



Subject card

Subject name and code	, PG_00052082						
Field of study	Nanotechnology						
Date of commencement of studies	October 2021	Academic year of realisation of subject			2023/2024		
Education level	first-cycle studies	Subject group			Obligatory subject group in the field of study Subject group related to scientific research in the field of study		
Mode of study	Full-time studies	Mode of delivery			at the university		
Year of study	3	Language of instruction			Polish		
Semester of study	6	ECTS credits			5.0		
Learning profile	general academic profile	Assessment form			assessment		
Conducting unit	Zakład fizyki układów nieuporządkowanych -> Instytut Nanotechnologii i Inżynierii Materiałowej -> Faculty of Applied Physics and Mathematics						
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Szymon Winczewski					
	Teachers	dr inż. Szymon Winczewski Jagoda Budnik					
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	45.0	0.0	0.0	60
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours		Self-study		SUM
	Number of study hours	60	6.0		59.0		125
Subject objectives	The main goal is to familiarise the students with atomistic simulation methods used in research on material qualities. During the course molecular dynamics methods are discussed. The goal is to familiarise the students with an array of simulation programs and other tools widely used in this field.						
Learning outcomes	Course outcome	Subject outcome			Method of verification		
	K6_U02	The student is able to critically analyse simulation results. The student is able to point out the limitations of the model used and propose corrections.			[SU1] Assessment of task fulfilment [SU3] Assessment of ability to use knowledge gained from the subject [SU5] Assessment of ability to present the results of task		
	K6_W06	The student understands the relation between microstructure and macroscopic properties of materials. The student knows, how the specificity of interatomic interactions influences the properties of materials. The student knows the basic thermodynamic response functions.			[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge		
	K6_W04	The student knows the tools for analysing the results of numerical calculations. The student knows how to present the obtained results in a form of a research report.			[SW3] Assessment of knowledge contained in written work and projects [SW1] Assessment of factual knowledge		
	K6_U03	The student is able to prepare and perform atomistic simulations using the programs presented during the course. The student is able to visualise the results of simulations using the graphical tools presented during the course.			[SU4] Assessment of ability to use methods and tools [SU1] Assessment of task fulfilment		

Subject contents	<p>1. Methods of defining atomic structures.</p> <p>2. Methods of visualising atomic structures (VMD and Ovito programs).</p> <p>3. Methods of describing interatomic interactions (Lennard-Jones potential, AIREBO force fields, multibody potentials).</p> <p>4. Numerical methods for solving equations of motion (classic and velocity Verlet algorithm).</p> <p>5. Simulation techniques: preparation and performance of simulations (LAMMPS program).</p> <p>6. Processing and presentation of simulation results (Gnuplot program).</p> <p>7. Statistical ensemble.</p> <p>8. Thermodynamic response functions.</p> <p>9. Methods of studying mechanical properties of atomic structures.</p> <p>10. Structure analysis methods.</p>														
Prerequisites and co-requisites	Student knows the basics of solid state physics and thermodynamics.														
Assessment methods and criteria	<table border="1" data-bbox="451 958 1487 1104"> <thead> <tr> <th data-bbox="451 958 794 992">Subject passing criteria</th> <th data-bbox="794 958 1141 992">Passing threshold</th> <th data-bbox="1141 958 1487 992">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="451 992 794 1025">Test in theory</td> <td data-bbox="794 992 1141 1025">50.0%</td> <td data-bbox="1141 992 1487 1025">25.0%</td> </tr> <tr> <td data-bbox="451 1025 794 1059">Written reports</td> <td data-bbox="794 1025 1141 1059">50.0%</td> <td data-bbox="1141 1025 1487 1059">25.0%</td> </tr> <tr> <td data-bbox="451 1059 794 1104">Solving assignments</td> <td data-bbox="794 1059 1141 1104">50.0%</td> <td data-bbox="1141 1059 1487 1104">50.0%</td> </tr> </tbody> </table>			Subject passing criteria	Passing threshold	Percentage of the final grade	Test in theory	50.0%	25.0%	Written reports	50.0%	25.0%	Solving assignments	50.0%	50.0%
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Recommended reading	Basic literature	<ol style="list-style-type: none"> 1. Dennis C. Rapaport, The Art of Molecular Dynamics Simulation, 2nd ed., Cambridge University Press, Oxford 2004. 2. Dieter W. Heerman, Podstawy symulacji komputerowych w fizyce, WNT, Warszawa 1997. 3. Furio Ercolessi, A molecular dynamics primer. 4. Vasily Bulatov, Wei Cai, Computer Simulations of Dislocations, Oxford University Press, Oxford 2006. 5. Daan Frenkel, Berend Smit, Understanding molecular simulation: from algorithms to applications, 2nd ed., Academic Press, 2002. 6. Andrew R. Leach, Molecular modelling: principles and applications, 2nd ed., Prentice Hall, 2001. 													
	Supplementary literature	none													
	eResources addresses	<p>Podstawowe</p> <p>https://enauczanie.pg.edu.pl/moodle/course/view.php?id=24373 - Komputerowe Modelowanie Materiałó 2022/2023 - on-line course on the e-Nauczanie platform</p> <p>Adresy na platformie eNauczanie:</p> <p>Komputerowe Modelowanie Materiałó 2023/2024 - Moodle ID: 37153</p> <p>https://enauczanie.pg.edu.pl/moodle/course/view.php?id=37153</p>													
Example issues/ example questions/ tasks being completed	<p>1. Defining and visualizing of simple atomic systems. 2. Analysis and graphical presentation of the scientific data. 3. Properties of argon dimer. 4. Thermodynamical properties of argon crystal (heat capacity, melting temperature, thermal expansion). 5. Mechanical properties of argon crystal.</p>														
Work placement	Not applicable														