COURSE DESCRIPTION CARD - SYLLABUS

Course name
Selected topics in materials modeling and simulation of physical processes [S1ETI2>WZzMMiSPF]

Course

Field of study
Education in Technology and Informatics

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
15

Laboratory classes
15

Other
0

Tutorials
0

Projects/seminars
0

Number of credit points

2,00

Coordinators

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Lecturers

Prerequisites

Knowledge of classical and quantum physics, chemistry, and mathematics within the scope covered in the technical informatics education program. Ability to solve simple problems based on acquired knowledge and the skill of obtaining information from specified sources. Proficiency in procedural programming.

Course objective

1.Providing students with fundamental knowledge and skills in the field of modeling and simulation.
2.Developing students' ability to analyze physical phenomena qualitatively and quantitatively using computer simulations.

Course-related learning outcomes

Knowledge:
As a result of the conducted classes, the student knows and understands:
basic methods of molecular modeling utilizing principles of quantum physics
methodology of computer simulations
basic definitions and classification of cellular automata according to Wolfram
example rules of cellular automata enabling simulation in various scientific domains

Skills:
As a result of the conducted classes, the student is able to:
correctly utilize standard analytical tools, including numerical and computational ones, to solve detailed physical and technical problems; able to critically assess the results of such analysis
choose the appropriate modeling method for an accurate description of material and physical processes, as well as determine the necessary computer resources for performing computational tasks
implement a selected simple and complex rule of cellular automata and simulate (visualize) the process that the rule mimicsconcisely describe the obtained simulation results and relate them to the behaviors of real systems

Social competences:
As a result of the conducted classes, the student will acquire the following social competencies:
can responsibly work on assigned tasks independently as well as in a team, assuming various roles within it
understands the need for and is aware of the opportunities for continuous self-improvement (undergraduate and graduate studies, postgraduate studies) - enhancing professional, personal, and social competencies

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

written exam
computer and oral presentation, evaluation of activity on exercises
<0–50)% unsatisfactory
<50–60)% - satisfactory;
<60–70)% - satisfactory plus;
<70–80)% - good;
<80–90)% - good plus;
<90–100> - very good.

Programme content

Participants will learn quantum models of molecules, computer methods of materials modeling at the atomic scale and apllication cellular automata (CA) technique in computer simulations.

Course topics

Part A.
1. Introduction to computer modeling and simulation.
2. Quantum models of molecules; construction and solving of the Schrödinger equation; the Kohn-Sham equation, the problem of describing multi-electron systems.
3. Contemporary methods of materials modeling at the atomic scale based on the theory of electronic density functional.
Part B.
1. Introduction to cellular automata (CA) technique: definitions, classifications and examples.
2. Apllication CA in w physics (Ising model, modeling surface growth) , biophysics (Penny model), social physics (evolution of public opinion) and chemistry (modeling catalytic reaction).
3. Apllication CA in transport modeling: lattice gas automata, granular flow, evacuation and wildfire.
4. Apllication CA in : fractals, diffusion-limited aggregation model (DLA), model of wildfire propagation.

Teaching methods

1. Lecture-conversation: multimedia presentation, simulation demonstrations.
2. Laboratory exercises: conducting computer modeling and simulations, individual projects, discussion, teamwork.

Bibliography

Basic:
1. Lecture notes (in polish)

2. Materials Modelling using Density Functional Theory, Giustino Feliciano, Oxford University Press
3. K. Kułakowski, Automaty komórkowe, OEN AGH (2000)
4. S. Wolfram, A New Kind of Science, Wolfram Media (2002)

Additional:
1. A Chemist's Guide to Density Functional Theory, Wolfram Koch, Max C. Holthausen, Wiley
2. D. Stauffer i inni, Biology, Sociology, Geology by Computational Physicists, Elsevier (2006)
3. D.P. Landau, K. Binder, A Guide to Monte Carlo Simulations in Statistical Physics, Cambridge University Press (2005)

Breakdown of average student's workload

	Hours	ECTS
Total workload	55	2,00
Classes requiring direct contact with the teacher	30	1,00
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	25	1,00