

FACULTY of Chemistry

SUBJECT CARD**Name of subject in Polish ... Numeryczne zastosowania w nano-inżynierii****Name of subject in English Numerical applications in nano-engineering****Main field of study (if applicable): ...Chemical engineering and technology.....****Specialization (if applicable): ...Advanced chemical engineering and green technology.....****Profile: academic****Level and form of studies: 2nd level****Kind of subject: obligatory****Subject code W03CET-SM2008W, W03CET-SM2008P****Group of courses NO**

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15		30		
Number of hours of total student workload (CNPS)	25		50		
Form of crediting (Examination / crediting with grade)	Exam		Crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points	1		2		
including number of ECTS points for practical classes (P)			2		
including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU)	0.6		1,2		

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge of mathematics, physics, and mass transfer phenomena at the bachelor's level (chemical engineering or related)
2. Understanding of numerical algorithms
3. Basic understanding of chemical thermodynamics

SUBJECT OBJECTIVES

C1 To familiarize students with the current state of nano-type research

C2 To understand future applications in nano-materials

C3 To familiarize students with specific properties in the nano-scale

C4 To introduce students to the modeling methodology of nano-porous materials

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

PEU_W01 – student understands the notion of nano-engineering and its role in future technologies
 PEU_W02 - student knows the current trends of nano-technology developments
 PEU_W03 - student knows how to model numerically the properties of nano-objects

relating to skills:
 PEU_U01 – student is able to find and understand the literature related to nanotechnology
 PEU_U02– student is able to discuss the current trends in nanotechnology
 PEU_U03 – student can design a numerical modeling analyze of nano-materials

PROGRAMME CONTENT

Lecture		Number of hours
Lec 1	Characteristics of the nano-scale properties.	2
Lec 2	Numerical projects: basic notions and definitions	2
Lec 3	Numerical projects in nano-materials.	2
Lec 4	Surface and deformations in nanoscale. Nanoporous materials.	2
Lec 5	Industrial applications of nanoporous materials	2
Lec 6	Characteristics of nanoporous materials: adsorption	2
Lec 7	Microscopic models of nanoporous materials and adsorption	2
Lec 8	Interpretation of simulations of adsorption and diffusion in nanoporous materials	1
	Total hours	15

Project		Number of hours
Proj 1	Definitions of models for simulations, basic Linux notions	4
Proj 2	Setting-up and optimalization of the input data	6
Proj 3	Examples of the Monte Carlo simulation methods	4
Proj 4	Simulation of adsorption in porous systems	6
Proj 5	Analysis of the simulation results: the role of adsorption energy	4
Proj 6	Transport in nanaopores	6
Proj 7	Adsorption in nanoporous systems	3
	Total hours	30

TEACHING TOOLS USED

N1. Multimedia presentation
 N2. Discussions and exercises
 N3. Consultations

EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT

Evaluation (F – forming during semester), P –	Learning outcomes code	Way of evaluating learning outcomes achievement
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concluding (at semester end)		
F (project)	PEU_U01 – U03	Grading based on the work on projects
P (lecture)	PEU_W01 -W03	Exam
PRIMARY AND SECONDARY LITERATURE		
LITERATURA PODSTAWOWA:		
[1] Akhlesh Lakhtakia, Nanometer structures: Theory, modeling and simulation, SPIE Press 2004		
LITERATURA UZUPEŁNIAJĄCA:		
Internet.		
SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)		
Bogdan Kuchta (bogdan.kuchta@pwr.edu.pl)		