Course Unit Descriptor

Study Programme: Physics

Course Unit Title: Crystal X-ray Diffraction and Structure Analysis

Course Unit Code: F18RSAK

Name of Lecturer(s): dr Olivera Klisurić

Type and Level of Studies: Bachelor Academic Degree

Course Status (compulsory/elective): elective

Semester (winter/summer): summer

Language of instruction: English

Mode of course unit delivery (face-to-face/distance learning): face-to-face

Number of ECTS Allocated: 6

Prerequisites:

Course Aims:

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:

Knowledge and Understanding:

- 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

Skills:

- 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:

Theory

Materials and materials properties. What is a crystal structure? Lattices and symmetries. Reciprocal lattice. Crystal symmetry. Point groups. Plane groups and space group. X-ray diffraction: geometry. X-ray diffraction: intensity. About crystal structures and diffraction patterns. Practical aspects of X-ray diffraction. Solving crystal structure. Limits of X-ray diffraction methods. Structure data bases.

Practice

Experimental exercises in the Laboratory of X-ray diffraction. Experimatal work on powder and single crystal diffractometer. Working with computer programs in the package WinGX.

Required Reading:

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 Contact Hours:	**Lectures:** 3	**Practical work:** 2

Teaching Methods:

Knowledge Assessment (maximum of 100 points):

Pre-exam obligations	points	**Final exam**	points
Active class participation		written exam	40
Practical work	10	oral exam	30
Preliminary exam(s)	20	…….	
Seminar(s)			

The methods of knowledge assessment may differ; the table presents only some of the options: written exam, oral exam, project presentation, seminars, etc.