



Subject card

Subject name and code	Materials Science - classical particle approach, PG_00071216						
Field of study	Nanotechnology, Nanotechnology						
Date of commencement of studies	February 2027	Academic year of realisation of subject				2027/2028	
Education level	second-cycle studies	Subject group				Specialty subject group 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	1	Language of instruction				English	
Semester of study	2	ECTS credits				4.0	
Learning profile	general academic profile	Assessment form				assessment	
Conducting unit	Division of Physics of Disordered Systems -> Institute of Nanotechnology and Materials Engineering -> Faculty of Applied Physics and Mathematics -> Faculties of Gdańsk University of Technology						
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Szymon Winczewski					
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	0.0	45.0	0.0	0.0	45
	E-learning hours included: 0.0						
	eNauczanie source address: <a href="https://enauczanie.pg.edu.pl/2025/course/view.php?id=1135">https://enauczanie.pg.edu.pl/2025/course/view.php?id=1135</a>						
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	45	2.0	53.0	100		
Subject objectives	An introduction to simulation methods used in the modeling of nanomaterials and nanostructures, with particular emphasis on molecular dynamics and molecular statics. The course includes practical training (illustrated with numerous examples and exercises) in commonly used simulation approaches, as well as instruction in the use of professional scientific software (VMD, gnuplot, LAMMPS, Ovito) and examples of application.						
Learning outcomes	Course outcome	Subject outcome			Method of verification		
	[K7_U03] has enhanced abilities of using advanced specialist software packages	The student is able to use professional scientific software employed for carrying out atomistic simulations.			[SU4] Assessment of ability to use methods and tools		
	[K7_W05] has in-depth knowledge of mathematical, numerical, and simulation methods - both classical and quantum - used in the modeling of nanostructures	The student is familiar with the molecular dynamics method and has an in-depth understanding of its principles of operation. The student is also aware of the advantages and limitations of this method.			[SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects		
	[K7_U02] has advanced skills in the design of nanomaterials and in conducting laboratory work related to the fabrication and characterization of nanostructures	The student is able to apply the molecular dynamics method to model the behavior of various nanomaterials and nanostructures and to predict their properties.			[SU1] Assessment of task fulfilment		
	[K7_U05] is able to plan and carry out theoretical and numerical calculations as well as simulations of phenomena and processes, critically analyze their results, draw conclusions, and formulate well-founded opinions in nanotechnology and related physical and natural sciences	The student is able to plan and carry out simulations that allow the investigation of a given nanomaterial or phenomenon. The student can analyze the simulation results and evaluate them critically, assessing their correctness and the adequacy of the applied simulation approach. The student is able to confront predictions obtained from simulations with reality and to propose ways to improve the applied approach/model.			[SU1] Assessment of task fulfilment [SU5] Assessment of ability to present the results of task		

Subject contents	<p>Course content – laboratory</p> <ol style="list-style-type: none"> <li>1. Defining and visualization of atomic systems.</li> <li>2. Introduction to the VMD program.</li> <li>3. Preparation, execution, and analysis of the results of MD simulations.</li> <li>4. Introduction to the LAMMPS program.</li> <li>5. Processing and presentation of simulation results.</li> <li>6. Introduction to the gnuplot program.</li> <li>7. Work on example problems involving the use of MD simulations in the modeling of nanomaterials and nanostructures, including graphene and graphene-like structures, fullerenes, and nanoparticles.</li> <li>8. Introduction to simulation approaches used in the study of various properties, including structural properties (structural parameters), mechanical properties (mechanical moduli, elastic constants), transport properties (diffusion coefficient, viscosity), and thermodynamic properties (specific heat, thermal conductivity coefficient, melting temperature).</li> </ol>																	
Prerequisites and co-requisites	The student is familiar with classical mechanics, thermodynamics, and materials science.																	
Assessment methods and criteria	<table border="1" data-bbox="448 461 1487 701"> <thead> <tr> <th data-bbox="448 461 794 495">Subject passing criteria</th> <th data-bbox="794 461 1141 495">Passing threshold</th> <th data-bbox="1141 461 1487 495">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="448 501 794 551">written tests assessing the required theoretical knowledge</td> <td data-bbox="794 501 1141 551">50.0%</td> <td data-bbox="1141 501 1487 551">10.0%</td> </tr> <tr> <td data-bbox="448 557 794 607">practical problems assessing the required practical skills</td> <td data-bbox="794 557 1141 607">50.0%</td> <td data-bbox="1141 557 1487 607">20.0%</td> </tr> <tr> <td data-bbox="448 613 794 647">work on assignments/project</td> <td data-bbox="794 613 1141 647">50.0%</td> <td data-bbox="1141 613 1487 647">50.0%</td> </tr> <tr> <td data-bbox="448 654 794 701">written reports from the completed assignments/project</td> <td data-bbox="794 654 1141 701">50.0%</td> <td data-bbox="1141 654 1487 701">20.0%</td> </tr> </tbody> </table>			Subject passing criteria	Passing threshold	Percentage of the final grade	written tests assessing the required theoretical knowledge	50.0%	10.0%	practical problems assessing the required practical skills	50.0%	20.0%	work on assignments/project	50.0%	50.0%	written reports from the completed assignments/project	50.0%	20.0%
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Example issues/ example questions/ tasks being completed	<ol style="list-style-type: none"> <li>1. Determination of the equilibrium structure of a selected graphene-like structure using the molecular statics method and energy minimization techniques.</li> <li>2. Determination of the elastic constants of a selected graphene-like structure based on molecular statics and the direct method.</li> <li>3. Determination of the equation of state of a nanomaterial and the properties associated with it.</li> <li>4. Determination of the melting temperature of a selected nanomaterial based on MD simulations.</li> <li>5. Determination, based on MD simulations, of the temperature dependence of the diffusion coefficient in a selected nanomaterial.</li> <li>6. Determination, based on MD simulations, of the specific heat of a selected nanomaterial.</li> <li>7. Determination, based on MD simulations, of the thermal conductivity of graphene.</li> </ol>																	
Practical activities within the subject	Not applicable																	

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