PhD STUDIES COURSE UNIT DESCRIPTION

Name of subject	Field of science, code	Faculty / Center	Department
Refinement of Crystalline and Magnetic Structures	Chemistry N 003	Faculty of Chemistry and Geosciences	Department of Inorganic chemistry
Student's workload	**Credits**	**Student's workload**	**Credits**
Lectures		Consultations	3
Independent study	7	Seminars	

Course annotation
The aim of the course is to convey theoretical and practical methods for determining the crystal and magnetic structure of materials from X-rays (XRD) and neutron diffraction data. Topics covered in the course: crystalline materials; magnetic materials; basics of crystallography; X-ray generation; neutron beam generation; X-ray and neutron radiation characteristics and application possibilities; diffractogram anatomy; determination of crystalline structure (XRD data): Le Bail refinement method and Rietveld analysis; sample preparation; experimental conditions; determination of magnetic properties; determination of crystalline and magnetic structure by Rietveld analyzing neutron diffraction data; visualization of crystalline and magnetic structures; instrumental file; determination of crystallite size; bond lengths and angles; single crystal diffraction; single crystal orientation. Determination of the crystal structure of at least 3 compounds selected by the student by Le Bail and Rietveld methods.
Reading list
1. Cullity, B. D, & Stock, Stuart R. (2014). Elements of x-ray diffraction (3rd ed.; Pearson new international edition., p. ii). Pearson. 2. Will, Georg. (2006). Powder diffraction: the Rietveld method and the two-stage method to determine and refine crystal structures from powder diffraction data (p. ix). Springer. 3. Furrer A., Mesot J., Strassle T. (2009) Neutron Scattering in Condensed Matter Physics, World Scientific. 4. Rodrigues-Carvajal J. (2000) An Introduction to the Program FullProf. 5. Pynn R. (1990) Neutron Scattering – A primer, LANSCE.

The names of consulting teachers	Science degree	Main scientific works published in a scientific field in last 5 year period
Ramūnas Skaudžius	Dr.	1. G. Inkrataite, M. Kemere, A. Sarakovskis, R. Skaudzius. Influence of Boron on the Essential Properties for New Generation Scintillators. *J. Alloy. Compd.* (2021) https://doi.org/10.1016/j.jallcom.2021.160002. 2. A.Pakalniškis, R. Skaudžius, D. V. Zhaludkevich, A. L. Zhaludkevich, D. O. Alikin, A. S. Abramov, T. Murauskas, V. Ya. Shur, A. A. Dronov, M. V. Silibin, A. Selskis, R. Ramanauskas, A. Lukowiak, W. Strek, D. V. Karpinsky, A. Kareiva. Morphotropic Phase Boundary in Sm-Substituted $BiFeO_3$ Ceramics: Local vs Microscopic Approaches. *J. Alloy. Compd.* (2021) https://doi.org/10.1016/j.jallcom.2021.159994. 3. G. Inkrataite, A. Zabiliute-Karaliune, J. Aglinskaite, P. Vitta, K. Kristinaityte, A. Marsalka, R. Skaudzius. Study of YAG : Ce and Polymer Composite Properties for Application in LED Devices. ChemPlusChem 85(7) (2020) 1504-1510, https://doi.org/10.1002/cplu.202000318. 4. A. Pakalniškis, A. Lukowiak, G. Niaura, P. Głuchowski, D.V. Karpinsky, D.O. Alikin, A.S. Abramov, A. Zhaludkevich, M. Silibin, A.L. Kholkin, R. Skaudžius, W. Strek, A. Kareiva.

		Nanoscale ferroelectricity in pseudo-cubic sol-gel derived barium titanate - bismuth ferrite ($BaTiO_3$– $BiFeO_3$) solid solutions. J. Alloy. Compd. 830 (2020) 154632, https://doi.org/10.1016/j.jallcom.2020.154632. 5. Karpinsky, D.V., Fesenko, O.M., Silibin, M.V., Dubkov, S.V., Chaika, M., Yaremkevich, A., Lukowiak, A., Gerasymchuk, Y., Stręk, W., Pakalniškis, A., Skaudzius, R., Kareiva, A., Fomichov, Y.M., Shvartsman, V.V., Kalinin, S.V., Morozovsky, N.V., Morozovska, A.N. Ferromagnetic-like behavior of Bi0.9La0.1FeO3–KBr nanocomposites. *Sci. Rep-UK.* 9 (2019) 10417, DOI: 10.1038/s41598-019-46834-0 6. M. Skruodiene, A. Katelnikovas, L. Vasylechko, R. Skaudzius, Tb^{3+} to Cr^{3+} Energy transfer in a co-doped $Y_3Al_5O_{12}$ host. *J. Lumin*. 208 (2019) 327-333. 7. J. Raudoniene, R. Skaudzius, A. Zarkov, A. Selskis, E. Garskaite, Wet-chemistry synthesis of shape-controlled Ag3PO4 crystals and their 3D surface reconstruction from SEM imagery. *Powder Technol.* 345 (2019) 26-34. 8. A. Smalenskaite, A.N. Salak, M.G.S.Ferreira, R.Skaudzius, A.Kareiva, Sol-gel synthesis and characterization of hybrid inorganic-organic Tb(III)-terephthalate containing layered double hydroxides. *Opt. Mat.* 80 (2018) 186-196. 9. A. Laurikenas, A. Katelnikovas, R. Skaudzius, A. Kareiva, Synthesis and characterization of Tb3+ and Eu3+ metal-organic frameworks with TFBDC2− linkers. *Opt. Mat.* 83 (2018) 363-369. 10. R. Skaudzius, M. Misevicius, V. Brimiene, M. Beniuse, G. Brimas, A. Kareiva, SEM (EDX) is an indispensable tool for the characterization of subcutaneous, preperitoneal and visceral adipose tissue of obese patients. *Chemija* 29 (2018) 67-80. 11. R. Skaudžius, D. Enseling, M. Skapas, A. Selskis, E. Pomjakushina, T. Jüstel, A. Kareiva, C. Rüegg. Europium–Enabled Luminescent Single Crystal and Bulk YAG and YGG for Optical Imaging. *Opt. Mat.* 60 (2016) 467-473. 12. M. Skruodiene, M. Misevicius, M. Sakalauskaite, A. Katelnikovas, R. Skaudzius. Doping effect of Tb^{3+} ions on luminescence properties of $Y_3Al_5O_{12}$:Cr^{3+} phosphor. *J. Lumin.* 179 (2016) 355-360. 13. R. Skaudzius, T. Juestel, A. Kareiva. Luminescence properties of Ln^{3+}–doped (Ce^{3+}, Eu^{3+}, Tb^{3+} or Er^{3+}) Mixed–Metals $Y_3(Al,In)_5O_{12}$ and $Y_3Al_{4.75}Cr_{0.25}O_{12}$ garnets synthesized by Sol–Gel method. *Mater. Chem. Phys.,* 170 (2016) 229-238.

Certified during Doctoral Committee session on September 28th, 2021. Protocol No. 610000-KT-142.
Committee Chairman prof. habil. dr. Aivaras Kareiva