UAB Universitat Autònoma de Barcelona

Solid State Chemistry

Code: 102507
ECTS Credits: 6

2025/2026

Degree	Type	Year
Chemistry	OT	4

Contact

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Teachers

Ramón Yáñez López

Teaching groups languages

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

Prerequisites

To have studied and passed the 3rd year course "Material Science"

Objectives and Contextualisation

"Solid State Chemistry" aims to expand the knowledge acquired with the obligatory subject of the third year "Material Science" by introducing significant concepts such as methods of preparation of materials and the physical properties of materials. Thus, at the beginning, the basic aspects of the synthesis of solid materials will be described, following with the study of their electrical, magnetic and optical properties. These properties will be related to their structural characteristics.

Competences

- Adapt to new situations.
- Be ethically committed.
- Communicate orally and in writing in one's own language.
- Learn autonomously.
- Manage, analyse and synthesise information.
- Manage the organisation and planning of tasks.
- Obtain information, including by digital means.
- Propose creative ideas and solutions.
- Reason in a critical manner

- Resolve problems and make decisions.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.
- Show initiative and an enterprising spirit.
- Show motivation for quality.
- Show sensitivity for environmental issues.
- Use IT to treat and present information.
- Use the English language properly in the field of chemistry.
- Work in a team and show concern for interpersonal relations at work.

Learning Outcomes

1. Adapt to new situations.
2. Be ethically committed.
3. Communicate orally and in writing in one's own language.
4. Describe the optical properties of materials and their most important applications.
5. Differentiate between the different types of solid electrical conductors and relate them with their structure, bonds and most important applications.
6. Distinguish the models of chemical bonding in solids and relate them with the physical and chemical properties of the same.
7. Interpret the magnetic behaviour of materials in accordance with their structure and bonds, and relate this with their most important applications.
8. Learn autonomously.
9. Manage, analyse and synthesise information.
10. Manage the organisation and planning of tasks.
11. Obtain information, including by digital means.
12. Propose creative ideas and solutions.
13. Read, analyse and extract information from texts in the English language on the different areas of the field of material chemistry.
14. Reason in a critical manner
15. Resolve problems and make decisions.
16. Show initiative and an enterprising spirit.
17. Show motivation for quality.
18. Show sensitivity for environmental issues.
19. Use IT to treat and present information.
20. Work in a team and show concern for interpersonal relations at work.

Content

6 ECTS: 31 hours of theory + 10 hours of exercises

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1. Chemical Bonding and Valence

- Hückel Theory of Molecular Orbitals and SALC
- Valence Bond Model
- First- and Second-Order Jahn-Teller Distortion
- Bond Valence

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2. Electronic Band Structure

- Band structure of a hydrogen atom chain

- Electronic structures of cyclic H molecules
- Translational symmetry and the Bloch function
- Quantum number *k*
- Visualization of crystal orbitals
- Band structure diagrams
- Density of States (DOS) plots
- Band structure of a chain of H_2 molecules
- Electrical and optical properties
- Metals, semiconductors, and insulators
- Direct vs. indirect band gap semiconductors
- Band structure representation in higher dimensions
- Two-dimensional crystal orbitals
- Three-dimensional crystal orbitals
- Band structures of two-dimensional materials
- Graphene
- Square lattice of CuO_2^{2-}
- Band structures of three-dimensional materials
- α-Polonium
- Diamond
- Elemental semiconductors
- Rhenium trioxide
- Perovskites

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3. Optical Materials

- Light, color, and electronic excitations
- Pigments, dyes, and gems
- Transitions between *d* orbitals (*d*-*a*-*d* excitations)
- Ligand field theory and crystal field theory
- Absorption spectra and spectroscopic terms
- Correlation diagrams
- Selection rules and absorption intensity
- Charge transfer excitations

- Ligand-to-metal charge transfer
- Metal-to-metal charge transfer
- Compound semiconductors
- Optical absorbance, band width, and color
- Electronegativity, orbital overlap, and band width
- Conjugated organic molecules
- Luminescence
- Photoluminescence
- Components of a phosphor
- Radiative return to the ground state
- Thermal quenching
- Lanthanide activators
- Non-lanthanide activators
- Energy transfer
- Sensitizers
- Concentration quenching and cross-relaxation
- Upconversion photoluminescence
- Electroluminescence
- Inorganic light-emitting diodes (LEDs)
- Organic light-emitting diodes (OLEDs)
- Materials for lighting
- Phosphors for fluorescent lamps
- Phosphor-converted white LEDs

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4. Dielectric and Nonlinear Optical Materials

- Dielectric properties
- Permittivity and dielectric susceptibility
- Polarization and Clausius-Mossotti equation
- Microscopic mechanisms of polarizability
- Frequency dependence of dielectric response
- Dielectric losses
- Dielectric polarizabilities and the additivity rule

- Crystallographic symmetry and dielectric properties
- Pyroelectricity and ferroelectricity
- Ferroelectricity in $BaTiO_3$
- Antiferroelectricity
- Piezoelectricity
- Local bonding considerations in non-centrosymmetric materials
- Second-order Jahn-Teller distortions with *d* cations
- Second-order Jahn-Teller distortions with s^2p cations
- Nonlinear optical (NLO) materials
- Nonlinear susceptibility and phase matching
- Notable materials for second harmonic generation (SHG):
    - KH_2PO_4
    - $KTiOPO_4$
    - Niobates and tantalates
    - Organic and polymeric NLO materials
    - Borates

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5. Magnetic Materials

- Magnetic materials and applications
- Physics of magnetism
- Bar magnets and atomic magnets
- Magnetic intensity, induction, energy, susceptibility, and permeability
- Unit systems in magnetism
- Types of magnetic materials
- Atomic origins of magnetism
- Electron motions contributing to magnetism and their quantization
- Atomic magnetic moments
- Magnetic moments of 3d ions in compounds
- Magnetic moments of 4f ions in compounds
- Note on magnetic moments of 4d and 5d metals in compounds
- Diamagnetism
- Paramagnetism

- Curie and Curie-Weiss paramagnetism
- Pauli paramagnetism
- Antiferromagnetism
- Superexchange interactions
- Ferromagnetism
- Ferromagnetic insulators and half-metals
- Ferromagnetic metals
- Superferromagnets
- Ferrimagnetism
- Frustrated systems and spin glasses
- Magnetoelectric multiferroics
- Molecular and organic magnets

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6. Conductive Materials

- Metals
    - Drude model
    - Free electron model
    - Fermi-Dirac distribution
    - Carrier concentration
    - Carrier mobility and effective mass
    - Fermi velocity
    - Scattering mechanisms
    - Band structure and conductivity of aluminum
    - Band structures and conductivity of transition metals
- Semiconductors
    - Carrier concentration in intrinsic semiconductors
    - Doping
    - Carrier concentrations and Fermi energies in doped semiconductors
    - Conductivity
    - p-n junctions
    - Light-emitting diodes and photovoltaic cells
    - Transistors

- Transition metal compounds
    - Electronic repulsion: Hubbard model
    - NaCl-type structure compounds
    - Perovskite structure compounds
- Organic conductors
    - Conductive polymers
    - Polycyclic aromatic hydrocarbons
    - Charge-transfer salts
- Carbon
    - Graphene
    - Carbon nanotubes

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7. Superconductivity

- Overview of superconductivity
- Properties of superconductors
- Origins of superconductivity and BCS theory
- Superconductors derived from C_{60}
- Molecular superconductors
- Perovskite superconductors: $BaBiO_3$
- Cuprate superconductors
    - La_2CuO_4 materials
    - $YBa_2Cu_3O_{7-\delta}$ ("YBCO" or "123") materials
    - Other cuprates
    - Electronic properties of cuprates
- Iron pnictides and related superconductors

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8. Energy Materials: Ionic Conductors, Mixed Conductors, and Intercalation Chemistry

- Electrochemical cells and batteries
- Fuel cells
- Conductivity in ionic compounds
- Superionic conductors
    - AgI: cationic superionic conductor
    - PbF_2: anionic superionic conductor

- Cationic conductors
    - Sodium beta-alumina
    - Other ceramic cationic conductors
    - Polymeric cationic conductors
- Proton conductors
    - Water-containing proton conductors
    - Acid salts
    - Perovskite proton conductors
- Oxide ion conductors
    - Fluorite-type oxide ion conductors
    - Perovskite and other oxide ion conductors
- Electrode materials for SOFCs and mixed conductors
- Intercalation chemistry and applications
    - Graphite intercalation chemistry
    - Lithium intercalation chemistry and battery electrodes
    - Lithium-ion batteries with oxide cathodes
    - Electrochemical characteristics of lithium batteries
    - Other electrode materials for lithium batteries

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Lectures	40	1.6	1, 8, 4, 5, 6, 7
Type: Supervised			
Tutorial	6	0.24	1, 8, 16, 17, 4, 5, 6, 9, 10, 7, 13, 2, 18, 11, 12, 14, 15, 20, 19
Type: Autonomous			
Preparation of work on the subject	18	0.72	1, 8, 16, 17, 4, 5, 6, 9, 10, 7, 13, 2, 18, 11, 12, 14, 15, 20, 19
Reading of texts	13	0.52	1, 8, 16, 17, 4, 5, 6, 9, 10, 7, 13, 2, 18, 11, 12, 14, 15, 20, 19
Study	65	2.6	1, 8, 16, 17, 4, 5, 6, 9, 10, 7, 13, 2, 18, 11, 12, 14, 15, 20, 19

The subject is given in the form of lectures and classroom practices. In addition, the students will have to do a bibliographical work and solve the questions posed by the teacher.

1) Lectures

Through the presentations of the teacher the student must acquire the own knowledge of this subject and complement them with the study of each subject treated with the help of the material that the professor provides through the Virtual Campus and the bibliography recommended The lectures will be open to the participation of the students, who will be able to ask the professor the questions and clarifications they need. The teacher can assign specific exercises or questions to the students to solve them (at home or in the classroom) and discuss them in the classroom. The presentations of the bibliographical works of the students will also be done in these classes and the participation of all the students will be invoked in the sessions of questions and discussions regarding the works.

2) Personal work
Students will be required to complete at least one assignment, problem set, evidence-based task and/or bibliographic research on topics proposed by the instructor.

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
Follow up assesments	25%	4	0.16	1, 8, 3, 16, 17, 4, 5, 6, 9, 10, 7, 13, 2, 18, 11, 12, 14, 15, 20, 19
Written exams	70	4	0.16	1, 8, 16, 17, 4, 5, 6, 7, 2, 18, 12, 14

Exams

For assessment purposes, the subject is divided into two parts.

Throughout the semester, two midterm exams will be administered, one for each part (ExP1 and ExP2), as well as a comprehensive make-up exam (ExG), all graded on a scale from 0 to 10.

Follow-up Work

During the semester, a number of follow-up assessments will be collected (individually or group-solved problems, short in-class quizzes, oral questions, etc.). The student will therefore obtain two follow-up scores (S1 and S2), which will be the weighted averages of the grades obtained in the follow-up activities for each part of the course.

Grades

Each part of the course will receive a grade (Not1 and Not2) calculated as:

- Not1 = 0.75 × ExP1 + 0.25 × S1
- Not2 = 0.75 × ExP2 + 0.25 × S2

The final grade (NF) will be calculated as:

- NF = (Not1 + Not2) / 2

To pass the course via the midterms, two conditions must be met:

1. The final grade (NF) must be ≥ 5.0
2. To be averaged, both ExP1 and ExP2 must be ≥ 4.5

If these requirements are not met, the student must take the make-up exam, which allows retaking one or both midterms, as the content of each part will be clearly separated and labeled (NotR1 and NotR2). The new final grade (NFR) will be calculated by replacing the ExP1 and/or ExP2 scores with those obtained in the make-up exam, ExR1 and/or ExR2.

To be eligible for the make-up exam, the student must have previously been assessed on activities that represent at least two-thirds of the total grade for the subject.

To pass the subject via the make-up exam, both of the following must be true:

1. The final grade (NFR) must be ≥ 5.0
2. To be averaged, both ExR1 and ExR2 must be ≥ 4.5

The final grade for the global exam is calculated as:

- NFR = (NotR1 + NotR2) / 2
- NotR1 = 0.75 × ExR1 + 0.25 × S1
- NotR2 = 0.75 × ExR2 + 0.25 × S2

Students who fail the course because they did not pass one of the sections, regardless of their overall average, will receive a maximum final grade of 4.5.

Students who pass the course through midterms but wish to improve their grade may take the global make-up exam, but they must complete the entire exam, i.e., both parts corresponding to each midterm. The grade from this exam will replace the average of the two midterms and will carry a weight of 85% (follow-up work grades cannot be recovered). In the global exam, students are not eligible for an "Honors Distinction" (Matrícula d'Honor).

Final grades of students who pass may be normalized from 0 to 10 (with a maximum grade of 10, preserving ranking order, and allowing for an increase of up to 1.5 points) in order to achieve a distribution among passing, good, excellent, and honors grades as deemed appropriate by the instructors.

If the student has only been assessed on a maximum of 33% of the activities and then withdraws, the final grade will be recorded as NOT EVALUABLE.

Single Assessment

Students who have opted for the single assessment modality must take a final exam covering the entire syllabus of the course. This will take place on the same day that students in the continuous assessment mode take the second midterm. The student's grade will be the score obtained on this exam.

If the final score is below 5, the student will have another opportunity to pass the course by taking the make-up exam, which will be held on a date set by the program coordination team. The student's grade will be the score obtained on this exam.

The same "Not Evaluable" criterion as for continuous assessment will apply.

Students must act honestly throughout the course. Dishonest behaviors (cheating, allowing others to cheat, or any action intended to distort an evaluation) in any follow-up activity or exam will result in a final grade of "Fail" with a score of 0 in the course, regardless of the other grades obtained. In particular, during written exams, mobile phones or any other telecommunication devices must be switched off and stored in bags or backpacks placed on the platform. If a student is found carrying any unauthorized device during an exam or follow-up test, they will be expelled from the room and receive a grade of "Fail" for the entire course.

Bibliography

R. J. D. Tilley "Understanding Solids" 2013, JohnWiley & Sons Ltd

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W.D. Callister "Introducción a la Ciencia e Ingenieria de Materiales" Reverté

D. R. Askeland "Ciencia e Ingeniería de Materiales" Paraninfo

A. R. West; Basic Solid State Chemistry; "Solid State Chemistry and its Applications" (Second edition) Wiley&Sons ISBN: 978-1-119-94294-8

L. E. Smart, E. A. Moore; "Solid State Chemistry: An Introduction" (Fourth Edition); CRC Press; ISBN-10: 1439847908

Software

None

Groups and Languages

Please note that this information is provisional until 30 November 2025. You can check it through this link. To consult the language you will need to enter the CODE of the subject.

Name	Group	Language	Semester	Turn
(TE) Theory	1	Catalan	second semester	morning-mixed