Zał. nr 5 do ZW 16/2020

FACULTY OF CHEMISTRY

SUBJECT CARD

Name of subject in Polish Nanostruktury w przemysłowych i numerycznych zastosowaniach
Name of subject in English Nanostructures in Industrial and Numerical Applications
Main field of study (if applicable): Chemical Nano-Engineering
Specialization (if applicable): ……..
Profile: academic
Level and form of studies: 2nd level, , full-time
Kind of subject: obligatory
Subject code …….
Group of courses NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30	30		30	
Number of hours of total student workload (CNPS)	60	60		30	
Form of crediting	crediting with grade*	crediting with grade*		crediting with grade*	
For group of courses mark (X) final course					
Number of ECTS points	2	2		1	
including number of ECTS points for practical classes (P)		2		1	
including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU)	1,4	1,4		0,7	

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

C1 Gaining basic knowledge of computational quantum chemistry
C2 Gaining knowledge how to select the proper computational technique for application in nano-engineering
C3 Application of computational quantum chemistry methods to model properties of light-driven molecular motors.

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SUBJECT OBJECTIVES

C1 Gaining basic knowledge of computational quantum chemistry
C2 Gaining knowledge how to select the proper computational technique for application in nano-engineering
C3 Application of computational quantum chemistry methods to model properties of light-driven molecular motors

SUBJECT EDUCATIONAL EFFECTS

related to knowledge:

PEK_W01 Student has knowledge regarding the variety of quantum-chemistry methods
PEK_W02 Student can choose the right computational approach to specific properties of nano-systems
PEK_W03 Student knows the basic principles of operation of light-driven molecular machines

related to skills:

PEK_U01 Student can work in the high-performance computing center environment
PEK_U02 Student can run efficiently quantum-chemistry programs
PEK_U03 Student can analyze the results of quantum-chemistry calculations
PEK_U04 Student can pinpoint the operation mechanism of light-driven molecular machines using computational quantum chemistry methods

related to social competences:

PEK_K01student understands the need to inform the public about the need to achieve the goals of development of nanoengineering
PEK_K02 student is able to work in a group, performing various roles including group leader
PEK_K03 student is aware of the social role of the engineer
PEK_K04 student is ready to critically evaluate his/her knowledge and received content

PROGRAMME CONTENT

	Lecture	**Number of hours**
Lec 1	Applications of computational quantum chemistry in modeling of nanostructures – an overview	
	The basics of molecular quantum mechanics	
	Hartree-Fock self-consistent-field method	
	Density functional theory. Kohn-Sham method.	
	Time-dependent density functional theory: formalism and applications.	
	Gaussian basis sets for molecular calculations	
	Methods to account for environmental effects	
	Electron correlation: Møller-Plesset perturbation theory	
	Electron correlation: Coupled-cluster theory	
	Electron correlation: Multiconfigurational self-consistent-field method	
	Applications: Modeling of excited states	
	Applications: Light-driven molecular motors (part 1)	
	Applications: Light-driven molecular motors (part 2)	
	Applications: Light-driven molecular motors (part 3)	
	Total hours	30

Classes		Number of hours
Cl	Introduction to high-performance computer center environment	
C2	Quantum chemistry computer tools: an introduction.	
C3	Building structures, geometry optimization, vibrational analysis	
C4	Building structures, geometry optimization, vibrational analysis (cont.)	
C5	Hartree-Fock self-consistent-field method	
C6	Density functional theory and its time-dependent extension	
C7	Methods to account for environmental effects	
C8	Møller-Plesset perturbation theory and coupled-cluster theory	
C9	Project 1: Modeling of spectra of molecules in solution (individual assignments)	
C10	Project 1: Modeling of spectra of molecules in solution (individual assignments)	
C11	Multiconfigurational self-consistent field method	
C12	Project 2: Light-driven molecular motors (individual assignments)	
C13	Project 2: Light-driven molecular motors (individual assignments)	
C14	Project 2: Light-driven molecular motors (individual assignments)	
C15	Project 2: Light-driven molecular motors (individual assignments)	
	Total hours	30

Laboratory		Number of hours
Lab 1		
Lab 2		
Lab 3		
Lab 4		
Lab 5		
…		
	Total hours	

Project		Number of hours
Proj 1	Introductory classes	
Proj 2	Individual assignments	
Proj 3	Application of multiscale modeling in nanotechnology	
Proj 4	Fundamentals of molecular dynamic simulations	
Proj 5	Thermostats and barostats	
Proj 6	Force-fields	
Proj 7	Modeling in transport using molecular dynamics	
Proj 8	Predicting properties using molecular dynamics	
Proj 9	Combining molecular dynamics with other modeling techniques	

Proj 10	Individual assignments (assessment part 1)	
Proj 11	Project 1: presentations	
Proj 12	Molecular machines and molecular dynamics (part 1)	
Proj 13	Individual assignments (assessment part 2)	
Proj 14	Molecular machines and molecular dynamics (part 2)	
Proj 15	Project 2: presentations	
	Total hours	30

TEACHING TOOLS USED
N1. Lecture with multimedia presentation N2. Hands-on sessions using computers N3. Preparation of reports

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 (lecture)	PEK_W01 - PEK_W03	Written evaluation
F1-F15 (class)	PEK_U01 - PEK_U04	Evaluation of individual reports
F1-F15 (Project)	PEK_U03 – PEK_U04 PEK_K01 – PEK_K04	Evaluation of the student's project presentation

PRIMARY AND SECONDARY LITERATURE
PRIMARY LITERATURE: N. Levine, „Quantum Chemistry", 7th Edition, Pearson Education, 2014. **SECONDARY LITERATURE:** Roos, R. Lindh, P. A. Malmqvist, V. Veryazov, P. O. Widmark, „Multiconfigurational Quantum Chemistry", 1st Edition, Wiley, 2016. Koch, M. C. Holthausen, „A Chemist's Guide to Density Functional Theory", 2nd Edition, Wiley, 2000.
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