

**DOCTORAL SCHOOL OF WROCLAW UNIVERSITY OF SCIENCE AND
TECHNOLOGY**

SUPERVISOR/TEAM/ DECLARING/CONDUCTING COURSE: Szczepan Roszak
DEPARTMENT: Chemical Department
SCIENTIFIC DISCIPLINE: Chemical Sciences

COURSE CARD

Course name in Polish: Chemia Teoretyczna i Obliczeniowa
Course name in English: Theoretical and computational chemistry
Course language Polish

University-wide general course type*:

The course is intended for all PhD students: YES / NO

- 1) **BASIC COURSE**
- 2) ~~**SPECIALIST COURSE**~~
- 3) ~~**SEMINAR**~~
- 4) ~~**HUMANISTIC COURSE**~~
- 5) ~~**LANGUAGE**~~

Subject code: NCQ100106W

* delete as applicable

	Lecture	Foreign language course	Seminar	Mixed forms
Number of hours of organized classes in university (ZZU)	30			
Grading	Exam	Exam	Oral presentation	Exam, inspection, evaluation classes
Number of ECTS points	0			

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic knowledge of physics and chemical sciences

COURSE OBJECTIVES

- C1. The student learn basics of quantum chemistry and is able for its practical application.
- C2. The course provides know-how for theoretical the determination of properties of molecules and materials and for modeling of chemical processes.
- C3. The course allows determining of usefulness of theoretical approaches for particular needs of student in his personal studies.

PROGRAM CONTENTS

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Form of classes – lecture (Lec)		Number of hours
Lec1	Basic concepts and postulates of quantum mechanics.	2
Lec2	Potential energy surfaces – molecular mechanics, chemical thermodynamics.	2
Lec3	Simple model problems, potential barrier, hydrogen bond, hydrogen oscillator- IR spectroscopy, quantum rotor – microwave spectroscopy.	4
Lec4	Hydrogen atom , spectroscopy of hydrogen.	2
Lec5	Variational method, orbital approximation, Slater determinant.	2
Lec6	The structure of many-electron atoms. Periodic system of elements.	2
Lec7	Hartree-Fock and Hartree-Fock-Roothaan approaches.	4
Lec8	Ab initio computations. Basis functions.	2
Lec9	Chemical bond – population analysis.	2
Lec10	Perturbation approach, molecular interactions.	2
Lec11	Electron correlation. Perspectives of computational chemistry.	4
Lec12	Available computer software and www pages , computer software in WCSS, PCSS, and ICM.	2
Total hours:		30

Form of classes – foreign language course (Lng)		Number of hours
Lng1		
Lng2		
Lng3		
..		
Total hours:		

Form of classes – seminar (Sem)		Number of hours
Sem1		
Sem2		
Sem3		
...		
Total hours:		

Form of classes – mixed forms (mix)		Number of hours
Mix1		
Mix2		
Mix3		
...		
Total hours		

TEACHING TOOLS USED
N1. Lectures N2. Discussion of particular practical problems.

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ACHIEVED SUBJECT LEARNING OUTCOMES		
Type of learning outcome	Code of learning outcome	Assessment of learning outcome
Knowledge	P8U_W	Is able to properly use foreign literature sources
Knowledge	P8S_WG	Possesses advanced knowledge regarding his discipline
Skills	P8S_UW	Is able to select and apply theoretical approaches for solving (or support experimental studies) chemical problems.
Social competence	P8U_K	Understands importance of scientific studies and teaching in the area of application of theoretical chemistry.

PRIMARY AND SECONDARY LITERATURE
<p><u>PRIMARY LITERATURE:</u></p> <p>[1] Introduction to Quantum Mechanics in Chemistry, M. A. Ratner, G. C. Schatz, Prentice-Hall, Upper Saddle River, NJ, 2000</p> <p>[2] Exploring Chemistry with Electronic Structure Theory, J. B. Foresman, A. Frish, Gaussian Inc., Pittsburgh, 1995.</p> <p>[3] Ab Initio Molecular Orbital Theory, W. J. Hehre, L. Radom, P. v R. Schleyer, J. A. Pople, Wiley, New York, 1996.</p> <p>[4] Ideas of Quantum Chemistry, L. Piela, PWN, Warszawa, 2012.</p> <p><u>SECONDARY LITERATURE:</u></p> <p>[1] Actual literature in scientific journals..</p> <p>[2] Theoretical and Computational Chemistry –lectures, S. Roszak, Wyd. Chemiczny, Politechnika Wroclawska, 2011.</p> <p>[3] Theoretical and Computational Chemistry –laboratory, S. Roszak, Wyd. Chemiczny, Politechnika Wroclawska, 2011.</p>
<p>SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)</p> <p style="text-align: center;">Szczepan Roszak; szczepan.roszak@pwr.edu.pl</p>