DOCTORAL STUDIES COURSE UNIT DESCRIPTION

Name of subject	Scientific Field	Faculty	Center/Institute/ Department
Theoretical Atomic Spectroscopy (8 ECTS credits)	Physics N 002	Faculty of Physics	Institute of Theoretical Physics and Astronomy
Student’s workload	Hours	Student’s workload	Hours
Lectures	20	Consultations	10
Individual study	160	Seminars	10

Course annotation
1. Introduction. Experimental background. Schrodinger equation. Central field approximation. Foundations of the angular momentum theory. Non-relativistic and relativistic atomic Hamiltonians and wave functions. Relativistic corrections and effects. 2. Many-electron atoms and ions. Coefficients of fractional parentage and grandparentage. Two and more shells of equivalent electrons. Antisymmetrization of wave function. 3. Energy level structure of atoms and ions. Classification of energy levels using various coupling schemes. Intermediate coupling. Optimization of the coupling scheme. Hyperfine structure of the energy spectra, isotopic and Lamb shifts. Correlation effects. 4. Radiative electronic transitions in atoms and ions. Line and oscillator strength, transition probability, lifetime and line intensity. Selection and sum rules for electronic transitions. Allowed and forbidden transitions. Peculiarities of electric dipole and quadruple as well as magnetic dipole transitions. 5. Interaction of atoms and ions with photons and electrons. Elastic and inelastic scattering. Classical, quantum, and semiclassical description of scattering. Cross section of scattering. Born approximation. Lippmann-Schwinger equation. Plane waves. Partial waves. Resonances. 6. Photoexcitation, photoionization, and photorecombination. Detailed balance principle. 7. Electron-impact excitation. Collision strength. Close coupling approximation. R-matrix method. Distorted-wave Born approximation. Plane-wave and Coulomb-wave Born approximation. Independent processes isolated resonances approach. 8. Electron-impact ionization. Time-dependent close-coupling method. Coulomb-Born and distorted wave approximations. Dielectronic capture and recombination. Autoionization.
List of literature
1. Cowan R.D. The Theory of Atomic Structure and Spectra. University of California Press, Berkeley, 1981. 2. Ch.Froese Fischer. The Hartree-Fock Method for Atoms (A Numerical Approach). John-Willey and Sons, New York -London-Sydney-Toronto, 1997. 3. Sakurai J. J., Napolitano J. Modern Quantum Mechanics. Addison-Wesley. 2011. 4. Friedrich H. Theoretical Atomic Spectroscopy. Springer. 2006. 5. Gordon W. F. Drake. Springer Handbook of Atomic Molecular and Optical Physics. Springer. 2006. 6. Boyle J. J., Pindzola M. S. Many-body Atomic Physics. Cambridge University Press. 1998. 7. Salzmann D., Atomic Physics in Hot Plasmas, Oxford University Press, 1998.

Consulting teachers	Scientific degree	Pedagogical name	Main scientific works published in a scientific field in last 5 year period
Valdas Jonauskas	Ph. D.	Assoc. Professor	1. Š. Masys, V. Jonauskas. The Crystalline Structure of Tensile Strained SrRuO3: A First-Principles Investigation. Crystal Growth & Design 18, 3397 (2018). DOI: 10.1021/acs.cgd.8b00113 2. V. Jonauskas, Electron-impact double ionization of the carbon atom, Astronomy & Astrophysics 620, A188 (2018). DOI: 10.1051/0004-6361/201834303 3. A. Kynienė, S. Kučas, Š. Masys, V. Jonauskas. Electron-impact ionization of Fe8+, Astronomy & Astrophysics 624, A14 (2019). DOI: 10.1051/0004-6361/201833762 4. V. Jonauskas, Š. Masys. Double- and triple-Auger processes in C1+, J. Quantitative Spectroscopy and Radiative Transfer 229, 11 – 16 (2019). DOI: 10.1016/j.jqsrt.2019.02.032 5. S. Kučas, P. Drabužinskis, A. Kynienė, Š. Masys and V. Jonauskas. Evolution of radiative and Auger cascades following 2s vacancy creation in Fe2+, J. Phys. B: At. Mol. Opt. Phys. 52, 225001 (2019). DOI: 10.1088/1361-6455/ab46fa 6. V. Jonauskas. Electron-impact ionization of Sn4+, J. Quantitative Spectroscopy and Radiative Transfer 239, 106659 (2019). DOI: 10.1016/j.jqsrt.2019.106659 7. A. Kynienė, S. Kučas, S. Pakalka, Š. Masys, and V. Jonauskas. Electron-impact single ionization of Fe3+ from the ground and metastable states, Phys. Rev. A 100, 052705 (2019). DOI: 10.1103/PhysRevA.100.052705 8. V. Jonauskas, A. Kynienė, S. Kučas, S. Pakalka, Š. Masys, A. Prancikevičius, A. Borovik, Jr., M. F. Gharaibeh, S. Schippers, and A. Müller. Electron-impact ionization of W5+, Phys. Rev. A 100, 062701 (2019). DOI: 10.1103/PhysRevA.100.062701 9. V. Jonauskas, Electron-impact single ionization of Si+, Astronomy & Astrophysics 642, A185 (2020). DOI: 10.1051/0004-6361/202038266 10. S. Kučas, A Kynienė, Š. Masys, V. Jonauskas, Multiple photoionization cross

			sections for Fe2+ K shell, Astronomy & Astrophysics 643, A46 (2020). DOI: 10.1051/0004-6361/202038762
Certified during Doctoral Committee session 02/02/2022, protocol No. (7.17 E) 15600-KT-32			
Committee Chairman prof. S. Juršėnas			