COURSE DESCRIPTION CARD - SYLLABUS

Course name
Advanced Materials Modeling Laboratory [S2FT2>ZLMM]

Course

Field of study	Year/Semester
Technical Physics	1/1
Area of study (specialization)	**Profile of study**
–	general academic
Level of study	**Course offered in**
second-cycle	Polish
Form of study	**Requirements**
full-time	compulsory

Number of hours

Lecture	Laboratory classes	Other
0	15	0
Tutorials	**Projects/seminars**	
0	0	

Number of credit points

1,00

Coordinators

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Lecturers

Prerequisites

Knowledge of quantum physics and solid-state physics, thermodynamics, and chemistry, necessary for understanding and analyzing the fundamental properties of materials and physicochemical processes on their surfaces. Familiarity with basic material modeling methods. Ability to solve simple problems based on existing knowledge and to gather information from designated sources. Competence in preparing, documenting, and presenting topics related to physics.

Course objective

1.To provide students with knowledge and skills in material modeling and simulation of physical processes, enabling them to describe selected material properties and interactions on their surfaces. 2. To develop students' ability to perform qualitative and quantitative analysis of physical processes occurring at the atomic level (such as bond formation, adsorption, intercalation, etc.) using material modeling. 3. To deepen the understanding of the relationship between the structure and properties of inorganic materials.

Course-related learning outcomes

Knowledge:
The student knows and understands:

1.the practical aspects of selected material modeling and simulation methods,
2.the material properties available in selected material modeling methods,
3. the limitations of selected material modeling methods,
4. the relationship between the structure and properties of materials.

Skills:
The student is able to:
1. use standard tools for material modeling and simulation, and obtain key properties of the modeled system,
2. identify the types of interactions between elements of the modeled structure and describe their impact on the material's properties,
3. correctly apply standard analytical tools to solve detailed physical problems and critically evaluate the results of such analysis,
4. select the appropriate modeling and simulation method for the accurate description of materials and physical processes, as well as determine the necessary computational resources to perform the required calculations..

Social competences:
The student has acquired competencies that allow them to:
1.responsibly work on an assigned task both independently and within a team, taking on various roles,
2. understand the need for and be aware of opportunities for continuous learning, enhancing professional, personal, and social competencies.

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

In terms of the methods used to verify the achieved learning outcomes, the following grading thresholds are applied:
50.1-60% - 3.0
60.1-70% - 3.5;
70.1-80% - 4.0;
80.1-90% - 4.5;
from 90.1% - 5.0
The assessment results from the preparation of a laboratory measurement protocol and/or oral response.

Programme content

Modeling material properties on the atomic scale based on selected material modeling and simulation methods. Description of selected topics in quantum chemistry and solid-state physics, surface physicochemistry, and thermodynamics using selected material modeling methods. The relationship between the structure and properties of materials.

Course topics

1. Practical aspects of modeling and simulation using selected computational methods.
2. Creating models of studied materials.
3. Modeling selected properties of materials.
4. Simulations of selected physical processes.
5. Interactions in materials, quantitative and qualitative analysis.
6. Analysis of the relationship between material properties and its structure.

Teaching methods

Conducting modeling and computer simulations, projects involving necessary calculations, data analysis, interpretation of results, and their presentation, discussions, and teamwork.

Bibliography

Basic:
1. Course materials (in Polish)

2. Materials Modelling using Density Functional Theory, Giustino Feliciano, Oxford University Press

Additional:
1. A Chemist's Guide to Density Functional Theory, Wolfram Koch, Max C. Holthausen, Wiley

Breakdown of average student's workload

	Hours	ECTS
Total workload	30	1,00
Classes requiring direct contact with the teacher	15	0,50
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	15	0,50