DESCRIPTION OF THE COURSE OF STUDY

Course code	**0531-2CHEM-C13-PCK**	
Name of the course in	Polish	Podstawy chemii kwantowej
	English	Introduction to quantum 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	**First-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 and physics**

3. DETAILED CHARACTERISTICS OF THE COURSE OF STUDY

3.1. Form of classes		Lectures, exercises
3.2. Place of classes		Classes in the teaching room of the UJK
3.3. Form of assessment		Lecture - exam, seminar- credit with grade
3.4. Teaching methods		Lecture, discussion
3.5. Bibliography	**Required reading**	„Introduction to Quantum Mechanics" D. J. Griffiths and D. F. Schroeter, Cambridge University Press, Third Edition 2018
	Further reading	"Principles of Quantum Mechanics" R. Shankar, Springer, Second Edition 1995

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 quantum mechanics needed for chemists.

SEMINAR

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

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

Lecture:

Physical construct of quantum mechanics. Postulates of quantum mechanics. Wave function. Operators. Schrödinger equation. Eigenfunctions and eigenvalues. Expectation value of the observable. Free particle. Particle in a box. Rigid rotor. Harmonic oscillator. Tunnelling effect. Schrödinger equation for hydrogen and hydrogen-like atoms. Perturbation theory. Variational principle. Electronic correlation. Born-Oppenheimer approximation. Spin. Pauli exclusion principle. Molecular orbital theory. Hückel molecular orbital theory.

Seminar:

Equation of wave function. Calculation of wavelength and frequency. Operators and their acting on wave function. Commutator of two operators. Conditions for linearity of an operator. Hermiticity of operators. Normalization factor of a wave function. Wave function orthogonalization. Calculation of quantum mechanical probability density of an electron. Pauli spin matrices. Calculation of transmission coefficient for a particle tunneling through a single potential barrier. Analysis of eigenfunctions of harmonic oscillator. Solving Schrödinger equation - particle in a box. Calculation of energy levels utilizing the Hückel molecular orbital theory.

4.3 Intended learning outcomes

Code	A student, who passed the course	Relation to learning outcomes
within the scope of **KNOWLEDGE:**		
W01	Student knows postulates of quantum mechanics	CHEMIA_W10
W02	Student knows harmonic oscillator Schrödinger equation	CHEMIA_W10
within the scope of **ABILITIES:**		
U01	Student can calculate normalization factor of a wave function	CHEMIA_U08
U02	Student can calculate commutator of two operators	CHEMIA_U08
U03	Student can solve Schrödinger equation for a free particle	CHEMIA_U08
within the scope of **SOCIAL COMPETENCE:**		
K01	Student is aware of the importance of quantum 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			Effort in class*		
	Form of classes			*Form of classes*			*Form of classes*		
	L	*E*	...	*L*	*E*	...	*L*	*E*	...
W01	+								
W02	+								
U01	+				+				
U02	+				+				
U03	+				+				
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, 50-60% 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
classes (C)* (including e-learning)	3	Credit with grade - test, 50-60% 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
others (...)* (including e-learning)	3	Credit with grade - test, 50-60% correct answers
	3,5	Credit with grade - test, 61-70% correct answers
	4	Credit with grade - test, 71-80% correct answers
	4,5	Credit with grade - test, 81-90% correct answers
	5	Credit with grade - test, 91-100% correct answers

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/	***45***	
Participation in lectures	20	
Participation in seminars	25	
INDEPENDENT WORK OF THE STUDENT/NON-CONTACT HOURS/	**55**	
Preparation for the lecture	10	
Preparation for the seminars	25	
Preparation for the exam	20	
TOTAL NUMBER OF HOURS	**100**	
ECTS credits for the course of study	**4**	

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

.....