COURSE DESCRIPTION CARD - SYLLABUS

Course name
Molecular modeling and simulation

Course

Field of study
Technical Physics

Year/Semester
3/5

Area of study (specialization)

Profile of study
general academic

Level of study
First-cycle studies

Course offered in
Polish

Form of study
full-time

Requirements
elective

Number of hours

Lecture	Laboratory classes	Other (e.g. online)
30	30	
Tutorials	Projects/seminars	

Number of credit points

5

Lecturers

Responsible for the course/lecturer:
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Wydział Inżynierii Materiałowej i Fizyki Technicznej

Responsible for the course/lecturer:

Prerequisites

Knowledge of quantum and classical physics at the level achieved after two years of study in the field of technical physics. The ability to solve simple physical problems based on the acquired knowledge, the ability to obtain information from indicated sources. Understanding the need to expand your competences, readiness to cooperate within the team.

Course objective

1. To provide students with basic knowledge and skills in the field of molecular modeling and simulation.

2. To develope students' skills in qualitative and quantitative analysis of physical phenomena occurring at the molecular level, based on computer simulations.

Course-related learning outcomes

Knowledge

The student knows and understands:

1) the basic principles of molecular modeling based on the laws of classical physics [K1_W01];

2) the basic methods of molecular modeling based on the principles of quantum physics, including the methods of quantum chemistry ("ab initio" and semi-empirical) and the methods based on the theory of electron density functional (DFT) [K1_W04];

3) the methodology of molecular dynamics simulations [K1_W01].

Skills

The student is able to:

1) correctly use standard analytical tools, including numerical and computational ones, to solve detailed physical and technical problems; can critically evaluate the results of such an analysis [K1_U09];

2) carry out molecular modeling and simulations with the use of standard software using classical and quantum methods [K1_U19];

3) choose the modeling method to solve a physical problem, as well as determine the necessary computer resources to perform a computational task [K1_U02, K1_U09, K1_U14].

Social competences

The student acquires competences allowing for:

1) responsible work on the assigned task, both independently and in a team, assuming various roles in it [K1_K01];

2) understanding the need and determining the possibilities of continuous training in order to improve professional and social competences [K1_K03].

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

Learning outcome (symbol)	Method of assessment	Assessment criteria	
Lecture:			
W01, W04, U09, K01, K03	close and open question test	3:	50.1%–70.0%
		4:	70.1%–90.0%
		5:	from 90.1%
Laboratory:			

U09, U14, U19, K01, K03	assessment of activity, reports	3:	50.1%–70.0%
		4:	70.1%–90.0%
		5:	from 90.1%

Programme content

1. Introduction to computer modeling and simulation.

2. Molecular modeling, types of models and their environment, kinds of calculations.

3. Classical models; concept of force field.

4. Quantum models; construction and solving the Schroedinger equation, the Kohn-Sham equation.

5. Algorithms of geometry optimization.

6. Simulations: molecular dynamics, Langevin dynamics, Monte-Carlo method.

7. Molecular docking - an element of computer aided drug design.

Teaching methods

Conversational lecture: multimedia presentation, simulation demonstrations.

Laboratory exercises: carrying out computer modeling and simulations, individual projects, discussion, team work.

Bibliography

Basic

1. Materials from lectures (in Polish)

2. Understanding Molecular Simulation. From Algorithms to Applications, D. Frenkel, B. Smit, Academic Press

Additional

1. Molecular Modeling Techniques in Material Sciences, J.-R. Hill, L. Subramanian, A. Maiti, Taylor&Francis 2005

2. Molecular Modeling and Simulation. An Interdisciplinary Guide, T. Schlick, 2nd edition, Springer 2010

3. http://www.molnet.eu (in Polish)

Breakdown of average student's workload

	Hours	ECTS
Total workload	125	5,0
Classes requiring direct contact with the teacher	65	
Student's own work (literature studies, preparation for laboratory classes, preparation for tests/exam, report preparation) [1]	60	

[1] delete or add other activities as appropriate