

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

Code	44611
Name	Nanochemistry and supramolecular chemistry
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2021 - 2022

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 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, 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 (TiO₂ 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

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 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. 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 adverse 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

Contents

The contents initially indicated in the teaching guide are maintained.

**Workload and temporary teaching planning**

Regarding the workload:

The different activities described in the Teaching Guide are maintained but the hours of dedication to each activity are changed, as shown in the following table:

ACTIVITY	Hours	% To be attended
Theory classes	40.00	70-100
Tutorials	5.00	70-100
Seminars	5.00	70-100
Study and independent work	75.00	0
TOTAL	125.00	

Regarding the temporary teaching planning:

The material to follow the theory/tutoring/classroom-seminar classes allows to continue the temporary teaching planning both in days and schedule, whether the teaching is face-to-face in the classroom or not.

Teaching Methodology

Theory courses: Theory classes and classroom tutoring will tend to the maximum possible face-to-face teaching, always respecting the health restrictions that limit the capacity of the classrooms to 50% of their usual occupation. Depending on the capacity of the classroom and the number of students enrolled, some of the students may need to follow the classes synchronously in an auxiliary classroom. If this situation arises, students will attend the main classroom or auxiliary classroom for weekly rotary shifts (preferably in alphabetical order). However, the rotation system will be fixed once the actual enrollment data is known, guaranteeing, in any case, that the percentage of face-to-face teaching of all students enrolled in the subject is the same.



The methodology used for non-face-to-face classes shall be:

1. Synchronously using virtual classroom tools (Teams, Blackboard ...)
2. Asynchronously using locut power-point presentations or other virtual classroom tools
3. Resolution of exercises and questionnaires

If there is a closure of the facilities for health reasons that totally or partially affects the classes of the course, they will be replaced by non-face-to-face sessions following the established schedules and using the tools of the virtual classroom.

Evaluation

The evaluation system described in the Teaching Guide of the subject in which the various evaluable activities have been specified as well as their contribution to the final grade of the subject is maintained.

If there is a closure of the facilities for health reasons affecting the development of any face-to-face evaluable activity of the subject, it will be replaced by a test of a similar nature that will be carried out in virtual mode using the computer tools licensed by the University of Valencia. The contribution of each evaluable activity to the final grade of the subject will remain unchanged, as set out in this guide.

References

The literature recommended in the Teaching Guide is maintained since it is accessible, and it is complemented by notes, slides and problems uploaded to the Virtual Classroom as material of the course.