workload (CNPS)	100	50	50		
Form of crediting (Examination / crediting with grade)	Exam	crediting with grade	crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points	3	2	2		
including number of ECTS points for practical classes (P)		2	2		
including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU)	1,3	0,7	1,4		

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. General Chemistry and Physics
2. Linear algebra and mathematical analysis
3. Fundamentals of physical and quantum chemistry

\

SUBJECT OBJECTIVES

C1 To acquaint students with fundamentals of molecular quantum mechanics.
C2 To acquaint students with modern methods of theoretical description of the electronic structure of atoms and molecules and to acquire the ability to apply these methods to determine the electronic structure and properties of molecular systems.
C3. Acquiring the ability to apply methods of theoretical chemistry to prediction and interpretation of selected spectral and thermodynamical properties of molecular systems.

SUBJECT EDUCATIONAL EFFECTS

related to knowledge:

Upon finishing the course, a student:
PEU_W01 - understands the problems and shortcomings of classical physics in the microscopic description,
PEU_W02 - knows the postulates of quantum mechanics and elements of the operator calculus,
PEU_W03 - can write the Schrödinger equation (SE) for model systems and for any molecular system,
PEU_W04 - knows the solutions of SE for the free particle, particle in model systems and for the hydrogen atom; understands the interpretation of these solutions,

PEU_W05 - knows the basic approximations used in the description of the electronic structure of molecular systems: the Born-Oppenheimer approximation and the basics of the variational and perturbational methods,
PEU_W06 - knows the basics of the theory of molecular orbitals,
PEU_W07 - has a basic knowledge of the solutions of the Hartree-Fock and Hartree-Fock-Roothan equations,
PEU_W08 - has basic knowledge of the theory of electron correlation and methods of its calculation (configuration interaction method, many-body perturbation theory, density functional theory),
PEU_W09 - has a basic knowledge of the theory of intermolecular interactions.

related to skills:
Upon finishing the course, a student:
PEU_U01 - can plan, carry out and interpret the results of calculations of the electronic structure of molecules within HF approximation and using selected methods taking into account electron correlation,
PEU_U02 - can predict the equilibrium structure of molecules,
PEU_U03 - can predict and interpret spectra of electronic states of molecules,
PEU_U04 - can interpret spectroscopic measurements based on quantum-chemical calculations,
PEU_U05 - can analyze the mechanisms of chemical reactions based on the results of quantum-chemical calculations.

related to social competences:
PEU_K01 student is ready to critically evaluate his/her knowledge and received content

PROGRAMME CONTENT

Lecture		Number of hours
Lec 1	**Introduction to molecular quantum mechanics.** Discussion of postulates of non-relativistic quantum mechanics. Definition of a wave function and its probabilistic interpretation. Definition of operators representing mechanical observables and elements of operator algebras. Time-dependent and time-independent Schrödinger's equation.	2
Lec 2	**Free particle and particle in model potentials.** Solving the Schrödinger equation for a free particle, particle in a box and in a harmonic potential.	2
Lec 3	**Hydrogen atom.** Solving the Schrödinger equation for a rigid rotator and hydrogen-like atoms.	2
Lec 4	**Molecular Hamiltonian.** Separation of the electronic and nuclear degrees of freedom. The adiabatic approximation and the Born-Oppenheimer approximation. The harmonic approximation. Normal modes analysis and interpretation of absorption spectra in the infrared range.	2
Lec 5	**Approximate methods of solving the Schrödinger equation I.** Variation calculus and its applications to model problems. Rayleigh-Ritz method. Molecular orbitals theory. Hückel method and its illustrative applications.	2
Lec 6	**Approximate methods of solving the Schrödinger equation II.** A time-independent perturbation theory. Perturbation in two-state and multi-state systems. Perturbation theory for degenerate reference states.	2
Lec 7	**Wave functions for many-electron systems.** Symmetry of the wave function. A determinantal wave function. The Slater-Condon rules. General expressions for matrix elements between Slater's determinants.	2
Lec 8	**The Hartree-Fock method.** The self-consistent field method. The Hartree-Fock-Roothan method. The charge density and matrix elements of the Fock operator.	2

Lec 9	**Molecular orbitals.** Elements of point group theory. Symmetry and nomenclature of molecular orbitals. Molecular orbitals diagrams for diatomic and polyatomic molecules. Walsh diagrams.	2
Lec 10	**Electronic correlation I.** Limitations of the Hartree-Fock method. Definition and methods for determining the electron correlation. The configuration interaction method.	2
Lec 11	**Electronic correlation II.** The Møller-Plesset perturbation theory. Elements of the coupled clusters method.	2
Lec 12	**The density functional theory.** One-particle density matrix and pair-density matrix. The Hohenberg-Kohn theorems. The Kohn-Sham method.	2
Lec 13	**The interaction of matter with electromagnetic radiation.** The fate of molecules in electronically excited states. Photochemical and photophysical processes in molecular systems. Jabłoński diagram. Absorption and fluorescence spectra in the UV and visible range**.** Fine structure of absorption and fluorescence spectra	2
Lec 14	**Processes of nonradiative deactivation of excited states.** Fermi's golden rule. Selection rules. Internal conversion. Conical intersections. Intersystem crossings. Excitation energy transfer - Förster's and Dexter's mechanisms. Natural and artificial light-harvesting systems. Photosynthesis.	2
Lec 15	**Intermolecular interactions.** The theory of intermolecular interactions. Hydrogen bond. Secondary structure of molecular systems, conformational analysis.	2
	Total hours	**30**

Classes		**Number of hours**
Cl 1	**Syllabus. Operator calculus**. Elements of linear algebra. Examining the properties of operators, operator eigenproblem.	2
Cl 2	**Solutions to the Schrödinger equation for model problems.**	2
Cl 3	**Simple applications of the variational principle to model problems.**	2
Cl 4	**Simple applications of the Rayleigh-Schrödinger perturbation theory** to model problems.	2
Cl 5	**Calculations of the electronic structure in the Hückel method for selected molecules I.** The π-electronic approximation and basic assumptions of the Hückel method for unsaturated hydrocarbons. Eigenproblem solution. Determination of molecular orbital coefficients for simple molecules.	2
Cl 6	**Calculations of the electronic structure in the Hückel model for selected molecules II.** Own problem in matrix form. Hamiltonian diagonalization and interpretation of eigenvalue and eigenvector spectra. Bond density and order matrix and population analysis.	2
Cl 7	**Hartree-Fock method I**. Slater-Condon rules. Solving problems within the Hartree-Fock method.	2
Cl 8	**Review and Test.**	1
	Total hours	**15**

Laboratory		**Number of hours**
Lab 1	**Work organization in a computer lab and a computing center.** Discussing the principles of health and safety at work. Distribution of accounts and basic information about available operating systems.	2
Lab 2	**Elements of the LINUX system I.** Basic information about the operating system. Selected BASH shell commands.	2

Lab 3	**Elements of the LINUX system II.** Support for selected text editors. Simple BASH shell scripts.	2
Lab 4	**Selected electronic structure calculation packages.** Preparation of batch files. Calculations of the electronic structure of atoms using the restricted and unrestricted Hartree-Fock method (HF). Structure of output files and interpretation of the results of calculations.	2
Lab 5	**Representation of the structure of molecular systems.** Orthogonal coordinates and internal coordinates on the example of Z-matrix.	2
Lab 6	**Accuracy of computational chemistry methods.** Selection of the basis functions. Comparison of the accuracy of selected ab initio methods and density functional theory methods. Validation of electronic structure calculation methods.	2
Lab 7	**Optimization of equilibrium geometry of molecules and analysis of normal-mode vibrations.** Discussion of gradient geometry optimization algorithms. Calculations of the harmonic frequencies' spectrum. Analysis of normal coordinates. Prediction and interpretation of infrared spectra.	2
Lab 8	**Molecular orbital theory.** Determination of potential energy curves for diatomic molecules in the HF method. Determination and interpretation of molecular orbital and Walsh diagrams. Charge-density population analysis.	2
Lab 9	**Configuration interaction method.** Calculation of electronic states' spectra using the configuration interaction method with single (CIS) and double excitations (CISD). Size-extensivity and size-consistency of the CI method. **Project I.** Calculations of the electronic states spectra and their interpretation for selected polyatomic molecules.	2
Lab 10	**Project I.** Calculations of the molecular structure and thermodynamical properties	2
Lab 11	**Mechanisms of chemical reactions.** Location of transition state geometry.	2
Lab 12	**Project II** – Calculations of electronic states spectra and their interpretation for selected polyatomic molecules.	2
Lab 13	**Work on individual projects I.**	2
Lab 14	**Work on individual projects II.**	2
Lab 15	**Work on individual projects III.**	2
	Total hours	30

TEACHING TOOLS USED
N1. Lecture at the blackboard N2. Multimedia presentation N3. Implementation of tasks / projects in the computer lab N4. Personal computers / resources of the computing center / specialized software

EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT

Evaluation (F – forming during semester), P – concluding (at semester end)	Learning outcomes code	Way of evaluating learning outcomes achievement
P	PEU_Lec01-	Final exam

	PEU_Lec15, PEU_K01	
F1	PEU_Cl01-PEU_Cl08, PEU_K01	Home assignments and test.
F2	PEU_La1-PEU_La15, PEU_K01	Individual projects
P		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] Engel, T., Reid, P., Quantum Chemistry and Spectroscopy, 3rd ed. ed. Pearson, Boston, 2013
[2] L. Piela, "Ideas of Quantum Chemistry" 3rd Edition, Elsevier, 2019
[3] D. O. Hayward, "Quantum Mechanics for Chemists", RSC, 2002

SECONDARY LITERATURE:

[1] R. W. Góra, teaching materials for the course: "Theoretical chemistry", 2019

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

Robert Góra, robert.gora@pwr.edu.pl