Coarse-grained molecular dynamics simulations of polyelectrolytes

Educational subject description sheet

Basic information

Study programme Fizyka (Physics of Advanced Materials for Energy Processing) **Speciality** - **Organizational unit** Faculty of Physics **Study level** Second-cycle programme **Study form** Full-time **Education profile** General academic	**Didactic cycle** 2023/24 **Subject code** 04FENS.28S.03278.23 **Lecture languages** English **Course type** Elective **Block** specialty subjects

Subject coordinator	Jarosław Kłos
Lecturer	Jarosław Kłos

Period	**Activities and hours**	**Number of ECTS points**
Semester 4	• Laboratories: 15, Graded credit	2

Goals

Code	Goal
C1	The classes are devoted to the main concepts in polymer physics and coarse-grained molecular dynamics simulations of polyelectrolytes

Subject learning outcomes

Code	Outcomes in terms of	Learning outcomes	Examination methods
Knowledge – Student:			
W1	can explain the general concept of the molecular dynamics simulation method and Langevin dynamics.	FEN_K2_W01, FEN_K2_W02, FEN_K2_W03	Project
W2	can explain the Kremer-Grest model of polymers.	FEN_K2_W01, FEN_K2_W02, FEN_K2_W03	Project
W3	can explain terms such as Verlet algorithm, periodical boundary conditions, cutoff radius, Verlet list, Ewald summation.	FEN_K2_W03	Project
W4	can explain what polyelectrolytes are.	FEN_K2_W01, FEN_K2_W02, FEN_K2_W04	Project
Skills – Student:			
U1	can write a LAMMPS script incorporating Langevin dynamics to simulate polyelectrolytes.	FEN_K2_U01, FEN_K2_U02, FEN_K2_U03, FEN_K2_U05	Project
U2	can carry out simulations of polyelectrolytes using a LAMMPS script.	FEN_K2_U01, FEN_K2_U02, FEN_K2_U03, FEN_K2_U05	Project

Study content

No.	Course content	Subject learning outcomes	Activities
1.	The molecular dynamics simulation method, the Langevin dynamics.	W1, W2, W3, W4, U1, U2	Laboratories
2.	The Kremer-Grest model of polymers, Coulomb interactions	W1, W2, W3, U1, U2	Laboratories
3.	Verlet algorithm, periodical boundary conditions, Ewald summation.	W1, W2, W3	Laboratories
4.	Introduction to LAMMPS scripts	U1, U2	Laboratories

Additional information

Activities	Teaching and learning methods and activities
Laboratories	Laboratory method

Activities	Credit conditions
Laboratories	The students will have to write their own LAMMPS script to simulate polyelectrolytes and test it. The final score will depend on the outcome of their work. The final score will be based on the Polish score scale: Very good (bdb; 5.0) Good plus (+db; 4.5) Good (db; 4.0) Satisfactory plus (+dst; 3.5) Satisfactory (dst; 3.0) Unsatisfactory (ndst; 2.0)

Literature

Obligatory

1. M. P. Allen and D. J. Tildesley, "Computer Simulation of Liquids". Clarendon Press 1989
2. Daan Frenkel and Berend Smit "Understanding Molecular Simulation". Academic Press 2001

Calculation of ECTS points

Activities	Activity hours*
Laboratories	15
Preparation for classes	10
Reading the indicated literature	5
Preparation of a project	20
Student workload	**Hours** 50
Number of ECTS points	**ECTS** 2

* academic hour = 45 minutes

Efekty uczenia się dla kierunku

Kod	Treść
FEN_K2_U01	The graduate can use their knowledge to formulate and solve complex and unusual problems in the field of physical sciences; select and apply appropriate methods and tools necessary to solve a given problem (including advanced IT techniques), as well as adapt existing methods and tools or develop completely new ones
FEN_K2_U02	The graduate can find the necessary information in the professional literature, databases and other sources, in particular in scientific journals basic to physics, and perform critical analysis, synthesis and creative interpretation of the collected information
FEN_K2_U03	The graduate can formulate and test hypotheses related to simple research problems in physics (plan and perform observations, experiments, theoretical calculations or computer simulations and critically evaluate and discuss the results obtained)
FEN_K2_U05	The graduate can use English in accordance with the requirements set out for level B2+ of the Common European Framework of Reference for Languages, as well as specialist English terminology in the field of physical sciences
FEN_K2_W01	The graduate knows and understands in-depth selected facts, phenomena, concepts and theories specific to physics and complex relationships between them (constituting advanced general knowledge in the field of physical sciences and representing both key and other selected issues in the field of advanced detailed knowledge in this discipline)
FEN_K2_W02	The graduate knows and understands in-depth selected research methods and tools as well as mathematical models used in physics
FEN_K2_W03	The graduate knows and understands in-depth selected computational methods and information technology tools and techniques used to solve complex problems in physics
FEN_K2_W04	The graduate knows and understands main development trends in the discipline of physical sciences