

**COURSE DATA****DATA SUBJECT****Code:** 44421**Name:** Basic concepts of supramolecular chemistry**Cycle:** Master's Degree / Doctorate**ECTS Credits:** 3**Academic year:** 2026-27**STUDY (S)**

Degree	Center	Acad. year	Period
2208 - Master's Degree in Molecular Nanoscience and Nanotechnology	Facultat de Química	1	First quarter

**SUBJECT-MATTER**

Degree	Subject-matter	Character
2208 - Master's Degree in Molecular Nanoscience and Nanotechnology	Basic concepts of supramolecular chemistry	COMPULSORY

**COORDINATION**

CORONADO MIRALLES EUGENIO

**SUMMARY**

It is intended that students acquire the basic knowledge related to supramolecular chemistry as a tool in building complex systems from well-defined units, the bottom-up approach.

**PREVIOUS KNOWLEDGE****RELATIONSHIP TO OTHER SUBJECTS OF THE SAME DEGREE**

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

**OTHER REQUIREMENTS**

Previous knowledge of chemistry, physics or materials science as taught in the degrees indicated in the recommended entry profile to the master's degree is required. Previous knowledge of molecular nanoscience and nanotechnology as taught in the Introduction Module is required.

**COMPETENCES / LEARNING OUTCOMES**

**2208 - Master's Degree in Molecular 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.

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 acquire supramolecular chemistry conceptual concepts necessary for the design of new nanomaterials and nanostructures.

To acquire the conceptual knowledge about molecular systems self-assembly and self-organisation.

To know the main biological and medical application in this area.

To know the methodological approaches used in Nanoscience.

To possess the necessary knowledge and abilities to continue with future studies in the PhD program in Nanoscience and Nanotechnology.

**DESCRIPTION OF CONTENTS**

1. Basic concepts in supramolecular chemistry: Molecular materials and supramolecular chemistry, supramolecular interactions, non-covalent interactions nature; General concepts in supramolecular chemistry, hostguest chemistry, topology, selectivity, co-operativity and preorganization, Functional features of supramolecular species, recognition, reactivity and selective transport, molecular self-assembly and self-association: chemical and biological examples; Cation, anion and neutral molecules recognition, dendrimers.
2. Binding constants. Concept. Measurement of binding constant: techniques: absorption spectroscopy, NMR, other techniques. Stoichiometry, job plot.
3. Receptors, coordination and the Lock and Key Analogy. The chelate and macrocyclic effects. Preorganization and complementarity. Nature of supramolecular interactions. Host-Guest chemistry: Crown ethers, Lariat Ethers, Podands, Cryptands, Spherands. Solution behaviour. Interactions with Alkali Metals and Transition Metals.
4. Nanoparticle synthesis. Tensioactives: monolayers, micelles, vesicles and capsules.
5. Molecular devices: molecular dyads and switches, logical doors, sensors. Signal amplification and



## 1. Basic concepts of supramolecular chemistry.

1. Basic concepts in supramolecular chemistry: Molecular materials and supramolecular chemistry, supramolecular interactions, non-covalent interactions nature; General concepts in supramolecular chemistry, hostguest chemistry, topology, selectivity, co-operativity and preorganization, Functional features of supramolecular species, recognition, reactivity and selective transport, molecular self-assembly and self-association: chemical and biological examples; Cation, anion and neutral molecules recognition, dendrimers.

2. Binding constants. Concept. Measurement of binding constant: techniques: absorption spectroscopy, NMR, other techniques. Stoichiometry, job plot.

antenna effect. Supramolecular chemistry in two-dimensional materials: graphene and beyond.

## WORKLOAD

### PRESENCIAL ACTIVITIES

Activity	Hours
Tutorials	5,00
Theory	15,00
Seminar	4,00
Other activities	2,00
<b>Total hours</b>	<b>26,00</b>

### NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	0,00
Individual or group project	0,00
Independent study and work	0,00
Preparation of lessons	10,00
Preparation for assessment activities	39,00
Resolution of case studies	0,00
<b>Total hours</b>	<b>49,00</b>

## TEACHING METHODOLOGY

The classes of this subject will be taught, together with the rest of the basic module, intensively during 3 weeks in January and each year at a different university.

During the **theory classes**, the teaching staff will give an overview of the subject under study, emphasising new or particularly complex aspects. The necessary bibliographical sources will be indicated for students to study the subject in depth.

The **practical classes** of this subject will be devoted to the organisation of seminars in which problems related to the theoretical content will be posed and solved. Likewise, practical cases and other topics related to the subject will be discussed with the students.



During these hours of practical activities, as far as possible, visits to laboratories and facilities related to the contents of the theoretical classes will be organised. This includes visits to nanomaterials fabrication laboratories.

After the intensive face-to-face classes, the lecturers will ask students a series of **questions** about the contents of the course that the student will have to solve.

Professors will hold **tutorials** with the students to resolve any doubts and questions they may have. These tutorials will take place in person or remotely (email, videoconference, telephone, etc.) depending on whether the student and teacher are from the same or a different university.

Through all these activities, students will acquire the competences described in the corresponding section. The basic competences will be worked on above all during the seminars.

## EVALUATION

The acquisition of the competences of the subject will be assessed by means of a written exam based on the questions posed to the students. The mark for this exam will represent 90% of the final mark for the subject.

Student participation during the training activities will represent 10% of the final grade.

In order to pass the course, it will be necessary to have attended 80% of the face-to-face training activities.

## REFERENCES

- J.W. Steed, J.L. Atwood: Supramolecular Chemistry. Wiley, 2000.
- J.M. Lehn, J.L. Atwood, J.E.D. Davies, D.D. Macnicol, F. Vogtle, D.N. Reinhoudt: Comprehensive Supramolecular Chemistry: Supramolecular Technology. Pergamon, 1996.
- T. Scharader, A.D. Hamilton: Functional Synthetic Receptors, Wiley-VCH, 2005.
- V. Balzani, M. Ventura, A. Credi: Molecular Machines, Wiley-VCH, 2003
- Jorio, M. S. Dresselhaus, G. Dresselhaus. Carbon Nanotubes. Springer, 2008.
- F. Langa, J.F. Nierengarten. Fullerenes: Principles and Applications. RSC Publishing, 2nd. Ed.



2011.

- J. Steed, D. R. Turner, K. J. Wallace, Core Concepts in Supramolecular Chemistry and Nanochemistry. Wiley, 2007.
- H.-J. Schneider, A. Yatsimirsky, Principles and Methods in Supramolecular Chemistry Wiley, 2000.
- Supramolecular Chemistry: From Molecules to Nanomaterials, ed. P. Gale and J. Steed, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2012
- Modern Supramolecular Chemistry, Eds. F. DIEDERICH, P. J. STANG; R. R. - TYKWINSKI; Wiley-VCH, Weinheim, 2008.
- "Supramolecular Chemistry: Fundamentals and Applications" - Editor: Fritz Vögtle, Jean-Marie Lehn, Christoph Schmuck. Wiley-VCH, 2012.
- "Supramolecular Chemistry: From Biological Inspiration to Biomedical Applications" - Editor: Philip A. Gale, Jonathan W. Steed. Elsevier, 2010.
- "Introduction to Supramolecular Chemistry" - Editor: P. A. Cox. Royal Society of Chemistry, 2016.