**COURSE UNIT (MODULE) DESCRIPTION**

| Course unit (module) title | Code |
|---|---|
| Classical and Quantum Molecular Dynamics | |

| Lecturer(s) | Department(s) where the course unit (module) is delivered |
|---|---|
| **Coordinator:** Assoc. Prof. Dr. Mindaugas Mačernis | Faculty of Physics |

| Study cycle | Type of the course unit (module) |
|---|---|
| First | Compulsory |

| Mode of delivery | Period when the course unit (module) is delivered | Language(s) of instruction |
|---|---|---|
| Face-to-face | 3rd semester | Lithuanian, English |

| Requirements for students | |
|---|---|
| **Prerequisites:** Quantum mechanics; Parallel calculation methods in Physics | **Additional requirements (if any):** None |

| Course (module) volume in credits | Total student's workload | Contact hours | Self-study hours |
|---|---|---|---|
| 5 | 140 | 64 | 76 |

| Purpose of the course unit (module): programme competences to be developed | | |
|---|---|---|
| Students will learn classical molecular dynamic (MD) and quantum molecular dynamic (QMD) theories with supercomputes. He will be able execute MD and QMD tasks for various molecular systems. | | |
| **Learning outcomes of the course unit (module)** | **Teaching and learning methods** | **Assessment methods** |
| The student is expected to be able to understand and run tasks classical molecular dynamic methods. | Lectures, laboratory works, independent work. | Laboratory works, exam. |
| The student is expected to be able to understand and run tasks quantum molecular dynamic methods. | Lectures, laboratory works, independent work. | Laboratory works, exam. |
| The student is expected to be able to understand and run tasks combined classical and quantum molecular dynamic methods. | Lectures, laboratory works, independent work. | Laboratory works, exam. |

| Content: breakdown of the topics | Contact hours | | | | | | | Self-study work: time and assignments | |
|---|---|---|---|---|---|---|---|---|---|
| | Lectures | Tutorials | Seminars | Exercises | Laboratory work | Internship/work placement | Contact hours | Self-study hours | Assignments |
| **1. MM simulation methods. Combined QM/MM simulation methods** | 8 | | | | | | 8 | 6 | Literature, tasks. |
| **2. Ab Initio molecular dynamics. Car-Parrinello method** | 8 | | | | | | 8 | 6 | Literature, tasks. |
| **3. Path-integral molecular dynamics** | 2 | | | | | | 2 | 2 | Literature, tasks. |

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|---|---|---|---|---|---|---|---|---|---|
| **4. Classical molecular dynamics with quantum degrees of freedom** | 2 | | | | | | 2 | 2 | Literature, tasks. |
| **5. Spatial structure in molecular liquids** | 2 | | | | | | 2 | 2 | Literature, tasks. |
| **6. Energy minimization by smoothing techniques** | 2 | | | | | | 2 | 2 | Literature, tasks. |
| **7. Molecular dynamics with DFT** | 2 | | | | | | 2 | 2 | Literature, tasks. |
| **8. Large scale parallel molecular dynamics simulations** | 2 | | | | | | 2 | 2 | Literature, tasks. |
| **9. Dynamic Monte Carlo simulations** | 2 | | | | | | 2 | 2 | Literature, tasks. |
| **10. Potential energy and free energy surfaces** | 2 | | | | | | 2 | 2 | Literature, tasks. |
| **11. Molecular dynamics tasks using AMBER package** | | | | 12 | | | 12 | 16 | Literature, tasks. |
| **12. Molecular dynamics tasks using Gaussian, Orca and other MD packages** | | | | 4 | | | 4 | 11 | Literature, tasks. |
| **13. Molecular dynamics tasks using NwChem package** | | | | 16 | | | 16 | 21 | Literature, tasks. |
| **Total** | **32** | | | **32** | | | **64** | **76** | |

| **Assessment strategy** | **Weight, %** | **Deadline** | **Assessment criteria** |
|---|---|---|---|
| Laboratory work | 30 | 1-16 weeks of semester | Students must complete and present reports for tasks. Work is completed during self-study hours. The tasks must be presented until the end of semester (80%). |
| Exam | 70 | 16th week of semester | Attendance requirements: practical work 90 %.<br>One self-study laboratory work which show MD usage level: project (P1). Final exam (one questions from MD theory). Exam mode – written answer (K1).<br><br>Final rating E = 0,5 K1 + 0,5 P1. |

| **Author** | **Year of publication** | **Title** | **Issue of a periodical or volume of a publication** | **Publishing place and house or web link** |
|---|---|---|---|---|
| **Compulsory reading** | | | | |
| Ed. Perla B. Balbuena, Jorrge M. Seminario | 2005 | Molecular Dynamics. From Classical to Quantum Methods | | Elsvier science, 946p ISBN0444829105 |
| Errol G. Lewars | 2011 | Computational Chemistry. Introduction to the Theory and Applications of Molecular and Quantum Mechanics | 2nd Edition | Springer, 664p ISBN9789048138609 |
| J. M. Thijssen | 2007 | Computational Physics | 2nd Edition | Cambridge University Press, 620p ISBN9780521833462 |
| **Optional reading** | | | | |
| William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery | 2007 | Numerical Recipes The Art of Scientific Computing | 3rd Edition | Cambridge University Press, 1235p ISBN9780521880688 |
| H. -P. Breuer, F. | 2010 | The Theory of Open | | Oxford University Press, |

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|---|---|---|---|---|
| Petruccione | | Quantum Systems | | 613p<br>ISBN9780199213900 |