COURSE DESCRIPTION CARD - SYLLABUS

Course name
Computer modeling of materials at the atomic scale [S1FT2>MKMwSA]

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

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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 computer modeling of materials, especially molecules and nanoparticles, at the atomic scale. 2. To develope students' skills in qualitative and quantitative analysis of physical phenomena occurring at the molecular and atomic level, based on computer simulations.

Course-related learning outcomes

Knowledge:
1. The student knows and understands the basic principles of molecular modeling based on the laws of classical physics
2. The student knows and understands the basic methods of atomic scale modeling based on the ideas

of quantum physics, including the first principles, semi-empirical and DFT methods (i.e. based on the theory of electron density functional)

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 computer 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:
open and close question test 3: 50.1%-70.0%
4: 70.1%-90.0%
5: from 90.1%
Laboratory:
assessment of activity, report 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, geometry optimization, molecular dynamics simulations, and molecular docking.

Course topics

1. Introduction to computer modeling and simulation of materials.
2. Modeling on the atomic scale: types of models and their environment, types of calculations.
3. Classical atomistic models; concept of force field.
4. Quantum models:
a) ab-initio and semi-empirical quantum chemistry methods;
b) methods based on the density functional theory (DFT) - Hohenberg-Kohn theorem, Kohn-Sham equation.
5. Comparison of classical and quantum methods.
6. Algorithms of geometry optimization.
7. Molecular dynamics simulations.
8. Elements of computer aided drug design - ligand docking.

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