



COURSE DESCRIPTION CARD - SYLLABUS

Course name

Molecular modeling and simulation [S1FT2>MiSM]

Course

Field of study

Technical Physics

Year/Semester

3/5

Area of study (specialization)

–

Profile of study

general academic

Level of study

first-cycle

Course offered in

Polish

Form of study

full-time

Requirements

elective

Number of hours

Lecture

30

Laboratory classes

30

Other

0

Tutorials

0

Projects/seminars

0

Number of credit points

4,00

Coordinators

dr hab. Arkadiusz Ptak prof. PP
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Lecturers

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 develop 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
- 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)
3) the methodology of molecular dynamics simulations

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
- 2) carry out molecular modeling and simulations with the use of standard software using classical and quantum methods
- 3) choose the modeling method to solve a physical problem, as well as determine the necessary computer resources to perform a computational task

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
- 2) understanding the need and determining the possibilities of continuous training in order to improve professional and social competences

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:

close and open question test 3: 50.1%-70.0%

4: 70.1%-90.0%

5: from 90.1%

Laboratory:

assessment of activity, reports 3: 50.1%-70.0%

4: 70.1%-90.0%

5: from 90.1%

Programme content

Fundamentals of atomic-scale computer modeling and simulation.

This includes the creation of molecular models, both classical and quantum, molecular dynamics simulations, and molecular docking.

Course topics

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	100	4,00
Classes requiring direct contact with the teacher	60	2,50
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	40	1,50