Zał. nr 5 do ZW 25/2019

Załącznik nr 4 do programu studiów

FACULTY OF CHEMISTRY

SUBJECT CARD

Name of subject in English: Nanostructures in Industrial and Numerical Applications
Main field of study (if applicable): Chemical and Process Engineering
Specialization (if applicable): Chemical Nano-engineering
Profile: academic
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code: ICC025007
Group of courses: YES

	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 (P) classes		2			1
including number of ECTS points for direct teacher-student contact (BK) classes	1	1			1

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge of the basic quantum mechanics

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_K01 student 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

Lectures		Number of hours
Lec 1	Applications of computational quantum chemistry in modeling of nanostructures – an overview	2
Lec 2	The basics of molecular quantum mechanics	2
Lec 3	Hartree-Fock self-consistent-field method	2
Lec 4	Density functional theory. Kohn-Sham method.	2
Lec 5	Time-dependent density functional theory: formalism and applications.	2
Lec 6	Gaussian basis sets for molecular calculations	2
Lec 7	Methods to account for environmental effects	2
Lec 8	Electron correlation: Møller-Plesset perturbation theory	2
Lec 9	Electron correlation: Coupled-cluster theory	2
Lec 10	Electron correlation: Multiconfigurational self-consistent-field method	2
Lec 11	Applications: Modeling of excited states	2
Lec 12	Applications: Light-driven molecular motors (part 1)	2
Lec 13	Applications: Light-driven molecular motors (part 2)	2
Lec 14	Applications: Light-driven molecular motors (part 3)	2
Lec 15	Exam	2
	Total hours	30

Classes		Number of hours
Class 1	Introduction to high-performance computer center environment	2
Class 2	Quantum chemistry computer tools: an introduction.	2
Class 3	Building structures, geometry optimization, vibrational analysis	2
Class 4	Building structures, geometry optimization, vibrational analysis (cont.)	2
Class 5	Hartree-Fock self-consistent-field method	2
Class 6	Density functional theory and its time-dependent extension	2
Class 7	Methods to account for environmental effects	2
Class 8	Møller-Plesset perturbation theory and coupled-cluster theory	2
Class 9	Project 1: Modeling of spectra of molecules in solution (individual assignments)	2
Class 10	Project 1: Modeling of spectra of molecules in solution (individual assignments)	2
Class 11	Multiconfigurational self-consistent field method	2
Class 12	Project 2: Light-driven molecular motors (individual assignments)	2
Class 13	Project 2: Light-driven molecular motors (individual assignments)	2
Class 14	Project 2: Light-driven molecular motors (individual assignments)	2

Class 15	Project 2: Light-driven molecular motors (individual assignments)	2
	Total hours	30

Seminar		Number of hours
Sem 1	Introductory classes	2
Sem 2	Individual assignments	2
Sem 3	Application of multiscale modeling in nanotechnology	2
Sem 4	Fundamentals of molecular dynamic simulations	2
Sem 5	Thermostats and barostats	2
Sem 6	Force-fields	2
Sem 7	Modeling in transport using molecular dynamics	2
Sem 8	Predicting properties using molecular dynamics	2
Sem 9	Combining molecular dynamics with other modeling techniques	2
Sem 10	Indivdual assignments (assessment part 1)	2
Sem 11	Project 1: presentations	2
Sem 12	Molecular machines and molecular dynamics (part 1)	2
Sem 13	Indivdual assignments (assessment part 2)	2
Sem 14	Molecular machines and molecular dynamics (part 2)	2
Sem 15	Project 2: presentations	2
	Total hours	30

TEACHING TOOLS USED

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

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

Evaluation (F – forming (during semester), P – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
P (lecture)	PEK_W01 - PEK_W03	Written evaluation
F1-F15 (class)	PEK_U01 - PEK_U04	Evaluation of individual reports
F1-F15 (seminar)	PEK_U03 – PEK_U04 PEK_K01 – PEK_K04	Evaluation of the student's project presentation

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] Ira N. Levine, „Quantum Chemistry", 7th Edition, Pearson Education, 2014.

SECONDARY LITERATURE:

[1] B. Roos, R. Lindh, P. A. Malmqvist, V. Veryazov, P. O. Widmark, „Multiconfigurational Quantum Chemistry", 1st Edition, Wiley, 2016.

[2] W. Koch, M. C. Holthausen, „A Chemist's Guide to Density Functional Theory", 2nd Edition, Wiley, 2000.

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

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