

Level: bachelor			
Course title: Crystal X-ray Diffraction and Structure Analysis			
Status: elective			
ECTS: 6			
Requirements: -			
Learning objectives: This course covers the following topics: X-ray diffraction: symmetry, space groups, geometry of diffraction, structure factors, phase problem, direct methods, Patterson methods, structure refinement, powder methods, limits of X-ray diffraction methods, and structure data bases.			
Learning outcomes: The overall competence is acquiring knowledge and students' ability for individual and team scientific research work in the field of applying physical concepts of X-ray diffraction and structure solution. The specific competences are, for example: <i>Knowledge and Understanding:</i> <ul style="list-style-type: none"> • define concepts such as lattice, point and space groups • be familiar with Bragg's Law and explain its the relation to crystal structure • identify and describe different diffraction methods • be familiar with crystal structure solution methods <i>Skills:</i> <ul style="list-style-type: none"> • the intellectual skills associated with the assimilation of educational subject matter; preparation of notes, revision material, the ability to access and utilise information from a variety of sources • ability to apply knowledge of math and physics • knowledge of contemporary issues 			
Syllabus: <i>Theoretical instruction</i> <ol style="list-style-type: none"> 1. Materials and materials properties 2. What is a crystal structure? 3. Lattices and symmetries 4. Reciprocal lattice 5. Crystal symmetry 6. Point groups 7. Plane groups and space group 8. X-ray diffraction: geometry 9. X-ray diffraction: intensity 10. About crystal structures and diffraction patterns 11. Practical aspects of X-ray diffraction 12. Solving crystal structure 13. Limits of X-ray diffraction methods 14. Structure data bases <i>Practical instruction</i> <ol style="list-style-type: none"> 1. Experimental exercises in the Laboratory of X-ray diffraction. Experimental work on powder and single crystal diffractometer. Working with computer programs in the package WinGX 			
Literature: <ol style="list-style-type: none"> 1. W. Borchardt-Ott, Crystallography, Springer, 2011 2. William Clegg, X-Ray Crystallography, Oxford University Press, 2015 3. W. Clegg (ed.), Crystal Structure Analysis, Oxford University Press, 2009 4. M. Ladd, R. Palmer, Structure Determination by X-ray Crystallography, Springer, 2013 5. G.S. Girolami, X-ray Crystallography, University Science Books, 2016 			
Weekly teaching load			Other:
Lectures: 3	Exercises: 2	Other forms of teaching:	