UNIVERSIDADE DA CORUÑA

Teaching Guide				
Identifying Data				2021/22
Subject (*)	Crystallography and Symmetry		Code	610G04006
Study programme	Grao en Nanociencia e Nanotecnoloxía			
Descriptors				
Cycle	Period	Year	Type	Credits
Graduate	2nd four-month period	First	Basic training	6
Language	SpanishGalician			
Teaching method	Face-to-face			
Prerequisites				
Department	Química			
Coordinador	Platas Iglesias, Carlos	E-mail	carlos.platas.iglesias@udc.es	
Lecturers	Bermúdez García, Juan Manuel Esteban Gomez, David Platas Iglesias, Carlos Señaris Rodriguez, Maria Antonia	E-mail	j.bermudez@udc.es david.esteban@udc.es carlos.platas.iglesias@udc.es m.senaris.rodriguez@udc.es	
Web				
General description	"Crystallography and Symmetry" is a subject of the second semester of the first year of the Degree in Nanoscience and Nanotechnology, which belongs to the Basic Training Module. This course aims at training students on knowing and learning to apply the fundamentals of point symmetry and spatial symmetry, become familiar with the world of crystals, with the most common structures of crystalline solids, with X-ray diffraction as a tool for characterizing solids, as well as with the relationship between crystallography and symmetry with other disciplines. These knowledge and skills will provide the theoretical and practical foundations necessary for the student to delve into the world of crystalline nanomaterials and their characterization by diffractometric and spectroscopic methods, in subsequent subjects of the degree in Nanoscience and Nanotechnology.			

Contingency plan	1. Modifications to the contents In principle, the contents of the course will be fully maintained. If necessary, for reasons of force majeure, a more general presentation of the contents of the course may be chosen, which in any case will cover all the most relevant aspects of the subject. 2. Methodologies *Teaching methodologies that are maintained The methodologies will be maintained but will be carried out in ?Online mode?, that is, using the ICT tools available to the Institution. In the event that part of the students cannot connect and follow the classes in real time, asynchronous means will be used (email, recordings of the expository sessions, more personalized tutorials ...). *Teaching methodologies that are modified The objective tests will be online tests that will be carried out using Moodle or equivalent tools, keeping track of them by Teams. 3. Mechanisms for personalized attention to students Students will be tutored through the Teams platform or through corporate email. 4. Modifications in the evaluation If all the students can follow on-line teaching activities without difficulty, students will be evaluated in the same way as the classroom teaching. Students who cannot follow synchronous online activities will be evaluated through equivalent activities carried out asynchronously. *Evaluation observations: None. 5. Modifications to the bibliography or webgraphy There are no modifications in the bibliography / webgraphy In-person classes, in the event of a capacity limitation as a result of updates to the regulations, two classrooms will be assigned to the course. Students will follow the lectures delivered by the instructor in one room, or virtually through TEAMS in the second room.

Study programme competences	
Code	Study programme competences
A3	CE3 - Reconocer y analizar problemas físicos, químicos, matemáticos, biológicos en el ámbito de la Nanociencia y Nanotecnología, así como plantear respuestas o trabajos adecuados para su resolución, incluyendo el uso de fuentes bibliográficas.
A5	CE5 - Conocer los rasgos estructurales de los nanomateriales, incluyendo las principales técnicas para su identificación y caracterización
A6	CE6 - Manipular instrumentación y material propios de laboratorios para ensayos físicos, químicos y biológicos en el estudio y análisis de fenómenos en la nanoescala.
A7	CE7 - Interpretar los datos obtenidos mediante medidas experimentales y simulaciones, incluyendo el uso de herramientas informáticas, identificar su significado y relacionarlos con las teorías químicas, físicas o biológicas apropiadas.
A8	CE8 - Aplicar las normas generales de seguridad y funcionamiento de un laboratorio y las normativas específicas para la manipulación de la instrumentación y de los productos y nanomateriales.
B4	CB4 - Que los estudiantes puedan transmitir información, ideas, problemas y soluciones a un público tanto especializado como no especializado
B6	CG1 - Aprender a aprender
B7	CG2 - Resolver problemas de forma efectiva.
B8	CG3 - Aplicar un pensamiento crítico, lógico y creativo.

C3	CT3 - Utilizar las herramientas básicas de las tecnologías de la información y las comunicaciones (TIC) necesarias para el ejercicio de su profesión y para el aprendizaje a lo largo de su vida
C7	CT7 - Desarrollar la capacidad de trabajar en equipos interdisciplinares o transdisciplinares, para ofrecer propuestas que contribuyan a un desarrollo sostenible ambiental, económico, político y social.
C8	CT8 - Valorar la importancia que tiene la investigación, la innovación y el desarrollo tecnológico en el avance socioeconómico y cultural de la sociedad

Learning outcomes			
Learning outcomes	Study programme competences		
Identify the main crystal forms, structures and systems.	A3 A5 A7	B6 B7 B8	C3 C8
Differentiate the main elements of symmetry and their nomenclature.	A5	B4	C3
Recognize the fundamentals of diffraction.	A3 A6 A8		C3 C7 C8
Solve basic crystallography problems.	A3 A5 A7	B7 B8	C3

Contents	
Topic	Sub-topic
Unit 1. Introduction.	Introduction to the world of crystals and symmetry. Its relevance in the field of nanoscience and nanotechnology.
Unit 2. Symmetry elements and operations.	Reflection, proper rotation, identity operation, inversion operation, improper rotation. Schönflies and Hermann-Mauguin notation. Exercises and problems.
Unit 3. Point symmetry groups.	Combination of elements and symmetry operations. Point symmetry groups. Character tables. Applications of point symmetry and group theory to solve simple problems.
Unit 4. Symmetry of crystals (I).	Introduction. Morphology and crystalline forms. Crystal systems. Crystal lattices. Unit cell. Bravais lattices. Miller indexes.
Unit 5. Symmetry of crystals (II).	Interaction of point symmetry and translation. Helical axes and sliding planes. The 230 space groups. Asymmetric unit coordinates, general, equivalent and special positions. Space group tables. Exercises and problems.
Unit 6. Common structures of crystalline solids	Packaging of rigid spheres model. Metal structures. AB structures: NaCl, CsCl, ZnS, NiAs. AB2 structures: TiO2, CaF2. Other structures of interest.
Unit 7. Introduction to X-ray diffraction.	Basic concepts of radiation-matter interaction. Bragg's law. X-ray powder diffractograms and their utility in the study of crystalline solids.

Planning				
Methodologies / tests	Competencies	Ordinary class hours	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A3 A5 A7 B4 B7 B8 C8	28	42	70
Laboratory practice	A5 A6 A7 A8 B6 B7 B8 C3 C7	12	12	24
Workshop	A5 B6 C7	4	14	18
Mixed objective/subjective test	A3 A5 A7 B4 B7 B8 C8	3	18	21

Objective test	A3 A5 A7 B4 B7 B8 C8	1	0	1
Seminar	A3 A5 C3 C7	3	12	15
Personalized attention		1	0	1
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	**Description**
Guest lecture / keynote speech	Lectures will be used to deliver the main the contents of each unit of the course, highlighting their most important aspects and paying particular attention to the fundamental concepts and / or those that are most difficult for students to understand. Lectures are interactive sessions, in which students are expected to participate by asking questions and requesting clarification of ideas or concepts.
Laboratory practice	They will focus on the preparation and study of crystalline substances, as well as their characterization by X-ray diffraction, and the interpretation of the results obtained using computer programs. The students will prepare a laboratory notebook in which they will describe the work done in the laboratory and the analysis of the results, as well as the main conclusions.
Workshop	An eminently practical training activity designed with the aim of addressing those aspects of the subject that are most difficult to understand. The work will be carried out individually or in groups under the direction of the teaching staff.
Mixed objective/subjective test	Final exam that will be carried out in the date fixed by the faculty board. Its content will include development and test questions, as well as problem exercises that will be similar to those analyzed throughout the course. Its objective is to obtain an evaluation of the level of knowledge and competences reached by the students, as well as to evaluate their capacity to relate them and to obtain an overview of the subject.
Objective test	Periodically, students will carry out a series of short tests in the problem solving sessions, which will include multiple-choice or short-answer questions. These tests are conceived both for the evaluation of the degree of acquisition of competences and for the consolidation of the contents presented in the lectures. This activity will allow not only to monitor the evolution of the students, but will also serve to detect those aspects of the subject that present a greater difficulty of understanding.
Seminar	These sessions will be dedicated to the resolution of problems and questions by the students, with the guidance of the teaching staff. These problems will be facilitated sequenced over time in accordance with the contents discussed in the lectures, and will be made available to the students with enough time so they can work on them before the corresponding face-to-face session.

Personalized attention	
Methodologies	**Description**
Mixed objective/subjective test Laboratory practice Seminar Workshop Objective test Guest lecture / keynote speech	The proposed teaching methodology is based on the work of the student, who becomes the main responsible for the own educational process. In order to optimize the effort of the student and obtain guidance during the process, it is extremely important to achieve close and constant interaction between teacher and student. Through this interaction and the different evaluation activities, the teacher will be able to determine to what extent the student is achieving the objectives proposed in each thematic unit and guide them in this regard. This orientation will be carried out through individual interviews that will take place during the tutoring hours of the teacher and / or at the most convenient times for the students. Obviously, and apart from these tutorials proposed by the teacher, students will be able to attend tutorials at their own request as many times as they wish and at times that are most convenient for them.

Assessment			
Methodologies	**Competencies**	**Description**	**Qualification**
Mixed objective/subjective test	A3 A5 A7 B4 B7 B8 C8	A test containing multiple-choice questions, short- and long-answer questions and problems, which will be similar to those presented throughout the course.	60

Laboratory practice	A5 A6 A7 A8 B6 B7 B8 C3 C7	The following aspects of laboratory work will be evaluated: - Organization of work and safety. - Attitude, scientific curiosity and degree of involvement in work. - Quality in the interpretation of the results. - Quality of the final report (laboratory notebook).	20
Seminar	A3 A5 C3 C7	The responses of the students and their individual or group participation in the corresponding face-to-face activities will be graded. Occasionally, and at the request of the teacher, the student must deliver problem sheets that can also be evaluated.	5
Workshop	A5 B6 C7	The activities carried out in workshops and the quality and frequency of the participation of the students will be evaluated.	5
Objective test	A3 A5 A7 B4 B7 B8 C8	Periodically, students will take a series of short tests, with multiple- answer or short-answer questions, during the seminar sessions. These objective tests are designed both to assess the degree of skill acquisition and to strengthen the contents seen in the lectures. This activity will not only monitor the evolution of the students, but will also serve as a tool to detect those aspects of the course that present a greater difficulty in understanding.	10

Assessment comments

Passing the course requires a minimum of 50 points, and at the same time the condition of obtaining a minimum of 45% of the Mixed Test score and a minimum of 40% in laboratory practices must be met. In the event that the minimum score is not reached in any of them, if the sum of the set is greater than or equal to 50 points, a failing grade will be awarded (4.5 out of 10 points). Since assessment is based on a continuous assessment model, the progression of the students throughout the semester will be specifically evaluated, with a maximum of 1 point that can be added to the final grade. The evaluation cannot be positive if students did not attended all the laboratory classes. The student will not be graded if the participation in activities that contribute to the overall grade is below 25% of the overall activities. The "second chance in July" is understood exclusively as a second chance to take the mixed-test: a second mixed-test is taken, representing 50% of the grade. The grades obtained in the other activities carried out during the course will be added to this grade. The honors will be awarded mainly to students who pass the subject at the first opportunity. It will only be awarded on the "second chance" if your maximum number is not covered on the first opportunity.

Students who qualify for the "Part Time Dedication Recognition and Academic Waiver of Attendance" in accordance with UDC regulations, must attend laboratory practices. The final grade for these students will consist of two parts: the grade obtained in the laboratory practices, which will contribute 20% to the final grade, and the mixed test, which will compute for the remaining 80%. These rating percentages will apply to both opportunities. In the case of exceptional, objectionable and duly justified circumstances, the responsible teacher may totally or partially exempt any student from participating in the continuous assessment process. Students who are in this circumstance must pass a specific exam that leaves no doubt about the achievement of the subject's competences.

According to the "Regulations of the regime of dedication to the study of undergraduate students at the UDC" (Art.3.be 4.5) and the "Rules of evaluation, review and claims of the qualifications of undergraduate and master's studies (Art 3 and 8b), students with recognition of part-time dedication and academic exemption from the attendance exemption must be able to participate in a training methodology and associated teaching activities that allow them to achieve the training objectives and competencies of the course. Therefore, they will participate in a personalized orientation system and evaluation tutorials that will serve, on the one hand, to guide the student's autonomous work and monitor their progress during the course, and on the other hand, to assess the degree of development of competence achieved.

The waiver percentage will be set in a first interview with the students, once their personal situation is known. In this way, a schedule will be established for the orientation tutorials, and the number of problem solving workshops that will be evaluated using this methodology will be determined (every two seminars or workshop sessions will be evaluated using 1 tutorial). Once known, their number will be weighted over the total and the number of tutorials in which these students must participate will be established. All of them will be agreed with the students according to their availability, according to the schedule of contents of the course and specifying the delivery times of the different materials that can be evaluated (problem sheets and questions). This material will be delivered to the student in advance through the Moodle platform according to the schedule agreed in the initial interview.

The tutoring sessions will be used to discuss aspects associated with both the contents of the course and the review of the tasks submitted, in addition to carrying out small assessment tests to verify whether students take advantage of these activities.

Sources of information	
Basic	- Sands, Donald E. (1974). Introducción a la cristalografía. Barcelona, Reverté - Smart, Lesley (2012). Solid state chemistry : an introduction. Boca Raton: CRC Press - Kettle, Sidney F.A. (2007). Symmetry and structure readable group theory for chemists. Hoboken: John Wiley - Borchardt-Ott, Walter (2011). Crystallography : an introduction . Berlin, Springer - Dept. de Cristalografía y Biol. Estruc. , CSIC (2020). Crystalografía. - Hargittai, István (1995). Symmetry through the eyes of a chemist. New York : Plenum Press
Complementary	- Müller, Ulrich (2013). Relaciones de simetría entre estructuras cristalinas : aplicaciones de la teoría de grupos cristalográficos en cristaloquímica. Madrid - DAVID J. WILLOCK (2009). Molecular Symmetry. Willey - Huheey, James E. (1997). Química inorgánica : principios de estructura y reactividad, Capítulo 3. México: Harla - Giacovazzo, C (2011). Fundamentals of crystallography. Oxford ; New York : Oxford University Press

Recommendations
Subjects that it is recommended to have taken before
Chemistry: Structure and Bonding/610G04005
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
Advanced Crystallography/610G04042 Techniques of Characterisation of Nanomaterials 2/610G04030 Techniques of Characterisation of Nanomaterials 1/610G04025 Solid State/610G04022 Spectroscopy/610G04017
Other comments
Students are encouraged to take the course "Structure and Bonding" (610G04005) before this one.Green Campus Program - Faculty of Sciences To achieve an immediate sustainable environment and comply with point 6 of the "Environmental Declaration of the Faculty of Sciences (2020)", the documentary works carried out in this course:a.- They will be requested mainly in virtual format and computer support.b.- If paper is used:- Plastics will not be used.- Double-sided prints will be made.- Recycled paper will be used.- The preparation of drafts will be avoided.