DOCTORAL STUDIES COURSE UNIT DESCRIPTION

Name of subject	Scientific Field	Center	Department
Selected Mathematical Methods and Numerical Modelling (8 ECTS credits)	Physics N 002	Center for Physical Sciences and Technology	Molecular Compound Physics
Student's workload	Hours	Student's workload	Hours
Lectures		Consultations	30
Individual study	170	Seminars	

Course annotation
Introduction. Relations between the theory and experiment. Physical models and numerical experiment. Outline of modeling. Variety of models. *Deterministic and stochastic dynamics.* One-step, diffusive and deterministic processes. Molecular dynamics. Verlet algorithm. Canonical and microcanonical ensembles. Markov processes. Chapmen-Kolmogorov equation. Master equation. Langevin and Fokker-Planck equations. Brownian dynamics. Monte Carlo method. Metropolis algorithm. *Disordered systems.* Concept of fractals. Fractal structure. Fractal kinetics. Fractal time. Percolation and Brownian particle motion in fractal. Dynamic disorder. Cellular automata. *Ill-posed problems.* Basics of solution regularization. Tichonov regularization. *Heuristic methods of model optimization.* Simulated annealing. Artificial neural networks. Genetic algorithms. Self-organized criticality model. Extremal optimization algorithm.Particle swarm optimization method.
List of literature
1. Xin-She Yang. Engineering optimization : an introduction with metaheuristic applications. John Wiley & Sons, Inc., Hoboken, New Jersey, 2010. 2. N.G. van Kampen. Stochastic processes in physics and chemistry. North-Holland, Amsterdam, 2004. 3. W.H.Press, S.A.Teukolsky, W.T.Vetterling & B.P.Flannery. Numerical recipes in Fortran. Art of scientific computing. Cambridge University Press. 2007. 4. H.Gould, J.Tobochnik. An introduction to computer simulation methods. Application to physical systems. (3rd edition). Addison-Wesley Publishing Company. N.Y. 2006

Consulting teachers	Scientific degree	Pedagogical name	Main scientific works published in a scientific field in last 5 year period
Jevgenij Chmeliov & Gediminas Trinkūnas	Dr.	Associate Prof.	1. S. Farooq, J. Chmeliov, G. Trinkunas, L. Valkunas, H. van Amerongen. Is There Excitation Energy Transfer between Different Layers of Stacked Photosystem-II-Containing Thylakoid Membranes? *J. Phys. Chem. Lett.* 2016, 6, 1406-1410. 2. J. Chmeliov, G. Trinkunas, H. van Amerongen, L. Valkunas Excitation migration in fluctuating light-harvesting antenna systems. *Photosynth Res*. 2016, 127, 49–60. 3. S. Farooq, J. Chmeliov, E. Wientjes, R. Koehorst, A. Bader, L. Valkunas, G.

			Trinkūnas, H. van Amerongen. Dynamic feedback of the photosystem II reaction centre on photoprotection. in plants. *Nature plants* 2018, 4, 225-231. 4. M. Tutkus, P. Akhtar, J. Chmeliov, F. Gorfol, G. Trinkunas, P.H. Lambrev, L. Valkunas. Fluorescence Microscopy of Single Liposomes with Incorporated Pigment-Proteins. *Langmuir*, 2018, 34, 14410-14418. 5. H. van Amerongen, J. Chmeliov, "Instantaneous Switching between Different Modes of Non-Photochemical Quenching in Plants. Consequences for Increasing Biomass Production", Biochimica et Biophysica Acta – Bioenergetics, 2020, 1861, 148119.
Certified during Doctoral Committee session 02/02/2022, protocol No. (7.17 E) 15600-KT-32			
Committee Chairman prof. S. Juršėnas			