



## COURSE UNIT (MODULE) DESCRIPTION

Course unit (module) title	Code
<b>Chemistry and Physics of <i>f</i> Elements</b>	

Lecturer(s)	Department(s) where the course unit (module) is delivered
<b>Coordinator: assoc. prof. dr. Arturas Katelnikovas</b> <b>Other(s):</b>	Faculty of Chemistry and Geosciences, Institute of Chemistry Naugardukas str. 24, LT-03225 Vilnius

Study cycle	Type of the course unit (module)
Second	Optional

Mode of delivery	Period when the course unit (module) is delivered	Language(s) of instruction
Face to face	3 <sup>rd</sup> semester	Lithuanian

Requirements for students	
<b>Prerequisites:</b> Finished bachelor studies in chemistry.	<b>Additional requirements (if any):</b>

Course (module) volume in credits	Total student's workload	Contact hours	Self-study hours
5	135	48	87

Purpose of the course unit (module): programme competences to be developed		
<p>A.1. ability to explain the principles of modern methods used for the characterization of classical and nanomaterials.</p> <p>B.1. ability to apply knowledge and suitable methods in research and practical work.</p> <p>B.2. ability to select appropriate methods of research and to interpret reasonably the results obtained through those methods.</p> <p>B.4. ability to work in the interdisciplinary areas and use the knowledge of different scientific fields in practical work.</p> <p>C.2. ability to analyze, make generalizations and critically evaluate scientific and practical information.</p> <p>D.3. ability to present clearly and scientifically knowledge and concepts of chemistry and nanochemistry to the professionals and non-professionals.</p>		
Learning outcomes of the course unit (module)	Teaching and learning methods	Assessment methods
<p>After successful completion of this course student should be able to:</p> <ul style="list-style-type: none"> <li>• Characterize the mining, separation and purification methods of rare earth elements;</li> <li>• Point out the importance of the rare earth metals in modern technologies;</li> <li>• Properly employ the various energy units (eV, cm<sup>-1</sup>, nm) in calculations;</li> <li>• Compare the optical properties of different rare earth ions;</li> <li>• Explain the differences between [Xe]4f<sup>n</sup> → [Xe]4f<sup>n</sup> and [Xe]4f<sup>n</sup> → [Xe]4f<sup>n-1</sup>5d<sup>1</sup> optical transitions;</li> <li>• Explain the defect influence on luminescent properties of optical materials;</li> <li>• Assign the lines and bands of rare earth ions in their emission and excitation spectra to certain optical</li> </ul>	<p>Lectures with demonstration of some chemical experiments;</p> <p>Laboratory work;</p> <p>Writing of laboratory work reports; Presenting and defending of these reports in classroom and answering related questions;</p> <p>Textbook reading.</p>	<p>All laboratory works must be accomplished, the reports must be written and defended.</p> <p>One midterm exam (multiple choice tasks, short answer tasks, complex tasks).</p> <p>Final exam (includes multiple choice tasks, complex tasks, graphical and calculation tasks).</p>

transitions; <ul style="list-style-type: none"> <li>• Prepare the plan of experiment and the list of necessary equipment;</li> <li>• Write the chemical reactions occurring during solid-state reaction method and sol-gel combustion reaction method;</li> <li>• Analyze and interpret the obtained results;</li> <li>• Explain the different optical properties of the same rare earth ion in various host matrixes;</li> <li>• Calculate the energy transfer efficiency from sensitizer to activator;</li> <li>• Compare the optical properties of divalent europium and trivalent cerium in various inorganic host matrixes.</li> </ul>		
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Content: breakdown of the topics	Contact hours					Total contact hours	Self-study hours	Self-study work: time and assignments
	Lectures	Seminars	Exercises	Laboratory work	Internship/work placement			Assignments
1. Introduction. Course objectives.	1					1	0	
2. Lanthanides in the periodic table of elements. Comparison of lanthanides with transition and alkaline metals. Rare earth metals containing minerals and their discovery. The distribution, resources, mining and purification of rare earth elements. Ionic radius, melting and boiling point temperature, and ionization energies as a function of atomic number of lanthanide metal/ion.	4					4	7	Textbook reading.
3. The properties of rare earth metals, their synthesis. Alloys. Binary compounds (oxides, halides, borides, carbides, nitrides, hydrides, sulphides).	3					3	5	Textbook reading.
4. Coordination compounds of the rare earth ions. Stability of complexes. Complexes with $\beta$ -diketonates. Complexes with EDTA and similar ligands. Complexes with N-ligands. The coordination numbers of rare earth complexes.  Laboratory work Synthesis and characterization of organic complexes of trivalent lanthanide ions.	4			4		8	10	Textbook reading. Preparation for laboratory works. Preparation of lab reports.
5. The synthesis method influence to optical properties of lanthanide ion doped inorganic materials. Solid state synthesis method. Precipitation method. Aqueous and non-aqueous sol-gel synthesis method. Sol-gel combustion method. Hydrothermal synthesis. Induction heating synthesis. Gas reduction/nitridation process.	4			4		8	20	Textbook reading. Preparation for laboratory works. Preparation of lab reports.

<p>Characterization of the optical materials. X-ray diffraction, IR spectroscopy, photoluminescence, thermoluminescence, scanning electron microscopy.</p> <p>Laboratory work Characterization of <math>(Y,Lu)_3Al_5O_{12}:Ce^{3+}</math> synthesized by solid state reaction and sol-gel combustion techniques.</p>								
<p>6. Physical properties of rare earth ions. Magnetic properties. Optical properties. Quantum numbers. Term symbols and their construction. Construction of term symbols of the rare earth ions at their ground state. Dieke diagram. Spectroscopic levels. <math>[Xe]4f^n \rightarrow [Xe]4f^n</math> and <math>[Xe]4f^n \rightarrow [Xe]4f^{n-1}5d^1</math> optical transitions. Factors influencing the optical properties of rare earth ions in different inorganic host matrixes: covalence, crystal-field strength, Stokes shift.</p> <p>Laboratory work Synthesis of <math>(Ba,Sr)_2SiO_4:Eu^{2+}</math> by solid state reaction method and investigation of Ba/Sr ratio influence to the luminescence properties of <math>Eu^{2+}</math> ion. Synthesis of <math>(Y,Lu)_2SiO_5:Ce^{3+}</math> by solid state reaction method and investigation of Y/Lu ratio influence to the luminescence properties of <math>Ce^{3+}</math> ion.</p>	8		4		12	25	Textbook reading. Preparation for laboratory works. Preparation of lab reports.	
<p>7. The evaluation of the optical properties of rare earth ion doped inorganic materials. Quantum yield, luminous efficacy, 1931 CIE colour space diagram, colour points. <math>Eu^{2+} \rightarrow Mn^{2+}</math> energy transfer. <math>Ce^{3+} \rightarrow Tb^{3+}</math> energy transfer. Downconversion. Downshifting. Upconversion. Influence of the host matrix site symmetry to the optical properties of rare earth ions.</p> <p>Laboratory work Investigation of <math>Eu^{2+} \rightarrow Mn^{2+}</math> energy transfer in <math>BaMgAl_{10}O_{17}</math> host matrix. Investigation of <math>Ce^{3+} \rightarrow Tb^{3+}</math> energy transfer in <math>GdMgB_5O_{10}</math> host matrix. Investigation of luminescence properties of <math>Eu^{3+}</math> ion in centre-symmetric and non-centre-symmetric compounds.</p>	8		4		12	20	Textbook reading. Preparation for laboratory works. Preparation of lab reports.	
	<b>32</b>		<b>16</b>		<b>48</b>	<b>87</b>		

Assessment strategy	Weight, %	Deadline	Assessment criteria
Laboratory works	50	Every 3-4 weeks	Safe work in the laboratory. Ability to get reliable results. All laboratory works must be accomplished, the reports

			must be written and defended. If failed, the student must repeat the laboratory work.
Final exam	50	January	Multiple choice tasks, short answer tasks, complex tasks, graphical and calculation tasks.

<b>Author</b>	<b>Year of publication</b>	<b>Title</b>	<b>Issue of a periodical or volume of a publication</b>	<b>Publishing place and house or web link</b>
<b>Compulsory reading</b>				
S. Cotton	2006	Lanthanide and Actinide Chemistry		John Wiley & Sons Ltd., Chichester, England
G. Blasse, B.C. Grabmaier	1994	Luminescent Materials		Springer-Verlag, Berlin, Germany
<b>Optional reading</b>				
C. Ronda (ed.)	2008	Luminescence. From Theory to Applications		WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany
W.M. Yen, S. Shionoya, H. Yamamoto (eds.)	2007	Phosphor Handbook (2 <sup>nd</sup> ed.)		CRC Press/Taylor & Francis, Boca Raton, USA