<table>
<tr><td>NAME OF THE COURSE</td><td colspan="5">Dynamics of atoms in gas and liquid phase</td></tr>
<tr><td>Code</td><td>PMP270</td><td>Year of study</td><td colspan="3">GU-1</td></tr>
<tr><td>Course teacher</td><td>Bernarda Lovrinčević, PhD, Assistant Professor</td><td>Credits (ECTS)</td><td colspan="3">5,0</td></tr>
<tr><td rowspan="2">Associate teachers</td><td rowspan="2"></td><td rowspan="2">Type of instruction (number of hours)</td><td>L</td><td>S</td><td>E</td><td>F</td></tr>
<tr><td>30</td><td>15</td><td>15</td><td></td></tr>
<tr><td>Status of the course</td><td>compulsory</td><td>Percentage of application of e-learning</td><td colspan="3">15%</td></tr>
<tr><td colspan="6">COURSE DESCRIPTION</td></tr>
<tr><td>Course objectives</td><td colspan="5">Basic understanding of the microscopic structure and dynamics of gaseous and liquid systems and their modeling using Monte Carlo and Molecular Dynamics simulations.</td></tr>
<tr><td>Course enrolment requirements and entry competences required for the course</td><td colspan="5">Basic knowledge in statistical mechanics, thermodynamics, classical mechanics, quantum physics and programming.</td></tr>
<tr><td>Learning outcomes expected at the level of the course (4 to 10 learning outcomes)</td><td colspan="5">1. Basic understanding of the microscopic structure and dynamics of liquids according to the ideas of statistical fluid physics.
2. Knowledge of basic and some of the advanced algorithms for calculating structural and thermodynamic quantities
3. Ability to model molecular systems in gaseous and liquid state
4. Ability to develop simple computer programs for simulation and analysis of simulation results
5. Understanding of computer experiments
6. Ability to use software packages for molecular dynamics simulation and data visualization programs</td></tr>
<tr><td>Course content broken down in detail by weekly class schedule (syllabus)</td><td colspan="5">1. Introduction to the course: basics of computer simulations, theory-experiment relationship. Basics of working in Linux.
2. Statistical description of the system: ensembles, probability density in phase space, time averaging and averaging over ensemble, ergot hypothesis.
3. N-particle density and N-particle distribution functions, 2-particle distribution function, radial distribution function (RDF), virial equation.
4. Introduction to simulations of molecular dynamics: three steps of simulation (initiation, equilibration, production). Example: molecular dynamics of rigid spheres.
5. Maxwell-Boltzmann velocity distribution in a system of rigid spheres. Code development and analysis of results.
6. Dynamic quantities in molecular dynamics: velocity-velocity correlation, diffusion coefficient: Green-Kubo and Einstein derivative.
7. Autocorrelation speed function: code generation and analysis of results.
8. Introduction to Monte Carlo simulations: an example of the Lennard-Jones system. Use of program code and analysis of results.
9. Monte Carlo simulation of fluid with modified potential: analysis of results and comparison with Lennard-Jones fluid.
10. Molecular dynamics of Lennard-Jones fluids and analysis of program code results.
11. Basic integration algorithms in molecular dynamics: calculation of particle positions and velocities.
12. Force fields in molecular dynamics: intramolecular and intermolecular potentials.
13. Basics of using a software package for molecular dynamics simulations.
14. Simulations of simple systems - water in liquid state. Results analysis and visualization.
15. Simulations of complex systems - protein in water. Results analysis and visualization.</td></tr>
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<tr><td>Format of instruction</td><td>☒ lectures
☒ seminars and workshops
☒ exercises
☐ on line in entirety
☐ partial e-learning
☐ field work</td><td>☒ independent assignments
☒ multimedia
☐ laboratory
☐ work with mentor
☐ homework assignments</td></tr>
<tr><td>Student responsibilities</td><td colspan="2">1. Attendance and commitment of students in class and preparation of assignments in class.
2. Doing homework.
3. Preparation of a seminar paper that includes independent modeling and simulation by the method of molecular dynamics of the selected physical problem and analysis of results.
4. Writing reports and seminar presentations.</td></tr>
<tr><td>Screening student work (name the proportion of ECTS credits for each activity so that the total number of ECTS credits is equal to the ECTS value of the course)</td><td colspan="2">
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<tr><th>Name</th><th>Ects</th><th>Name</th><th>Ects</th><th>Name</th><th>Ects</th></tr>
<tr><td>Class attendance</td><td>1</td><td>Research</td><td>1</td><td>Experimental work</td><td></td></tr>
<tr><td>Oral exam</td><td></td><td>Report</td><td></td><td>Homework assignments</td><td>1</td></tr>
<tr><td>Seminar essay</td><td>1</td><td>Essay</td><td></td><td></td><td></td></tr>
<tr><td>Tests</td><td></td><td>Practical training</td><td>1</td><td></td><td></td></tr>
<tr><td>Written exam</td><td></td><td>Project</td><td></td><td></td><td></td></tr>
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<tr><td>Grading and evaluating student work in class and at the final exam</td><td colspan="2">1. Written part of the seminar paper - 35%.
2. Presentation of the seminar paper - 35%.
3. Exercises - 30%.</td></tr>
<tr><td>Required literature (available in the library and via other media)</td><td colspan="2">
<table>
<tr><th>Title</th><th>Number of copies in the library</th><th>Availability via other media</th></tr>
<tr><td>J.-P. Hansen and I. R. McDonald, Theory of simple liquids, Academic Press, 2006.</td><td>0</td><td>YES</td></tr>
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</td></tr>
<tr><td>Optional literature (at the time of submission of study programme proposal)</td><td colspan="2">J. M. Haile: Molecular dynamics simulation, John Wiley & Sons, New York, 1992.
K. Huang, Statistical Mechanics, Wiley, New York 1963.
P. Allen & D. Tildesley, Computer Simulation of Liquids, Clarendon, Press, Oxford, 1987.
Scientific papers.</td></tr>
<tr><td>Quality assurance methods that ensure the acquisition of exit competences</td><td colspan="2">Exam results statistics and student evaluation through a survey conducted by the University of Split.</td></tr>
<tr><td>Other (as the proposer wishes to add)</td><td colspan="2"></td></tr>
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