



## Subject card

|   |  |  |   |                                     |         |   |     |
|---|--|--|---|-------------------------------------|---------|---|-----|
| Subject name and code                       | AI in modelling and simulations of materials and nanomaterials, PG_00071218  |  |   |                                     |         |   |     |
| 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<br>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                            |                                     |         | 2.0   |     |
| Learning profile                            | general academic profile   |  | Assessment form                         |                                     |         | assessment  |     |
| Conducting unit                             | Division of Theoretical Physics and Quantum Informaton -> Institute of Physics and Applied Computer Science -> Faculty of Applied Physics and Mathematics -> Faculties of Gdańsk University of Technology  |  |   |                                     |         |   |     |
| Name and surname of lecturer (lecturers)    | Subject supervisor   |  | dr inż. Paweł Syty                      |                                     |         |   |     |
|   | Teachers   |  |   |                                     |         |   |     |
| Lesson types                                | Lesson type  | Lecture  | Tutorial                                | Laboratory                          | Project | Seminar   | SUM |
|   | Number of study hours  | 0.0  | 0.0                                     | 0.0                                 | 26.0    | 4.0   | 30  |
|   | 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  | 30   |   | 2.0                                 |         | 18.0  | 50  |
| Subject objectives                          | The aim of the project part is to develop practical skills in independent and team-based problem solving in the field of materials science and nanotechnology using advanced artificial intelligence methods. Students will learn to design, implement and verify AI models on real material data and interpret the results obtained in a physical context. The classes prepare students to conduct scientific research and work in R&D teams where AI is an integral tool for material analysis and design. The aim of the seminar is to develop practical skills in presenting and discussing the results of one's work. |  |   |                                     |         |   |     |

| Learning outcomes | Course outcome  | Subject outcome   | Method of verification  |
|-------------------|---|---|---|
|                   | [K7_W05] has in-depth knowledge of mathematical, numerical, and simulation methods - both classical and quantum - used in the modeling of nanostructures  | The student has in-depth knowledge of artificial intelligence, machine learning, and data analysis methods used in modeling and simulation of materials and nanomaterials, including methods integrating classical and quantum approaches, and understands their mathematical and numerical foundations in the context of physical and material problems.   | [SW1] Assessment of factual knowledge<br>[SW2] Assessment of knowledge contained in presentation                  |
|                   | [K7_K01] is able to cooperate and work effectively in a group, assuming different roles depending on changing needs. Adheres to the principles of professional ethics and demonstrates creativity and entrepreneurship. Is capable of self-assessment as well as constructive evaluation of the work of others. | The student is able to effectively collaborate in a project team on research tasks using AI methods in materials science and nanotechnology, taking on various organizational and substantive roles, adhering to the principles of research ethics and responsible use of AI, demonstrating creativity, initiative, and the ability to self-assess and constructively evaluate the work of others, as well as to present and discuss the results of their own research. | [SK1] Assessment of group work skills<br>[SK4] Assessment of communication skills, including language correctness |
|                   | [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, implement, and perform calculations and simulations using artificial intelligence tools on real material data, critically analyze and validate the obtained results in light of the laws of physics and chemistry, draw reasonable conclusions, and formulate substantive opinions on phenomena and processes in nanotechnology.   | [SU2] Assessment of ability to analyse information<br>[SU1] Assessment of task fulfilment                         |

| Subject contents  | <p>Course content – project</p> <p>General assumptions</p> <ul style="list-style-type: none"> <li>- Form: team project (23 people) or individual project</li> <li>- Nature: research and design</li> <li>- Tools: Python, ML/DL libraries, material data analysis tools</li> <li>- Data: real or semi-synthetic from the field of materials science/nanotechnology</li> <li>- Final result: <ul style="list-style-type: none"> <li>- working ML/AI model</li> <li>- technical and research report</li> <li>- presentation of results</li> </ul> </li> </ul> <p>Implementation stages</p> <p>1 Definition of the research problem</p> <ul style="list-style-type: none"> <li>- selection of a problem in the field of: <ul style="list-style-type: none"> <li>- prediction of material/nanostructure properties</li> <li>- experimental data analysis</li> <li>- material design</li> </ul> </li> <li>- determination of: <ul style="list-style-type: none"> <li>- input and output variables</li> <li>- physical significance of the problem</li> </ul> </li> <li>- identification of data and model limitations</li> </ul> <p>2 Representation of material data</p> <ul style="list-style-type: none"> <li>- selection and implementation of descriptors</li> <li>- data preprocessing</li> </ul> <p>3 Building and training an ML/DL model</p> <ul style="list-style-type: none"> <li>- implementation and comparison of at least two approaches: <ul style="list-style-type: none"> <li>- classical ML (e.g., Random Forest, Gradient Boosting)</li> <li>- deep learning model (e.g., GNN, CNN)</li> </ul> </li> <li>- selection of architecture and hyperparameters</li> <li>- validation</li> </ul> <p>4 Integration of physical knowledge</p> <ul style="list-style-type: none"> <li>- introduction of physical constraints: <ul style="list-style-type: none"> <li>- data filtering</li> <li>- modification of the loss function</li> <li>- interpretation of results in physical terms</li> </ul> </li> <li>- analysis of the consistency of predictions with physical expectations</li> </ul> <p>5 Uncertainty analysis and interpretability</p> <ul style="list-style-type: none"> <li>- estimation of prediction uncertainty</li> <li>- model interpretation</li> <li>- critical assessment of result reliability</li> </ul> <p>6 Material/nanostructure design and optimization</p> <ul style="list-style-type: none"> <li>- application: <ul style="list-style-type: none"> <li>- Bayesian optimization</li> <li>- generative algorithms</li> </ul> </li> <li>- search for structures with specified properties</li> <li>- analysis of design trade-offs</li> </ul> <p>7 Integration with experimental/simulation data</p> <ul style="list-style-type: none"> <li>- data analysis: <ul style="list-style-type: none"> <li>- microscopic</li> <li>- spectroscopic</li> <li>- simulation</li> </ul> </li> <li>- construction of a surrogate model</li> <li>- acceleration of calculations/analysis</li> </ul> <p>8 Documentation of results</p> <ul style="list-style-type: none"> <li>- technical report containing: <ul style="list-style-type: none"> <li>- problem description</li> <li>- methodology</li> <li>- analysis of results</li> <li>- limitations, prospects</li> </ul> </li> </ul> |                               |  |                          |                   |                               |  |       |       |   |       |       |  |       |       |
|---|--|-------------------------------|--|--------------------------|-------------------|-------------------------------|--|-------|-------|---|-------|-------|--|-------|-------|
| Prerequisites and co-requisites   | <p>Course content – seminar</p> <p>Oral presentation of the results of the project developed as part of the project component. Duration of a single project presentation approximately 15-20 minutes (including discussion).</p>   |                               |  |                          |                   |                               |  |       |       |   |       |       |  |       |       |
| Assessment methods and criteria   | <table border="1"> <thead> <tr> <th data-bbox="448 1621 794 1653">Subject passing criteria</th> <th data-bbox="794 1621 1141 1653">Passing threshold</th> <th data-bbox="1141 1621 1477 1653">Percentage of the final grade</th> </tr> </thead> <tbody> <tr> <td data-bbox="448 1653 794 1711">Assessment of progress in project implementation</td> <td data-bbox="794 1653 1141 1711">50.0%</td> <td data-bbox="1141 1653 1477 1711">30.0%</td> </tr> <tr> <td data-bbox="448 1711 794 1794">Assessment of the quality of the completed project, including project documentation</td> <td data-bbox="794 1711 1141 1794">50.0%</td> <td data-bbox="1141 1711 1477 1794">50.0%</td> </tr> <tr> <td data-bbox="448 1794 794 1854">Evaluation of project presentations during the seminar</td> <td data-bbox="794 1794 1141 1854">50.0%</td> <td data-bbox="1141 1794 1477 1854">20.0%</td> </tr> </tbody> </table>   |                               |  | Subject passing criteria | Passing threshold | Percentage of the final grade | Assessment of progress in project implementation | 50.0% | 30.0% | Assessment of the quality of the completed project, including project documentation | 50.0% | 50.0% | Evaluation of project presentations during the seminar | 50.0% | 20.0% |
| Subject passing criteria  | Passing threshold  | Percentage of the final grade |  |                          |                   |                               |  |       |       |   |       |       |  |       |       |
| Assessment of progress in project implementation                                    | 50.0%  | 30.0%                         |  |                          |                   |                               |  |       |       |   |       |       |  |       |       |
| Assessment of the quality of the completed project, including project documentation | 50.0%  | 50.0%                         |  |                          |                   |                               |  |       |       |   |       |       |  |       |       |
| Evaluation of project presentations during the seminar                              | 50.0%  | 20.0%                         |  |                          |                   |                               |  |       |       |   |       |       |  |       |       |
| Recommended reading   | <p>Basic literature</p> <ul style="list-style-type: none"> <li>- Kritesh Kumar Gupta, Sudip Dey, Tanmoy Mukhopadhyay, Machine Learning in Nanoscale Materials Design, Springer, 2025</li> <li>- Kunal Roy, Arkaprava Banerjee, Materials Informatics II, Springer, 2025</li> </ul>   |                               |  |                          |                   |                               |  |       |       |   |       |       |  |       |       |

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|  | Supplementary literature   | - Yuling An, Machine Learning in Materials Informatics: Methods and Applications, American Chemical Society, 2022<br>- Yuan Cheng, Tian Wang, Gang Zhang, Artificial Intelligence for Materials Science, Springer, 2021 |
|  | eResources addresses   |   |
| Example issues/<br>example questions/<br>tasks being completed | <ul style="list-style-type: none"> <li>- Prediction of mechanical properties of nanocomposites</li> <li>- Analysis of TEM and SEM images using CNN</li> <li>- Design of nanostructures with a specified energy gap</li> <li>- Surrogate modeling for DFT simulations</li> <li>- Active learning in material experiment planning</li> </ul> |   |
| Practical activities within<br>the subject                     | Not applicable   |   |

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