DOCTORAL STUDIES COURSE UNIT DESCRIPTION

| Name of subject | Scientific Field | Center | Department |
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| **Thermodynamics of Open Systems** (8 ECTS credits) | Physics N 002 | Center for Physical Sciences and Technology | Molecular Compounds Physics |
| Student's workload | Hours | Student's workload | Hours |
| Lectures | | Consultations | 40 |
| Individual study | 160 | Seminars | |

| Course annotation |
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| Introduction. Open systems. Irreversibility. Historical overview of the structure formation in nonlinear nonequilibrium systems.<br>Basics of thermodynamics. Laws of thermodynamics. Equations, which follows from conservation laws. Kinetic equations describing the transport phenomena (Navier-Stokes, heat permeability, diffusion). Linear response to the external action. Time symetry and Onsager reciprocal relations. Fluctuation-dissipation theorem. Relaxation processes. Local equilibrium. Nonlinear thermodynamics: general criterion of evolution.<br>Basics of mathematics description of self-organization. Dynamical variables. Fundamental equations. Spatially homogeneous systems. Phase space and phase trajectories. Crytical points. Stability according to Liapunov. Systems with one and two degrees of freedom. Classification of the crytical points. Auto-oscillations. Limiting cycle. Bifurcations. Analysis of the nonlinear equations in the vicinity of bifurcation. Dynamical equations of spatially inhomogeneous systems. Criteria of solution stability.<br>Time-dependent structures and static instability. Compressed bar. Laser generation. Bistability in chemistry. Triger. Optical bistability. Basics of catastrophe theory. Analogy with phase trasitions. Mechanical auto-oscillations. Auto-oscillations in electric circuit. Dynamics of populations. Belousov-Zhabotinsky reactions and other models of chemical reactions. Oscillations in biology. MAthematical models of evolution.<br>Spatial structures. General theory of structural organization for the systems far from equilibrium. Bernard effect. Prigogine-Lefever-Nicolis model. Dissipation structures in biology. Morphogenesis. Auto-oscillation phenomena. Switchover waves. Running pulses.<br>Stochastic description. Relative probability. Marcovian processes. Chepmen-Kolmogorov equations. Kinetic equation. Langevin equation. Fokker-Planck equation. Stationary solutions of Fokker-Planck equation. Nonequilibrium phase trasitions. Generalized Ginzburg-Landau equaiton. Nonequilibrium phase transitions at the presence of external fields.<br>Dynamical chaos. Turbulence. Chaos. Strange attractors. |
| List of literature |
| 1. Yu.L. Klimontovich. Statistical Theory of Open Systems: Volume 1: A Unified Approach to Kinetic Description of Processes in Active Systems (Fundamental Theories of Physics). Springer, 1994.<br>2. G. Nicolis, i. Prigogine, Exploring complexity. W. H. Freeman and Co., New York, 1985.<br>3. J. J. Kaladė ir L. Valkūnas. Matematinis modeliavimas ir sinergetiškos pagrindai. Vilniaus universiteto vadovėlis, Vilnius, 2009.<br>4. Г.Николис, И.Пригожин. Самоорганизация в неравновесных системах. Мир, М. 1979.<br>5. H. Haken. Synergetics: Introduction and Advanced Topics, Berlin, Heidelberg, Springer, 2004. |

6. R. Kubo, M. Toda, N. Hashitsume. Statistical physics II, Springer-Verlag, Berlin Heidelberg, 1991.
9. L. E. Reichl. A modern course in statistical physics, John Wiley & Sons, Ins., New Jork (1998).

| Consulting teachers | Scientific degree | Pedagogical name | Main scientific works published in a scientific field in last 5 year period |
|---|---|---|---|
| Leonas Valkunas | habil. Dr. | Prof. | 1. A. Gelzinis, L. Valkunas. "Analytical derivation of equilibrium state for open quantum system", *J. Chem. Phys*., 2020, 152 (5), 051103.<br>2. Y. Braver, L. Valkunas, A. Gelzinis. "Benchmarking the forward–backward trajectory solution of the quantum-classical Liouville equation", *J. Chem. Phys*., 2020, 152 (21), 214116.<br>3. J. Chmeliov, A. Gelzinis, M. Franckevičius, M. Tutkus, F. Saccon, A. V. Ruban, L. Valkunas. "Aggregation-related nonphotochemical quenching in the photosynthetic membrane", *J. Phys. Chem. Lett*., 2019, 10 (23), 7340-7346.<br>4. A. Gelzinis, R. Augulis, V. Butkus, B. Robert, L. Valkunas. "Two-dimensional spectroscopy for non-specialists", *Biochim. Biophys. Acta (BBA)-Bioenergetics*, 2019, 1860 (4), 271-285.<br>5. M. J. Llansola-Portoles, K. Redeckas, S. Streckaité, C. Ilioaia, A. A. Pascal, A. Telfer, M. Vengris, L. Valkunas, B. Robert. "Lycopene crystalloids exhibit singlet exciton fission in tomatoes", *Phys. Chem. Chem. Phys*., 2018, 20 (13), 8640-8646.<br>6. D. Abramavicius, V. Chorošajev, L. Valkunas. "Tracing feed-back driven exciton dynamics in molecular aggregates", *Phys. Chem. Chem. Phys.*, 2018, 20 (33), 21225-21240.<br>7. S. Farooq, J. Chmeliov, E. Wientjes, R. Koehorst, A. Bader, L. Valkunas, G. Trinkunas, H. van Amerongen. "Dynamic feedback of the photosystem II reaction center on photoprotection in plants", *Nature Plants*, 2018, 4, 225–231. |

Certified during Doctoral Committee session 02/02/2022, protocol No. (7.17 E) 15600-KT-32

Committee Chairman prof. S. Juršėnas