

## COURSE SYLLABUS

### Chemistry of Molecular Materials

2324-2-F5401Q051

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#### Aims

objectives

Molecular materials are rapidly gaining momentum, both in terms of scientific research and technological applications. Aim of the course is to provide a detailed knowledge of the structure properties relationships ruling the behaviour of such materials, with particular emphasis on electronic, optical and optoelectronic properties.

Knowledge and understanding

At the end of the course the student:

1. Understands the concept of conjugation in organic materials and correlates the extension of conjugation with optical, electrical and optoelectronic properties
2. Understands the concept of non-covalent bond and is capable of understanding its influence in the solution and solid-state aggregation behavior of organic materials
3. Can distinguish between electron donating and electron accepting residues in organic molecules. Can reason on their influence on electrical, optical and optoelectronic properties.
4. Can design organic conjugated materials for a specific purpose, given a series of conditions defining the required behaviour

Applying Knowledge and understanding:

The student:

1. Knows the basic working principles of organic electro/optic modulators, thin film transistors, electrochromic devices, solar cells, oleds, luminescent solar collectors, photodetectors. Based on such knowledge, the student is capable of proposing strategies to improve the performances of the same.
2. Knows the working principle of organic photoresists and can apply the concept in most documented industrial and research applications of the same

3. Is capable of independently gathering additional information on any one of the topics described during classes.
4. Knows and critically evaluates the literature of the field.
5. Understands the peer reviewing process and is capable of providing a report in the peer reviewing spirit

#### Making judgments.

Given the structure of a conjugated molecule or polymer, the student is capable of qualitatively estimating the corresponding optical, electrical and optoelectronic properties. On the other end, given a certain function that an organic molecule is required to perform, the student can propose known and original organic derivatives in principle capable of performing it. The student is also capable of estimating the influence of the environment on the properties of isolated and aggregated molecules.

#### Communication skills.

The student is trained in the reading, understanding and summarizing of scientific literature. Particular emphasis is given to the capability of providing concise and complete information. The student possesses the specific terminology of the field, thus being in the position of discussing with counterparts possessing both a chemical and a physical/engineering background. He possesses a "problem solving" attitude.

#### Learning skills.

The Student is able to extend what has been learned in classes to case studies not covered during the course. He is in particular able to autonomously manage the wide literature dedicated to the conjugated materials. He knows the research tools of the dedicated literature, including patents.

## Contents

Non-covalent interactions and molecular aggregates and solids: dipole-dipole, ion-dipole, hydrogen bonding, coordinative bonding and van der Waals interactions. Examples of host-guest interactions in solution: crown ethers, coronands, cryptands, calixarenes and resorcinarenes, rotaxanes and catenanes. Materials for nonlinear optics: theoretical background. Molecular materials for optoelectronics. Push-pull derivatives and BLA model. Bulk materials (poled polymers and sol-gel, Langmuir-Blodgett films, self-assembled superlattices). Two-photon absorbing materials and related applications (up-converted lasing and imaging, optical limiting, 3D microfabrication). Synthesis and characterization of organic semiconductors. Transport properties in charge transfer complexes. Conducting polymers (polyacetylene, PPV, polyetherocycles). Electrochemical and oxidative polymerizations. Cross-coupling polymerizations.

Electrochromic materials and devices: background and design criteria for molecular and polymeric materials. Specific issues with device assembly. Materials for displays and lighting: Working principle and device architecture of OLEDs. Molecular materials polymeric materials. Solid state down-converting devices. Luminescent solar concentrators. Organic rechargeable batteries. Elements of organic materials for bioimaging and photodynamic therapy.

## Detailed program

The course is organized in class activities, guided reading activities and corresponding in-class discussion.

- Elements of conjugated materials design (building blocks)
- Elements of supramolecular chemistry (non-covalent interactions)
- Conjugated molecules and materials having Nonlinear Optical Behavior
- Photoresists
- Organic polymeric semiconductors and conductors
- Electrochromic materials

- Organic Field Effect Transistors
- Scientific literature and databases
- Luminescent solar collectors
- Photodynamic therapy
- Organic solar cells (DSSC, perovskite, bulk heterojunction)
- Charge transfer complexes
- Organic light emitting devices

Students are invited to take part to guided readings activities thus organized:

Homework – guided reading

- During classes you will have to repeat this exercise for few different papers
- Active discussions amongst fellow student in class will be organized.
- You will have to provide a referee report for a scientific paper that you assume is not in the final published form but rather at the submitted to the referees step

## Prerequisites

Molecular based materials require an interdisciplinary approach. Elements of

- Materials science
- Organic chemistry
- Inorganic chemistry
- Physical chemistry
- Medicinal chemistry, environmental chemistry, physics.... (depending on the application) could be required

## Teaching form

The course is organized as follows:

- 5 CFU of in class activities, guided reading activities and corresponding in-class discussion;
- 1 CFU of laboratory teaching

## Textbook and teaching resource

- Jonathan W. Steed, David R. Turner, Karl J. Wallace, Core Concepts in Supramolecular Chemistry and Nanochemistry, John Wiley&Son
- Nanoscale Science and Technology, R.Kelsal, I.Hamley, M.Geoghegan. John Wiley and Sons, Chichester, 2005
- Nanochemistry, G.A Ozin and A.C. Arsenault. Royal Society of Chemistry Publishing, Cambridge 2006.
- Kirk-Othmer encyclopedia of chemical technology (<http://onlinelibrary.wiley.com/book/10.1002/0471238961>)
- Annotated slides (on moodle)
- Registration of standard classes (on moodle)
- Video lessons (on moodle)

## **Semester**

second semester.

## **Assessment method**

- Single oral exam.
- Evaluation of the guided readings assignments

during the exam the student will have to answer general questions on the topics discussed in both standard and video lesson. Questions will focus on the capability to reorganize the concepts discussed in classes. Students will be encouraged to reason on the possible use of their notions in practical examples/applications.

## **Office hours**

generally in the afternoon between 14:30 and 17:30 but visits on appointment are strongly suggested.

## **Sustainable Development Goals**

AFFORDABLE AND CLEAN ENERGY | INDUSTRY, INNOVATION AND INFRASTRUCTURE

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