

**COURSE DATA****Data Subject**

Code	44417
Name	Introduction to the Master on Molecular Nanoscience and Nanotechnology: Basic concepts
Cycle	Master's degree
ECTS Credits	6.0
Academic year	2023 - 2024

Study (s)

Degree	Center	Acad. year	Period
2208 - M.D. in Molecular Nanoscience and Nanotechnology	Faculty of Chemistry	1	First term

Subject-matter

Degree	Subject-matter	Character
2208 - M.D. in Molecular Nanoscience and Nanotechnology	1 - Introduction to the Master's Degree in molecular nanoscience and nanotechnology: Basic concepts	Obligatory

Coordination

Name	Department
CORONADO MIRALLES, EUGENIO	320 - Inorganic Chemistry

SUMMARY

The objective of this subject is to ensure that all the students share a certain degree of knowledge on Chemistry and Physics needed to understand the basic concepts of Nanoscience, regardless of the previous training that could have previously acquired.

PREVIOUS KNOWLEDGE



Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

There are no specified enrollment restrictions with other subjects of the curriculum.

OUTCOMES

2208 - M.D. in Molecular Nanoscience and Nanotechnology

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- To possess the necessary knowledge and abilities to continue with future studies in the PhD program in Nanoscience and Nanotechnology.
- For students from field of knowledge (e.g. chemistry) to be able to scientifically communicate and interact with colleagues from another field (e.g. physics) in the resolution of problems laid out by the Molecular Nanoscience and Nanotechnology.
- To know the fundamentals of solid state physics and supramolecular chemistry necessary on molecular nanoscience.
- To know the methodological approaches used in Nanoscience.

LEARNING OUTCOMES

The objective of this subject is to ensure that all the students share a certain degree of knowledge on Chemistry and Physics needed to understand the basic concepts of Nanoscience, regardless of the previous training that could have previously acquired. This is necessary since most of the students would have a degree in scientific or technological topics such as Biology, Biochemistry or Chemical Engineering, alongside Physics and Chemistry, and the objectives and contents of their education can be very different from each other.

Students following this course must:

1. Acquire the capacity to use the basic language to describe the structure and chemical bonding or organic and inorganic molecules, including non-bonding intermolecular interactions.



2. Acquire the capacity to use the basic language of Theoretical and Computational Chemistry relative to the previous item.
3. Acquire basic knowledge on the computation of thermodynamical properties from statistical concepts.
4. Acquire the capacity to use the basic language of structure and bonding in Solid State Physics.
5. Acquire the capacity to use the basic language to describe the electronic structure of solid systems
6. Acquire the capacity to use the basic language of Physical Optics in relation with the interactions between the electromagnetic radiation and solid systems.
7. Acquire the capacity to use the basic language to describe electric and magnetic properties of materials.

DESCRIPTION OF CONTENTS

1. Basics concepts in chemistry

1. Principles of reactivity: Chemical equilibria (4 hours)
 - 1.1. General concepts in aqueous solutions
 - 1.2. Introduction to acid-base, oxidation-reduction, complex formation and precipitation reactions
2. Coordination Chemistry (9 hours)
 - 2.1 Introduction
 - 2.2. Structures of the coordination compounds
 - 2.3 Bond theory
 - 2.4. Kinetics and reaction mechanisms in coordination compounds
3. Organic Chemistry (9 hours)
 - 3.1. Constitution of organic compounds: hydrocarbon backbone and functional groups. Basic rules of nomenclature. Basic concept on stereochemistry: Chirality and optical activity. Conformation and configuration. Enantiomers and diastereoisomers.
 - 3.2. Electronic delocalization. Resonance. Aromaticity. Acid-base properties of organic compounds. Structure-acidity relationship.
 - 3.3. 3D structure: Stereochemistry and chirality.
4. Structure determination (4 hours)
 - 4.1. Concepts on symmetry. Symmetry groups.
 - 4.2. Vibrations in molecules. Infrared and Raman spectroscopies. IR spectra of organic and inorganic compounds. Characteristic vibration zones. Factors controlling frequency groups. Main functional groups and characteristic frequencies. Hydrogen bonding. Characteristic frequencies of coordination and organometallic compounds. Ligand coordination. Stereochemistry around a central atom.
 - 4.3. Other spectroscopies and spectrometries. Nuclear Magnetic Resonance (NMR) spectroscopy. General aspects. Basic description of NMR phenomena. Chemical shift. Mass Spectrometry. Fundamentals. Experimental techniques in mass spectrometry.

**2. Basics concepts in physics.**

1. Crystal structure and reciprocal space (6 hours)
 - 1.1. Interactions among the atoms in a solid
 - 1.2. Crystal structure: unit cell and Bravais lattices.
 - 1.3. Diffraction techniques and reciprocal space
2. Vibrations in molecules and crystals (4 hours)
 - 2.1. Small oscillations around the equilibrium
 - 2.2. Normal vibrational modes in molecules
 - 2.3. Infinite systems. Wave equation. Phonons in crystals.
 - 2.4. Damped and forced oscillations. Resonances.
3. Electronic structure of solids (8 hours)
 - 3.1. Introduction to Quantum Physics. Wave function. Operators and states. Probability amplitudes. Schrödinger equation.
 - 3.2. Quantum confinement and bound states.
 - 3.3. Bands in solids. Effective mass. Density of States.
4. Electromagnetism in materials (8 hours)
 - 4.1. Electric and magnetic forces on charges in motion
 - 4.2. Electrostatics: Gauss Law.
 - 4.3. Magnetostatics: Amperes Law
 - 4.4. Electromagnetic induction: Faradays law.
 - 4.5. Maxwell equation and electromagnetic waves.
 - 4.6. Dielectric constant and electric polarization in materials: Conductors and dielectrics.
 - 4.7. Magnetic susceptibility and magnetic properties of solids
5. Physical properties of solids (4 hours)
 - 5.1. Charge transport: Drudes model and Ohms law.
 - 5.2. Optical properties of solids. Absorption and emission of light. Interband transitions. Plasmons.
 - 5.3. Mechanical properties of solids. Elasticity and Youngs modulus.
 - 5.4. Seminar

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Seminars	12,00	100
Tutorials	8,00	100
Development of group work	60,00	0
Preparing lectures	30,00	0
TOTAL	150,00	



TEACHING METHODOLOGY

Theory classes, participatory lectures

Articles discussion.

Chaired debate or discussion.

Practical cases or seminar problems discussion.

Seminars.

Individual works development.

EVALUATION

EVALUATION

Attendance and active participation in seminars.	10-20%
Continuous evaluation.	10-20%
Questions answering	10-20%
Individual work development.	60-70%

REFERENCES



Basic

- R.H. Petrucci. QUIMICA GENERAL : PRINCIPIOS Y APLICACIONES MODERNAS 11. Ed. Pearson. 2017
Guía docente M1 - 54070 pág. 10
Martin Silberberg, Patricia Amateis . Chemistry: The Molecular Nature of Matter and Change 8th Edition. 2017. MacGrawHill. 2017. ISBN1259631753
L Cademartiri, G. A. Ozin, Principles of Nanochemistry John Wiley & Sons, 2009 .
P.J. Collings, Liquid Crystals: Naturers delicate of Mater. 2ª Ed., Princenton University Press, 2002.
E.H Wichmann, B.P.C. Física cuántica (Curso de Física de Berkeley) · 2020
C. Kittel, P. McEuen ·Introduction to Solid State Physics. Wiley. 2018
Ulman, An Introduction to Ultrathin Organic Films: from Langmuir-Blodgett to Self-Assembly, Academic Press, San Diego, 1991.
Allen J. Bard, Integrated Chemical Systems: A Chemical Approach to Nanotechnology, Wiley, John & Sons,1994.
Nanoscopic Materials. Emil Roduner. RSC Publishing, 2006

Additional

- (UT 1.1) Petrucci. Química general e inorgánica.Tomo 1
(UT 1.2) Glen E. Rodgers. Química Inorgánica. Introducción a la Química de la Coordinación, del estado sólido y descriptiva. Capítulos 1 a 5
(UT 1.3.) J. E. McMurry, Organic Chemistry, 8th Edition; Brooks/Cole, 2012
P. Y. Bruice, Química Orgánica, 8ª Edición; Pearson-Prentice Hall, México, 2008
(UT 1.4.) Spectrometric Identification of Organic Compounds, R.M. Silverstein, F.X. Webster, D. Kiemle, 7th Ed., John Wiley and Sons, 2004.Infrared and Raman Spectra of Inorganic and Coordination Compounds, K. Nakamoto, 6th Ed., John Wiley and Sons, 2009. Libro de tablas: Determinación Estructural de Compuestos Orgánicos. E. Pretsch, P. Bühlmann, C. Affolter, A. Herrera, R. Martínez, Editorial Masson, Barcelona, 2004.