DESCRIPTION OF THE COURSE OF STUDY

Course code	0531.6.CHEM.2.B/C.CT	
Name of the course in	Polish	Chemia teoretyczna
	English	Theoretical chemistry

1. LOCATION OF THE COURSE OF STUDY WITHIN THE SYSTEM OF STUDIES

1.1. Field of study	**Chemistry**
1.2. Mode of study	**Full-time studies**
1.3. Level of study	**Second-cycle studies**
1.4. Profile of study*	**General academic**
1.5. Person/s preparing the course description	**Dr. hab. Pawel Rodziewicz, Assoc. Prof.**
1.6. Contact	**pawel.rodziewicz@ujk.edu.pl**

2. GENERAL CHARACTERISTICS OF THE COURSE OF STUDY

2.1. Language of instruction	**English**
2.2. Prerequisites*	**Completed course in mathematics, physics and introduction to quantum chemistry**

3. DETAILED CHARACTERISTICS OF THE COURSE OF STUDY

3.1. Form of classes		Lectures, seminar, laboratory (in silico)
3.2. Place of classes		Classes in the teaching room of the UJK
3.3. Form of assessment		Lecture - exam, seminar- credit with grade, laboratory - credit with grade
3.4. Teaching methods		Lecture, discussion, practical exercises
3.5. Bibliography	**Required reading**	„Quantum Mechanics in chemistry" G. C. Schatz, Dover Publications, First Edition 2002
	Further reading	"Molecular Simulations: Fundaments and Practise" S. Alavi, Wiley-VCH, First Edition 2020

4. OBJECTIVES, SYLLABUS CONTENT AND INTENDED LEARNING OUTCOMES

4.1. Course objectives ***(including form of classes)***

LECTURE

The aim of the lecture is to present the basic issues related to theoretical chemistry needed for chemists.

SEMINAR

The aim of the seminar is to solve tasks and problems related to the content introduced during the lecture.

LABORATORY

The aim of the laboratory (in silico) is to apply computational methods to calculate energetic, structural and spectroscopic properties of molecules by creating input file, running calculations and analysis of the output.

4.2. Detailed syllabus ***(including form of classes)***

Lecture:
Schrödinger equation for model systems. Semi-empirical quantum chemistry methods. Hartee-Fock method. Post-HF methods. Electronic structure of atoms and diatomic molecules. Basis sets. Density functional theory (DFT). Potential energy surface (PES). Geometry optimization. Population analysis. Bond order. Electronegativity. Force field (FF). Molecular mechanics. Binding and interaction energy. Interactions in condensed matter. Periodic boundary conditions. Canonical ensemble and its usage for calculation of thermodynamic functions.

Seminar:
Energy level degeneracy. Eigenvalues and eigenvectors. Gram-Schmidt method for orthonormalizing of vectors. Interatomic and intermolecular potential for mutual interactions. Calculation of a strength of covalent and non-covalent interactions. Calculation of different thermodynamic functions.

Laboratory (in silico):
Construction of 3D models of molecules. Internal and cartesian coordinates. Preparation of the Input file. Setting up DFT and FF-based calculations. Analysis of the Output file. Visualization of the atomic and molecular orbitals and electronic

density. Conformational analysis. Global and local energy minima. Calculation of binding and interaction energy. Calculation and visualization of radial distribution function (RDF). Calculation of spectroscopic properties (IR spectra). Visualization of crystal structure. Application of periodic boundary conditions in condensed matter. Visualization of different carbon allotropes: diamond, fullerene, graphite, graphene, carbon nanotubes.

4.3 Intended learning outcomes

Code	A student, who passed the course	Relation to learning outcomes
within the scope of **KNOWLEDGE:**		
W01	Student knows fundaments of density functional theory (DFT) and post-HF methods.	CHEMIA_W07
W02	Student knows techniques for geometry optimization and analysis of potential energy surface	CHEMIA_W07
within the scope of **ABILITIES:**		
U01	Student can calculate energetic properties, including binding and interaction energy	CHEMIA_U04
U02	Student can calculate eigenvalues and eigenvectors	CHEMIA_U04
within the scope of **SOCIAL COMPETENCE:**		
K01	Student is aware of the importance of theoretical chemistry and is aware of the need to constantly acquire knowledge and skills related to the work of a chemist	CHEMIA_K01

4.4. Methods of assessment of the intended learning outcomes

Teaching outcomes *(code)*	Method of assessment (+/-)																				
	Exam written			Test			Project*			Effort in class*			Self-study*			Group work*			Others* e.g. standardized test used in e-learning		
	Form of classes			*Form of classes*			*Form of classes*			*Form of classes*			*Form of classes*			*Form of classes*			*Form of classes*		
	L	*S*	*L*	*L*	*S*	*L*	*L*	*S*	...	*L*	*S*	*L*	*L*	*S*	...	*L*	*S*	...	*L*	*S*	.. .
W01	+																				
W02	+																				
U01	+				+	+															
U02	+				+	+															
K01											+	+									

4.5. Criteria of assessment of the intended learning outcomes

Form of classes	Grade	Criterion of assessment
lecture (L) (including e-learning)	3	Written exam, 51-60% points
	3,5	Written exam, 61-70% points
	4	Written exam, 71-80% points
	4,5	Written exam, 81-90% points
	5	Written exam, 91-100% points
seminar (S)	3	Credit with grade - test, 51-60% points
	3,5	Credit with grade - test, 61-70% points
	4	Credit with grade - test, 71-80% points
	4,5	Credit with grade - test ,81-90% points
	5	Credit with grade - test, 91-100% points
laboratory (L)	3	Credit with grade - test, 51-60% points
	3,5	Credit with grade - test, 61-70% points
	4	Credit with grade - test, 71-80% points
	4,5	Credit with grade - test, 81-90% points
	5	Credit with grade - test, 91-100% points

5. BALANCE OF ECTS CREDITS – STUDENT'S WORK INPUT

Category	Student's workload	
	Full-time studies	Extramural studies
NUMBER OF HOURS WITH THE DIRECT PARTICIPATION OF THE TEACHER /CONTACT HOURS/	***75***	**50**
Participation in lectures	30	20
Participation in seminars	15	10
Participation in laboratories	30	20
INDEPENDENT WORK OF THE STUDENT/NON-CONTACT HOURS/	**50**	**75**
Preparation for the lecture	5	10
Preparation for the seminars	15	20
Preparation for the laboratories	10	15
Preparation for the exam	20	30
TOTAL NUMBER OF HOURS	**125**	**125**
ECTS credits for the course of study	**5**	**5**

Accepted for execution *(date and legible signatures of the teachers running the course in the given academic year)*

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