COURSE OFFERED

Name of the course	Polish	**Modelowanie reaktywności chemicznej za pomocą symulacji dynamiką molekularną**
	English	**Modeling of Chemical Reactivity with Molecular Dynamics Simulations**

1. LOCATION OF THE COURSE OF STUDY WITHIN THE EDUCATION SYSTEM

1.1. Section [1]	Section of Exact and Natural Sciences
1.2. Discipline[2]	Chemical Sciences
1.3. Type of education	Stationary
1.4. Level of education	Doctoral School
1.5. Person preparing the course description	dr hab. Paweł Rodziewicz, prof. UJK
1.6. Contact	pawel.rodziewicz@ujk.edu.pl

2. GENERAL CHARACTERISTICS OF THE COURSE OF STUDY

2.1. Type of course [3]	specialized subjects in the discipline
2.2. Language of the course	English

3. DETAILED CHARACTERISTICS OF THE COURSE OF STUDY

3.1. Type of classes[4]		lecture
3.2. The number of hours[5]		15h
3.3. Location of classes		lecture room at the institute of chemistry
3.4. Type of assessment		pass with a grade
3.5. Didactic methods		presentation and discussion
3.6. Literature	**basic**	1. D. Marx, J. Hütter, “Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods”, Cambridge University Press, 2009 2. A. R. Leach, “Molecular Modelling: Principles and Applications”, Pearson, 2001
	supplementary	1. M. P. Allen, D. J. Tildesley, “Computer Simulation of Liquids”, Oxford, 2017 2. Scientific articles from journals available in the "Web of Science" database regarding ab initio molecular dynamics methods and their applications

[1] Section of Humanities:, Social Sciences, Section of Exact and Natural Sciences, Section of Medical and Health Sciences, Section of Arts.

[2] History,Linguistics, Literary Studies, Medical Sciences, Health Sciences, Political and Administrative Sciences, Legal Sciences, Security Sciences, Pedagogy, Communication and Media Studies, Management and Quality Studies, Biological Sciences, Chemical Sciences, Physical Sciences, Earth and related Environmental Sciences, Visual Arts and Artwork Conservation, Musical Arts.

[3] General courses, domain specific subjects in the section, disciplinary subjects in the sections, specialized subjects in the discipline.

[4] Classes, lecture, seminar.

[5] Consistent with the education program at the Doctoral School
Jan Kochanowski University in Kielce.

4. OBJECTIVES, SYLLABUS CONTENT AND INTENDEND LEARNING OUTCOMES

4.1. Course objectives (including the form of classes)

C01 Gaining extended knowledge of molecular dynamics methods and their application to the description of chemical reactions.

C02 Acquiring the ability to properly select molecular dynamics methods to describe chemical processes and analyze the obtained data.

4.2. Syllabus content

1. Newton, Langevin and Hamilton equations. Calculating the forces acting on atoms.
2. Verlet and leap-frog algorithm. Time step selection procedure.
3. Assumptions of Born-Oppenheimer and Car-Parrinello molecular dynamics method.
4. Born-von Karman boundary conditions. Pseudopotentials.
5. Constrained molecular dynamics in the description of rare events.
6. Calculating free energy using metadynamics.
7. Trajectory analysis methods. Radial distribution function.
8. Calculation of barriers and construction of energy paths in chemical reactions.

5. SUBJECT LEARNING OUTCOMES

Learning outcomes	A doctoral student who has passed the subject:	Reference to the learning outcomes of Doctoral School (according to the training program at the Doctoral School)
in the area of KNOWLEDGE:		
W01	The doctoral student possesses in-depth knowledge of molecular dynamics methods, encompassing theoretical foundations, general issues, and selected specific topics relevant to the scientific discipline in which the doctoral dissertation is being prepared.	SD_W01
W02	The doctoral student has advanced knowledge of development trends in the applications of molecular dynamics methods in describing the energetics of chemical reactions in disciplines related to the research being pursued.	SD_W02
in the area of SKILLS:		
U01	The doctoral student can define the goal and subject of research using molecular dynamics methods, as well as formulate research hypotheses in the discipline where the doctoral dissertation is being prepared.	SD_U01
U02	The doctoral student can effectively use a foreign language in research or project activities.	SD_U07
in the area of SOCIAL COMPETENCE:		
K01	The doctoral demonstrates entrepreneurial thinking and actively takes initiative.	SD_K04

6. METHODS OF ASSESSMENT OF THE INTENDED LEARNING OUTCOMES

	METHOD OF ASSESSMENT (+/-)

SUBJECT LEARNING OUTCOMES	Oral/written exam			Kolokwium			Project			activity in class			Own work			Group work			Others		
	The type of classes			*The type of classes*			*The type of classes*			*The type of classes*			*The type of classes*			*The type of classes*			*The type of classes*		
	L	*C*	*S*	*L*	*C*	*S*	*L*	*C*	*S*	*L*	*C*	*S*	*L*	*C*	*S*	*L*	*C*	*S*	*L*	*C*	*S*
W01							+														
W02							+														
U01							+						+								
U02							+						+								
K01							+						+								

7. CRITERIA OF ASSESSMENT OF THE INTENDED LEARNING OUTCOMES

Form of classes	Grade	Criterrion of assessment
Lecture (L) [6]	3,0	obtaining 51-60% of the total number of points for completing of own project
	3,5	obtaining 61-70% of the total number of points for completing of own project
	4,0	obtaining 71-80% of the total number of points for completing of own project
	4,5	obtaining 81-90% of the total number of points for completing of own project
	5,0	obtaining 91-100% of the total number of points for completing of own project

Accepted for execution

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[6] Niepotrzebne usunąć.