

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

<b>Code</b>	44421
<b>Name</b>	Basic concepts of supramolecular chemistry
<b>Cycle</b>	Master's degree
<b>ECTS Credits</b>	3.0
<b>Academic year</b>	2023 - 2024

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. year</b>	<b>Period</b>
2208 - M.D. in Molecular Nanoscience and Nanotechnology	Faculty of Chemistry	1	First term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
2208 - M.D. in Molecular Nanoscience and Nanotechnology	5 - Basic concepts of supramolecular chemistry	Obligatory

**Coordination**

<b>Name</b>	<b>Department</b>
CORONADO MIRALLES, EUGENIO	320 - Inorganic Chemistry

**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

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

## OUTCOMES

### 2208 - M.D. in 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 possess the necessary knowledge and abilities to continue with future studies in the PhD program in 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.
- To know the methodological approaches used in Nanoscience.
- 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.

## LEARNING OUTCOMES

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.

## DESCRIPTION OF CONTENTS

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

## WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	15,00	100
Tutorials	5,00	100
Seminars	4,00	100
Other activities	2,00	100
Preparation of evaluation activities	39,00	0
Preparing lectures	10,00	0
<b>TOTAL</b>	<b>75,00</b>	

## TEACHING METHODOLOGY

- Theory classes, participatory lectures
- Articles discussion.
- Chaired debate or discussion.
- Practical cases or seminar problems discussion.
- Seminars.
- Problems.
- Laboratory practices and demonstrations and visit to installations.
- Experts conferences.
- Attendance to courses, conferences and round tables.

## EVALUATION

Written exam about the subject basic contents	70-90%
Attendance and active participation in seminars.	0-10%



Questions answering	10-20%
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## REFERENCES

### Basic

- 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.