COURSE (MODULE) DESCRIPTION

Course Title	Code
Magnetic Resonance Spectroscopy	

Annotation
Magnetic resonance is a very broad field of science due to its wide range of applications in chemistry, physics, materials science, medicine, and other fields. The most commonly used experimental methods are Nuclear Magnetic Resonance (NMR) spectroscopy, Electron Paramagnetic Resonance (EPR) spectroscopy, and Magnetic Resonance Imaging (MRI). During the course, students will be introduced to classical and quantum theories of magnetic resonance, as well as modern experimental methods. They will learn to understand the principles of experimental techniques and analyse NMR and EPR spectra. Theoretical examples in lectures will be supplemented with experimental research examples. During laboratory work, students will become familiar with and record NMR and EPR spectra using modern scientific equipment.

Lecturer	Department
dr. Vytautas Klimavičius	Faculty of Physics, Institute of Chemical Physics

Study Level	Course Type
Master‘s	Compulsory

Type	Semester	Language
Auditorium	III (Autumn) semester	Lithuanian, English

Prerequisites	

Credits	Total Workload	Contact Workload	Independent Workload
5	140	48	92

Course Aim		
The course is intended to introduce nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR) spectroscopy, classical magnetic resonance theory, quantum mechanical magnetic resonance theory, applications of magnetic resonance in materials science and biosciences, the principles of NMR tomography in medicine, and hyperpolarization techniques.		
Aims of the Course	**Teaching Methods**	**Assessment**
Gain knowledge on Magnetic Resonance, and its applications	Lectures, Seminars, Laboratory Work	Exam, Cumulative score from Seminars and Laboratory work.
To be able to analyse experimental data.		

Topics	Contact Workload							Individual Work and Tasks	
	Lectures	Consultations	Seminars	Exercises	Laboratory work	Practical	Total	Individual Work	Tasks

1. Introduction Historical aspects, atoms in a magnetic field, the Stern–Gerlach experiment, nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR).	2						**2**	**0**	
2. Classical Magnetic Resonance Theory Spin magnetic moments, spin magnetization, Larmor precession, spin–lattice (T_1) and spin–spin (T_2) relaxation, magnetic field pulses, free induction decay.	4						**4**	**8**	Analysis of Scientific Literature.
3. Quantum Mechanical Magnetic Resonance Theory Vector algebra, matrices, Hilbert space and spin operators, NMR Hamiltonians, Liouville space and super operators.	6						**6**	**12**	Analysis of Scientific Literature.
4. High-Resolution NMR Structure of high-resolution spectra, influence of magnetic field homogeneity on spectra, decoupling of nuclear interactions, 1D and 2D experiments, applications of NMR in chemistry, materials science, and biosciences.	4		2		4		**10**	**20**	Analysis of Scientific Literature and Seminar Preparation
5. Solid-State NMR Anisotropic interactions in solids, NMR spectra of single crystals and powders, magic angle spinning (MAS), cross-polarization (CP), 1D and 2D experiments, applications in materials science and biosciences	4		2		4		**10**	**20**	Analysis of Scientific Literature and Seminar Preparation
6. Principles of NMR Tomography Magnetic field gradients, the operating principle of a tomograph, and applications of tomography in medicine.	2		2				**4**	**8**	Analysis of Scientific Literature and Seminar Preparation
7. EPR Spectroscopy Hyperfine interactions, continuous-wave and pulse methods, applications in materials science and biosciences.	2		2		4		**8**	**16**	Analysis of Scientific Literature and Seminar Preparation
8. Hyperpolarization Techniques Dynamic Nuclear Polarization (DNP), parahydrogen-induced polarization (PHIP), applications in materials science and biosciences	2		2				**4**	**8**	Analysis of Scientific Literature and Seminar Preparation
Total	**26**		**10**		**12**		**48**	**92**	

Assessment	weight %	Period	Criteria
Seminars	25	All Semester	During the seminar, the results of independently completed tasks are presented. Knowledge is assessed based on the completed tasks: quality and accuracy of the provided information (5 points), presentation style and delivery (2 points), and responses to additional questions (3 points). A 10-point grading system is used.
Laboratory work	25	All Semester	During laboratory work, students will be introduced to high-resolution, solid-state NMR and EPR experimental techniques, record NMR and EPR spectra, and process them. Knowledge is assessed based on completed tasks:

			analysis of recorded spectra (5 points), quality of the laboratory report (2 points), and responses to additional questions (3 points). A 10-point grading system is used.
Exam	50	Exam Session	5 open-ended questions. Answers may require a formula or an explanatory diagram. Each correctly answered question is worth 2 points; incorrect answers receive 0 points. A 10-point grading system is used.

Author	Year	Title	Number	Publisher or Online Link
Compulsory Literature				
1. Malcolm H. Levitt	2008	Spin Dynamics: Basics of Nuclear Magnetic Resonance		John Wiley & Sons Ltd, The Atrium, Southern Gate Chichester, England
2. J. Keeler	2002	Understanding NMR Spectroscopy		Wiley, The Atrium, Southern Gate Chichester, England
3. V. I. Chizhik ,Y. S. Chernyshev, A. V. Donets, V. V. Frolov, A. V. Komolkin, M. G.Shelyapina	2014	Magnetic Resonance and Its Applications		Springer International Publishing Switzerland
4. Vladimir I. Bakhmutov	2011	Solid-State NMR in Materials Science: Principles and Applications		CRC Press
5. K.Müller, M. Geppi	2021	Solid State NMR: Principles, Methods, and Applications		Wiley
Additional Literature				
1. R. E. Wasylishen, S. E. Ashbrook, S. Wimperis	2012	NMR of Quadrupolar Nuclei in Solid Materials		John Wiley & Sons Ltd, Ltd The Atrium, Southern Gate Chichester, England
2. C P. Slichter	1990	Principles of Magnetic Resonance		Springer