Faculty of Chemistry

SUBJECT CARD

Name of subject in Polish	**Modelowanie molekularne**
Name of subject in English	**Molecular modeling**
Main field of study (if applicable):	Biotechnology, Chemistry
Specialization (if applicable):	Bioinformatics, Medicinal Chemistry
Profile:	academic
Level and form of studies:	2nd level, full-time
Kind of subject:	obligatory
Subject code	CHC024006
Group of courses	NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15		30		15
Number of hours of total student workload (CNPS)	60		60		30
Form of crediting	Examination		crediting with grade		crediting with grade
For group of courses mark final course with (X)					
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	0,5		1		0,5

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

Basic knowledge of atomic and molecular structure concepts
Basic knowledge of analytic geometry
Basic knowledge of computer science
Basic knowledge of organic chemistry

SUBJECT OBJECTIVES

C1 Teaching construction of 3-D molecular models
C2 Teaching applications of quantum chemistry methods
C3 Teaching elementary concepts of the theory of intermolecular interactions
C4 Teaching modeling techniques of molecular aggregates
C5 Teaching modeling chemical reactions

SUBJECT LEARNING OUTCOMES

Relating to knowledge:

PEK_W01 – knowledge of construction of 3-dimensional molecular models and their transformations
PEK_W02 – knowledge of elementary molecular modeling methods and limits of their applications.
PEK_W03 – knowledge of major components of intermolecular interaction energy
PEK_W04 – knowledge of modeling drugs and biocatalysts

Relating to skills:

PEK_U01 – ability of construction of 3-D molecular model starting from assumed hybridization type
PEK_U02 – ability to predict molecular structure and properties
PEK_U03 – ability to predict possibile structures of molecular aggregates
PEK_U04 – ability to analyse protein-ligand interactions
PEK_U05 – ability to model dynamic properties of molecular aggregates

relating to social competences:

PEU_K01 – ability to comprehend, critically assess and communicate the information from scientific sources related to modeling of biological systems of molecules and their properties.

PROGRAM CONTENT

Lectures		Number of hours
Lec 1	Basic concepts. Interdisciplinary charakter of molecular modeling. Typical molecular modeling tasks. Molecular structure sources. Algorithms used in construction of 3-D molecular models with examples. Hybridization. Coordinate transformations. Basic concepts of molecular graphics. Visualization techniques. Literature review.	2
Lec 2	Basic concepts of quantum chemistry. Review of quantum chemistry computational methods. Hueckel Molecular Orbitals and ab intio methods. Theoretical prediction of physical properties and structures.	2
Lec 3	Construction of molecular models – exercises and test	2
Lec 4	Basic concepts of the theory of intermolecular interactions. Perturbation theory. Characteristics of major components of intermolecular interaction components.	2
Lec 5	Hydrogen bonding. Molecular charge distribution and electrostatic models. Force fields.	2
Lec 6	Predicting properties and structure of molecular aggregates – exercises and test.	2
Lec 7	Modeling interactions in receptors and enzyme active centers. Drug design techniques. Molecular dynamice. Homology modeling.	2
Lec 8	Analysis of enzyme catalytic activity and biocatalyst design.	1
	Total hours	15

Laboratory		Number of hours
Lab 1	Introduction and lab organization. Editing of molecular structures.	2
Lab 2	Preparing molecular dynamics simulations	2
Lab 3	Preparing molecular dynamics simulations	2
Lab 4	Analysis of molecular dynamics trajectories	2
Lab 5	Computational task #1.	2
Lab 6	Force field parametrization of arbitral organic molecules: initial topology, atom types and non-bonding parameters	2
Lab 7	Force field parametrization of arbitral organic molecules: optimization of atomic charges	2
Lab 8	Force field parametrization of arbitral organic molecules: bonding parameters	2
Lab 9	Computational task #2.	2
Lab 10	Receptor-ligand docking and virtual screening	2

Lab 11	Quantum mechanical calculation of interaction energies	2
Lab 12	Computational task #3.	2
Lab 13	Introduction to hybrid QM/MM modeling	2
Lab 14	Modeling energy profile of a reaction using QM/MM methods	2
Lab 15	Computational task #4	2
	Total hours	30
Seminar		Number of hours
Se1	Student seminars: protein structure prediction, homology modeling	2
Se2	Student seminars: superimposing molecules, docking, predicting protonation state	2
Se3	Student seminars: modeling receptors, sensors, molecular switches, molecular motors	2
Se4	Student seminars: use of genetic algorithms and neural nets in molecular modeling	2
Se5	Student seminars: drug design techniques	2
Se6	Student seminars: modeling IR, Raman, UV, NMR spectra	2
Se7	Student seminars: modeling chemical Reaction and transition states	2
Se8	Student seminars: biocatalyst design	1
	Total hours	15

TEACHING TOOLS USED

N1 Lecture with multimedia presentation
N2 Solving problems
N3 Use of software
N4 Student multimedia presentation
N5 Preparing report

EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT

Evaluation (F – forming (during semester), P – concluding (at semester end)	Learning outcomes number	Way of evaluating learning outcomes achievement
F_Lec1	PEK_W01, PEK_W02, PEK_U01	Test with problem solving
F_Lec2	PEK_W02, PEK_W03, PEK_W04, PEK_U01, PEK_U03	Test with problem solving
C_Lec	PEK_W01, PEK_W02, PEK_W03, PEK_W04, PEK_U01, PEK_U03	F_Lec1+F_Lec2, or final exam (test with problem solving, 24 score points): Score Grade 12-14 3,0 15-16 3,5 17-18 4,0 19-20 4,5 21-22 5,0 23-24 5,5
F_Lab1	PEK_W04, PEK_U05	Computational task #1:
F_Lab2	PEK_W01, PEK_W04, PEK_U01, PEK_U04	Computational task #2
F_Lab3	PEK_W04, PEK_U03, PEK_U04	Computational task #3
F_Lab4	PEK_W04, PEK_U02	Computational task #4
C_Lab	PEK_U01, PEK_U02, PEK_U03, PEK_U04, PEK_U05, PEK_W01, PEKW04	F_Lab1+F_Lab2+F_Lab3+F_Lab4 Total score Grade 14-16 3,0 17-19 3,5

		20-22 4,0 23-25 4,5 26-28 5,0
F_Sem	PEU_K01	Preparation and presentation of seminar on individual topic; Active participation in discussion of presentations of other students
C_Sem	PEU_K01	Final grade

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] L. Piela, Quantum Chemistry Ideas, Elsevier, 2010
[2] A.R. Leach, Molecular Modeling:Principles and Applications, (2-nd Ed), Prentice Hall, 2001
[3] H.D. Hotje, Molecular modeling. Basic principles and applications, (3-rd Ed), Wiley, 2008
[4] T. Schlick, Molecular modeling and simulation, Springer, 2002.

SECONDARY LITERATURE:

[1] F. Jensen, Introduction to computational chemistry, Wiley, 2006 (2-nd Ed)
[2] J.M. Goodman, Chemical Applications of Molecular Modeling, RSC, 1999.
[3] J.P. Doucet, J. Weber, Computer-Aided Molecular Design, 1996,Academic Press, 1996
[4] G.H. Grant, W.G. Richards, Computational chemistry, Oxford Sci. Publ., 1995

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

Paweł Kędzierski, Pawel.Kedzierski@pwr.edu.pl