

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

<b>Code</b>	44611
<b>Name</b>	Nanochemistry and supramolecular chemistry
<b>Cycle</b>	Master's degree
<b>ECTS Credits</b>	5.0
<b>Academic year</b>	2018 - 2019

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. year</b>	<b>Period</b>
2218 - M.U. en Química	Faculty of Chemistry	1	Second term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
2218 - M.U. en Química	6 - Nanochemistry and supramolecular chemistry	Optional

**Coordination**

<b>Name</b>	<b>Department</b>
ROMERO MARTINEZ, FRANCISCO MANUEL	320 - Inorganic Chemistry

**SUMMARY**

The field *Nanochemistry and Supramolecular Chemistry* is represented by an optional 5 cr. subject, which is included in the academic/research programme of the Master of Chemistry. It is scheduled in the second semester. After the study of the basic aspects of Supramolecular Chemistry in the Advanced Chemistry module (1st semester), this subject concerns essentially Nanochemistry and some additional topics of Supramolecular Chemistry related to the nanoworld.

The term nanochemistry was coined by Prof. Ozin (University of Toronto, Canada) as a "sub-discipline of solid state chemistry that emphasizes the synthesis...of preparing little pieces of matter with nanometer sizes in one, two or three dimensions." With respect to Physics and Engineering, where the nanometric size is reached by miniaturization and by fragmentation of macroscopic objects, Chemistry is already placed at the subnanometric scale in such a way that, starting from molecules, nanoscopic objects are built by assembly of smaller units. This assembly relies on the presence of intermolecular interactions at multiple length scales and Supramolecular Chemistry appears as a powerful conceptual tool for rationalizing these phenomena.



Why are we interested in the nanometric dimension? In nanomaterials, a vast majority of atoms lie at the surface and they are subject to interactions that are markedly different to those present in the bulk. This is why these materials show very remarkable physical (electronic, optic, magnetic, mechanic) properties that find important applications in the field of non-linear optics, photonics, or information storage and processing. Chemical properties are also very different for these nanoobjects in comparison with bulk substances, and these novel properties are relevant in areas such as catalysis, sensing or environmental issues.

Nanochemistry is already present in the consumer market, in products such as sunscreen lotions (TiO<sub>2</sub> nanoparticles), resistant and ultralight fibers (carbon nanotubes), new drugs, pollution studies, soil remediation, etc.

## 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 specific requirements to study this subject.

## OUTCOMES

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- Be able to solve complex chemistry problems, whether in the academic, research or industrial application areas at a specialization or masters-level.
- Possess the necessary skills to develop multidisciplinary activities within the field of chemistry at the master's level.
- Be able to design, perform, analyse and interpret experiences and complex data in the environment of chemistry at a specialization level.
- Acquire advanced knowledge to assess the importance of chemistry in health, the environment, new materials and energy.
- Acquire the necessary advanced knowledge to assess the importance of chemistry in economic and social development in a context of specialization.

## LEARNING OUTCOMES

- Know the fundamental aspects of nanochemistry and supramolecular chemistry.
- Know the methods of synthesis of nanomaterials.
- Understand the physical and chemical properties of nanomaterials.
- Establish the applications of the nanoworld in: architecture and civil engineering, cosmetics, adhesives, coatings, medicine, and in the preservation and restoration of artistic and cultural heritage.



- Know how to choose the most appropriate technique for the analysis of nanomaterials.
- Describe the main techniques of preparation of samples for the identification and quantification of nanomaterials in different matrices of interest (industrial, environmental).
- Know the applications of supramolecular chemistry: transport, catalysis, sensors and molecular machines.

## DESCRIPTION OF CONTENTS

### 1. Supramolecular Chemistry

- 1.1.- Recognition of neutral molecules. Cyclodextrins and cucurbiturils. Molecular tweezers. Cyclophanes. Molecular covalent cavities and capsules. Carcerands and hemicarcerands. Dendrimers.
- 1.2.- Chemosensors and optical and electrochemical dosimeters. Design. Mechanisms of recognition-transduction to a macroscopic signal. Application examples.
- 1.3.- Molecular self-assembly via template effect. Kinetic and thermodynamic considerations. Types of templates. Hydrophobic effect. Helicates, grids, catenanes and rotaxanes, molecular knots and boxes.
- 1.4.- Supramolecular devices. Switching systems. Molecular machines based on rotaxanes and catenanes. Interface between molecular and macroscopic worlds: anchoring of supramolecular systems on surfaces.

### 2. Inorganic nanoparticles and nanorods

- 2.1.- Introduction to nanoparticle synthesis: processes of nucleation and growth. Importance of surface phenomena. Control over size and shape. Synthesis of silica and polydimethylsiloxane nanoparticles. Applications.
- 2.2.- Nanoparticles and nanorods of gold and other noble metals. Synthetic methods. Optical properties: surface plasmon resonance. Anisotropy effects. Nanoparticles of cadmium selenide: quantum dots. Carbon nanoparticles.
- 2.3.- Nanoparticles and nanorods of metal oxides. Methods of synthesis of titania nanoparticles: optical and electronic properties. Applications. Iron oxide nanoparticles: preparation and magnetic properties. Ferrofluids.
- 2.4.- Carbon nanotubes. Synthesis and characterization. Mechanical and electrical properties.

### 3. Graphene and other 2D materials

- 3.1.- Synthesis and characterization of graphene: chemical vapour deposition (CVD) and chemical etching. Nanographene. Nucleation and vertical growth. Synthesis of aqueous dispersions of graphene. Functionalization of graphene: covalent and non-covalent chemistry. Graphene oxide. Graphene and hydrogenated graphene.
- 3.2.- Physicochemical properties and applications of graphene: electronic, magnetic, and transport properties. Electrochemistry of graphene and graphenoids. Applications in solar cells and energy conversion and storage. Graphene-based catalysis. Selective capture of CO<sub>2</sub>.
- 3.3.- Graphene analogues: silicene, germanene, stanene and phosphorene. Layers of inorganic materials (metal dichalcogenides, graphitic phase of ZnO, coordination polymers).



3.4.- Nanosheets of double hydroxides (LDH). Introduction. Preparation of LDH precursors. Size. Shape. Delamination of 3D LDH systems.

#### 4. Analytical control of nanomaterials

4.1.- Aims and types of tests: analysis of synthetic nanomaterials, intermediate and consumer products; analysis of nanomaterials in samples of biomedical and environmental interest. Qualitative analysis, quantitative analysis, characterization. Sample preparation: digestion; extraction, (ultra)centrifugation.

4.2.- Microscopy (TEM, SEM, AFM, otras) and spectrometric (XPS, Raman, DLS, fluorescencia, ET-AAS, ICP-AES e ICP-MS, UV/vis) techniques.

4.3.- Separation techniques (FFF, SEC, hydrodynamic chromatography, CE). Other techniques: voltammetric, microbalances, etc.

4.4.- Applications: food analysis, materials for healthcare and other consumer goods; analysis of environmental samples; nanotoxicity studies.

#### 5. Bionanochemistry

5.1.- Methods of bioconjugation of inorganic nanoparticles. The bio-nano interface. Protein corona. Cell internalization of nanoparticles. Pharmacokinetics and biodistribution. Imaging techniques of nanoparticles in vivo.

5.2.- Biomedical applications of inorganic nanoparticles in therapy and clinical diagnosis. Theranostics. Nanoparticles as vectors in drug delivery. Liposomal formulations. Biosensors. Tissue engineering.

5.3.- Nanomaterials toxicity. Mechanisms of action. Allergy and genotoxicity. Strategies for mitigation of adverse effects. Nanoparticles and environment.

5.4.- Case study: Analysis of companies in the bionano sector present in the consumer market or in advanced phases of clinical trials.

### WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Tutorials	5,00	100
Seminars	5,00	100
Development of individual work	15,00	0
Study and independent work	30,00	0
Readings supplementary material	10,00	0
Preparation of evaluation activities	20,00	0
<b>TOTAL</b>	<b>125,00</b>	





## TEACHING METHODOLOGY

The following teaching methodology will be applied for this subject:

- Lecture by teacher, including conducted class discussions.
- Seminars intended to solve practical exercises and examples of applications.
- Tutorials, aimed towards an individual assessment of the understanding of the subject by the students.

Besides, Aula Virtual (Moodle) platform will be used for communication and sharing of information inside the group.

## EVALUATION

Marks will be calculated as the weighted average of the scores obtained in the final exam (70%) and in the continuous assessment of activities related to this subject performed throughout the term (30%). A minimum mark of 4.5 must be achieved in the two parts.

There will be only one final exam, containing five questions, related to the five thematic units (UT) that appear in the programme.

## REFERENCES

### Basic

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- SUPRAMOLECULAR CHEMISTRY. F. Vögtle. John Wiley, New York, 1991.
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- CORE CONCEPTS IN SUPRAMOLECULAR CHEMISTRY AND NANOCHEMISTRY. J. W. Steed, D. R. Turner, K. Wallace, John Wiley & Sons, Chichester, 2007.
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- A TEXTBOOK OF NANOSCIENCE AND NANOTECHNOLOGY. T. Pradeep, McGraw Hill Education, New Delhi, 2012.



- ANALYTICAL CHEMISTRY: A MODERN APPROACH. R. Kellner, J. M. Mermet, M. Otto, M. Valcárcel, H. M. Widmer, Wiley-VCH, Weinheim, 2004.
- GRAPHENE. J. Warner, F. Schaffel, M. Rummeli, A. Bachmatiuk. Elsevier, 2012.

#### **Additional**

- CROWN ETHERS AND CRYPTANDS. G. Gokel, RSC Publishing, Cambridge, 1991.
- MACROCYCLIC CHEMISTRY. B. Dietrich, P. Viout, J.-M. Lehn, VCH, Weinheim, 1993
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- GOLD NANOPARTICLES FOR BIOLOGY AND MEDICINE. D. A. Giljohann, D. S. Seferos, W. L. Daniel, M. D. Massich, P. C. Patel, C. A. Mirkin, Angew. Chem. Int. Ed. 2010, 49, 3280.
- MAGNETIC NANOPARTICLES: DESIGN AND CHARACTERIZATION, TOXICITY AND BIOCOMPATIBILITY, PHARMACEUTICAL AND BIOMEDICAL APPLICATIONS. L. H. Reddy, J. L. Arias, J. Nicolas, P. Couvreur, Chem. Rev. 2012, 112, 5818-5878.