**COURSE OFFERED**

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|---|---|---|
| **Name of the course** | Polish | **Nowoczesne metody badawcze** |
| | English | **Modern research methods** |

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

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|---|---|
| **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

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|---|---|
| **2.1. Type of course** [3] | Domain specific subjects in the section |
| **2.2. Language of the course** | English |

## 3. DETAILED CHARACTERISTICS OF THE COURSE OF STUDY

| | | |
|---|---|---|
| **3.1. Type of classes**[4] | | lecture/seminar |
| **3.2. The number of hours**[5] | | 10h/10h |
| **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. H.-D. Höltje, W. Sippl, D. Rognan, G. Folkers, "Molecular Modeling: Basic Principles and Applications, 3rd Edition", Wiley, 208<br>2. D. Frenkel, B. Smit, "Understanding Molecular Simulation From Algorithms to Applications", Academic Press, 2002 |
| | **supplementary** | 1. T. Schlick, "Molecular Modeling and Simulation An Interdisciplinary Guide 2nd edition", Springer, 2010<br>3. A. R. Leach, "Molecular Modelling: Principles and Applications", Pearson, 2001 |

## 4. OBJECTIVES, SYLLABUS CONTENT AND INTENDEND LEARNING OUTCOMES

4.1. Course objectives (including the form of classes)

C01 Gaining extended knowledge of the use of in silico research in describing the properties of systems in chemistry, biology and other experimental sciences.

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[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.

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| C02 Acquiring the ability to analyze the phenomena utilizing molecular modeling based methods. |

4.2. Syllabus content

1. In silico research methodology.
2. Roots and general ideas of molecular modeling.
3. Atomistic approaches in the natural sciences.
4. Computational methods used in the in silico research.
5. Cluster approach and periodic boundary conditions.
6. Interatomic and intermolecular interactions in the gas phase, liquid and solid.
7. Visualization of structure and electronic properties of molecules.
8. Computational ways to describe energetic, structural and spectroscopic properties of molecular systems (gas phase, liquid and solid).
9. Thermodynamics vs. kinetics. Statistical analysis.
10. Molecular dynamics based on molecular mechanics. Force field.

Seminar serves as a platform for discussion on the use of molecular modeling techniques to unravel phenomena present in the research of doctoral students.

## 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 has advanced knowledge of development trends in the application of molecular modeling in disciplines related to the research being pursued. | SD_W02 |
| W02 | The doctoral student has expanded knowledge of in silico research methodologies, including statistical analysis of results. | SD_W03 |
| **in the area of SKILLS:** | | |
| U01 | The doctoral student is capable of utilizing knowledge from various disciplines to identify, formulate, and creatively solve complex problems or undertake research project tasks. | SD_U03 |
| U02 | The doctoral student can design and conduct educational activities, utilizing modern teaching methods and tools. | SD_U11 |
| **in the area of SOCIAL COMPETENCE:** | | |
| K01 | The doctoral student is able to justify the significance of knowledge in addressing cognitive and practical problems. | SD_K02 |
| K02 | The doctoral student can fulfill the obligations of a researcher and creator toward society, as well as initiate actions in the public interest. | SD_K03 |

## 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* | *E* | *S* | *L* | *C* | *S* | *L* | *C* | *S* | *L* | *C* | *S* |
| W01 | | | | | | | | + | | | | | | | | | | | | | |
| W02 | | | | | | | | + | | | | | | | | | | | | | |
| U01 | | | | | | | | + | | | | | | + | | | | | | | |
| U02 | | | | | | | | + | | | | | | + | | | | | | | |
| K01 | | | | | | | | + | | | | | | + | | | | | | | |
| K02 | | | | | | | | + | | | | | | + | | | | | | | |

## 7. CRITERIA OF ASSESSMENT OF THE INTENDED LEARNING OUTCOMES

| Form of classes | Grade | Criterrion of assessment |
|---|---|---|
| **Classes (C)** [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 |
| **Lecture (L)** | Pass/ failed | Attendance at at least 80% of lectures required |

**Accepted for execution**

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[6] Niepotrzebne usunąć.