UAB
Universitat Autònoma de Barcelona

Crystallography

Code: 106812
ECTS Credits: 6

2024/2025

Degree	Type	Year
2504602 Nanoscience and Nanotechnology	OB	1

Contact

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Teachers

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Teaching groups languages

You can view this information at the end of this document.

Prerequisites

The course has no previous prerequisites, apart from basic knowledge of mathematics, physics and chemistry. Basic knowledge is required in:

- Chemical formulation

- Valence and bonding

- Matrix algebra

- Vector algebra

- Wave physics

- Physics of waves

Objectives and Contextualisation

This course provides fundamentals about the organization of atoms in solid state.

The objectives are:

I. Acquisition of basic knowledge for the description of the crystal structure of solids. The aspects to consider are:

1- The crystal lattice and its mathematical description.

2- Crystal symmetry and its mathematical description.

II. To know the basics of X-ray diffraction of crystals as an experimental technique that allows access to the crystalline structure of solids.

III. Acquisition of spatial vision of crystalline structures and their symmetry.

IV. To learn how to perform simple tasks with crystallography software.

V. To learn how the type of bond is related to the crystal strcuture and to know the most important structural types.

VI. To get the the bases to be able to relate the physical properties of matter with its crystalline structure, inclusing nanosize effects

Learning Outcomes

1. CM13 (Competence) Apply chemical knowledge to solve quantitative and qualitative problems, using bibliographic sources when necessary.
2. CM14 (Competence) Work collaboratively to plan and organise the basic tasks carried out in a physicochemical analysis laboratory.
3. KM25 (Knowledge) Recognise and describe the geometrical patterns and symmetry that characterise a crystalline medium.
4. SM22 (Skill) Explain the variation in properties of the chemical elements and their compounds, based on the periodic table groups and crystal structure.

Content

(topic order may change)

1. Reticular theory

2. Point symmetry

3. Spatial symmetry

4. Crystal structures

5. Crystal morphology

6. X-ray diffraction

7. Real crystal and crystal size effects

Practical sessions

(the order and content could change)

Session 1: Point symmetry with crystallographic models

Session 2: Point symmetry with interactive PDFs

Session 3: Plane symmetry groups

Session 4: Visualization of crystal structures with VESTA

Session 5: Powder Diffraction

Session 6: Crystallography databases

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Laboratory	12	0.48	
Lectures	35	1.4	
Tutorials	5	0.2	
Type: Autonomous			
Independent work	87	3.48	

Lectures consists of explanations from the teachers together with questions and discussions with the students.

In the tutorials students are split in two groups. The tutorials consist of solving exercises and problems previously provided to the students. Once the exercises are done in class, the solutions will be available on the virtual campus.

In the laboratories students are split in three groups. If possible, laboratories will take place in spaces that facilitate group work or in classrooms that allow the use of computers (electrified classrooms or PC classrooms). The students will have a script to carry out with the support of the teaching staff. The correct result will be provided either in the classroom itself or in the virtual campus.

The students' independent work consists on working by himself/herself on all the aspects previously seen in the classroom either in lectures, tutorial or laboratories. Lecture presentations, reference material, bibliography, solved exercises and crystallography software (either in computer classrooms or as free software) will be available for the students for this purpose.

The Virtual Campus is used for communication with the students. It is also the place where laboratory scripts, specific reference material, lecture presentations, grades, etc. will be stored. The lecture presentations constitute a basis for the lectures. In any case they replace the attendance to the lectures.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Deliveries	20 - 30 %	4	0.16	CM13, CM14, KM25, SM22
Mid-term exam 1	35 - 40 %	2	0.08	CM13, KM25, SM22
Mid-term exam 2	35 - 40 %	2	0.08	CM13, KM25, SM22
Recovery exam	35 - 40 % each part	3	0.12	CM13, KM25, SM22

The evaluation of the course includes both continuous evaluation and a final or recovery exam.

Continuous assessment comprises two mid-term exams, the first one is scheduled for the first half of April and the second in June. Each exam represents 40% of the overall qualification. Continuous assessment also includes the assessment of assignments, class attendance, exercises, assignment or quiz set in class. These assignments represent 20% of the overall grade.

The course can be passed in the continuous assessment, without the need to take the final exam if an overall grade of 5 is reached. The make-up exam in June is an opportunity redo one or two mid-term exams. In this case, the grade obtained in the make-up exam will replace the corresponding partial exam. Assessable deliveries are not recoverable.

Students who do not assists to any exam will be considered as not avaluable.

Single assessment

The single assessment (for students who requested it) will take place on the day of the second mid-term exam. This assessment will consist of:

1.-Completion of an exam for the entire subject (70% of the overall grade).

2.-The delivery of a work to be done with crystallographic software (10% of the overall grade).

3.-An oral test where crystal models will be presented and questions will be asked about their symmetry (20% of the overall grade).

In case of failing to pass, the students will have the right to take a second exam where the grade will replace the grade of the first exam. This second exam will preferably take place on the same day as the make-up exams. Both the assignment and the oral test cannot be recovered.

Bibliography

Books

· An introduction to Mineral Science

A. PUTNIS, Cambridge University Press

· Fundamentals of Crystallography

C. GIACOVAZZO, Oxford University Press

· Space groups for solid state scientists

G. BURNS, A. M. GLAZER, Elsevier

· The Basics of Crystallography and Diffraction

C. HAMMOND, Oxford University Press

· Crystallography

WALTER BORCHARDT-OTT, Springer Verlag

· Estructura atómica y enlace químico

JAUME CASABÓ I GISPERT, Editorial Reverté

• An Introduction to Crystal Chemistry

R.C. EVANS, Cambridge University Press

• Cristal·lografia. Teoria Reticular, Grups Puntuals i Grups Espacials

SALVADOR GALÍ MEDINA, Edicions de la Universitat de Barcelona

• International Tables for Crystallography. Volume A: Space-Group Symmetry (teaching edition)

T. HAHN, editor, The International Union of Crystallography, D. Reidel Publishing Company

Web sites

https://www.uab.cat/web/la-divulgacio/grups-puntuals-de-simetria-1345664584325.html

http://www.iucr.org International Union of Crystallography

http://www.iucr.org/education/pamphlets Teaching pamphlets

http://reference.iucr.org/dictionary/Main_Page Diccionari de cristal·lografia

http://it.iucr.org/ International Tables for Crystallography, accés només al campus

http://www.xtal.iqfr.csic.es/Cristalografia/ Instituto de Química Física Rocasolano

http://www.crystallography.net/cod/ Crystallography Open Database

http://rruff.geo.arizona.edu/AMS/amcsd.php American Mineralogist Crystal Structure Database

Software

Interactive PDF: https://www.uab.cat/web/la-divulgacio/grups-puntuals-de-simetria-1345664584325.html

VESTA: https://jp-minerals.org/vesta/en/

Quiztallography (Android) https://play.google.com/store/apps/details?id=aax.uab.quiztallography&pli=1

Language list

Name	Group	Language	Semester	Turn

(PAUL) Classroom practices	1	Catalan	second semester	afternoon
(PAUL) Classroom practices	2	Catalan	second semester	afternoon
(PLAB) Practical laboratories	1	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	2	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	3	Catalan	second semester	morning-mixed
(TE) Theory	1	Catalan	second semester	afternoon