

## **COURSE DATA**

Data Subject		
Code	44611	
Name	Nanochemistry and supramolecular chemistry	
Cycle	Master's degree	
ECTS Credits	5.0	
Academic year	2019 - 2020	

Study (s)		
Degree	Center	Acad. Period
		year
2218 - M.U. en Química	Faculty of Chemistry	1 Second term

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

#### Coordination

Name Department

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 o 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, mecanic) 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 ( $TiO_2$  nanoparticles), resistent 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

Prior knowledge of chemistry is required, at the level taught in the qualifications listed in the recommended profile for admission of candidates to the Masters Degree.

### **OUTCOMES**

#### 2218 - M.U. en Química

- 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 aplications of the nanoworld in: architecture and civil engineering, cosmetics, adhesives, coatings, medecine, 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 tecniques of preparation of samples for the identification and quantification of nanomaterials in differents 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. Nanoparticles, nanorods and bidimensional materials

- 2.1.- Introduction to the synthesis of nanoparticles: nucleation and growth processes. Importance of surface phenomena. Control of form and size. Self-assembly. Defects. Synthesis of silica and polydimethylsiloxane nanoparticles. Applications.
- 2.2.- Gold nanoparticles. Synthesis methods. Optical properties: surface plasmon resonance. Effects of anisotropy. Nanoparticles of cadmium selenide: quantum dots.
- 2.3.- Nanoparticles of metal oxides. Methods of synthesis of iron oxide nanoparticles: preparation and magnetic properties. Ferrofluids.
- 2.4.- Carbon nanoforms. Surface effects. Shapes. Mechanical and electrical properties.
- 2.5.- Graphene analogues: Exfoliation methods. Boron Nitride. Transition metal dicalcogenides (TMDC). Oxides of transition metals. Semiconductors. Phosphorene.
- 2.6.- Nanosheets of double hydroxides (LDH). Introduction. Preparation of LDH precursors. Size. Shape. Delamination of 3D LDH systems.



#### 3. Analytical control of nanomaterials

- 3.1.- 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.
- 3.2.- Microscopy (TEM, SEM, AFM, otras) and spectrometric (XPS, Raman, DLS, fluorescencia, ET-AAS, ICP-AES e ICP-MS, UV/vis) techniques.
- 3.3.- Separation techniques (FFF, SEC, hydrodynamic chromatography, CE). Other techniques: voltammetric, microbalances, etc.
- 3.4.- Applications: food analysis, materials for healthcare and other consumer goods; analysis of environmental samples; nanotoxicity studies.

### 4. Bionanochemistry

- 4.1.- 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.
- 4.2.- Biomedical applications of inorganic nanoparticles in therapy and clinical diagnosis. Theranostics. Nanoparticles as vectors in drug delivery. Liposomal formulations. Biosensors. Tissue engineering.
- 4.3.- Nanomaterials toxicity. Mechanisms of action. Allergy and genotoxicity. Strategies for mitigation of advers effects. Nanoparticles and environment.
- 4.4.- 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
TOTAL	125,00	

## **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 a series of questions related to the four thematic units (UT) that appear in the programme.

The minimum overall grade to pass the subject will be 5.0.

### **REFERENCES**

#### **Basic**

- SUPRAMOLECULAR CHEMISTRY. J.W. Steed, J. L. Atwood. John Wiley & Sons, New York, 2000.
- SUPRAMOLECULAR CHEMISTRY. F. Vögtle. John Wiley, New York, 1991.
- SUPRAMOLECULAR ELECTROCHEMISTRY. A.E. Kaifer, M. Gómez-Kaifer. VCH, Weinheim, 1999.
- SUPRAMOLECULAR PHOTOCHEMISTRY. V. Balzani, F. Scandola, Ellis Harwood, New York, 1999.
- CORE CONCEPTS IN SUPRAMOLECULAR CHEMISTRY AND NANOCHEMISTRY. J. W. Steed, D. R. Turner, K. Wallace, John Wiley & Sons, Chichester, 2007.
- NANOCHEMISTRY. L. Cademartiri, G. A. Ozin, WILEY-VCH, Weinheim, 2009.
- CONCEPTS OF NANOCHEMISTRY. G. A. Ozin, A. Arsenault, L. Cademartiri, RSC Publishing, Cambridge, 2008.
- NANOMATERIALS CHEMISTRY. C. N. R. Rao, A. Müller, A. K. Cheetham, Wiley-VCH, Weinheim, 2007.
- 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
- INORGANIC NANOPARTICLES. Synthesis, Applications and Perspectives. C. Altavilla, E. Ciliberto, CRC Press, Boca Raton, 2007.
- Special Issue on CARBON NANOTUBES. Acc. Chem. Res. 2002, 35, 997-1113.
- HONEYCOMB CARBON: A REVIEW OF GRAPHENE. M. J. Allen, V. C. Tung, R. B. Kaner, Chem. Rev. 2010, 110, 132-145.
- INORGANIC ANALOGUES OF GRAPHENE. C. N. R. Rao, A. Nag, Eur. J. Inorg. Chem. 2010, 4244-4250.
- Z. Liu, R. Ma, M. Osada, N. Iyi, Y. Ebina, K. Takada, T. Sasaki, J. Am. Chem. Soc. 2006, 128, 4872-4880.
- R. Ma, Z. Liu, K. Takada, N. Iyi, Y. Bando, T. Sasaki, J. Am. Chem. Soc. 2007, 129, 5257-5263.
- ANALYTICAL METHODS TO ASSESS NANOPARTICLE TOXICITY. B. J. Marquis, S. A. Love, K. L. Braun, C. L. Haynes, Analyst 2009, 134, 425-439.
- COMPARATIVE ADVANTAGES AND LIMITATIONS OF THE BASIC METROLOGY METHODS APPLIED TO THE CHARACTERIZATION OF NANOMATERIALS. P. Linkok, M. Artemyev, A. E. Efimov, I. Nabiev, Nanoscale 2013, 5, 8781-8798.
- 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.

## **ADDENDUM COVID-19**

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

#### 1. Contents

The contents initially collected in the teaching guide are maintained.



Prior to March 13, 22 face-to-face sessions had been taught out of a total of 24, which means 91.7% of teaching. The remaining 2 sessions have been taught online.

## 3. Volume of work and temporary planning of teaching

Workload and time planning are maintained on scheduled days and times.

### 3. Teaching methodology

The teaching methodology indicated in the teaching guide is maintained. The face-to-face teaching is replaced by: Study of the material provided by the teachers in the Virtual Classroom, synchronous videoconferences, resolution of doubts in forums and email.

#### 4. Evaluation

The weight of this subject will be maintained in accordance with the provisions of the original teaching guide.

A) Exam: 70%

B) Continuous evaluation actions: 30%

In the case of not being able to make an in-person evaluation, the exams of the first and second calls will be carried out online using the means available for it.

### 5. Bibliography

The bibliography described to the students in the Teaching Guide is maintained. To this bibliography we must add the material that the teachers had uploaded to the Virtual Classroom. Students who do not have the books can access the Service online.