

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

<b>Código</b>	44417
<b>Name</b>	Introducción al máster en nanociencia y nanotecnología molecular: Conceptos básicos
<b>Cycle</b>	Master's degree
<b>ECTS Credits</b>	6.0
<b>Curso académico</b>	2016 - 2017

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. year</b>	<b>Period</b>
2208 - M.U. en Nanociencia y Nanotecnología Molecular	FACULTY OF CHEMISTRY	1	First term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
2208 - M.U. en Nanociencia y Nanotecnología Molecular	1 - Introduction to the Master's Degree in molecular nanoscience and nanotechnology: Basic concepts	Obligatory

**Coordination**

<b>Name</b>	<b>Department</b>
CORONADO MIRALLES, EUGENIO	320 - QUÍMICA INORGÁNICA

**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

### 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 of 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
<b>TOTAL</b>	<b>150,00</b>	

**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

- G.A. Ozin, A.C. Arsenault: Nanochemistry. The Royal Society of Chemistry, 2005.
- P.J. Collings, Liquid Crystals: Nature's delicate order of Matter. 2<sup>a</sup> Ed., Princeton University Press, 2002.
- 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.
- (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, 8<sup>a</sup> 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.