UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Chemistry of Molecular Materials

2627-2-F5402Q029

Aims

General objectives

Molecular materials are rapidly gaining ground, both in terms of scientific research and technological applications. The course aims to provide detailed knowledge of the relationships between the structure and properties that govern the behaviour of such materials, with particular attention to electronic, optical, and optoelectronic properties.

Knowledge and understanding

At the end of the course the student:

Understands the concept of conjugation in organic materials and correlates the extent of conjugation with optical, electrical and optoelectronic properties
Understands the concept of non-covalent bonds and can understand its influence on the aggregation state of molecules and polymers in the solid state and in solution
Can distinguish between electron donors and acceptors residues in organic molecules. Can reason about their influence on electrical, optical and optoelectronic properties.
Can design organic conjugated materials for a specific purpose, based on a set of conditions that define the required behaviour

Knowledge and ability of understanding

The student:

Knows the basic operating principles of organic electro/optical modulators, thin film transistors, electrochromic devices, solar cells, OLEDs, photodetectors, and organic batteries. Based on this knowledge, the student is able to propose strategies to improve their performance.
Can independently collect additional information on any of the topics described during the lessons.
Can design and modify a proposed molecular structure so that it can be applied in different devices.

Autonomy of judgment

Given the structure of a conjugated molecule or polymer, the student is able to qualitatively estimate the corresponding optical, electrical and optoelectronic properties. Conversely, given a certain function that a given organic molecule must perform, the student can propose organic derivatives known in literature and original capable of performing it. The student is also able to estimate the influence of the environment on the properties of isolated and aggregated molecules.

Communication skills

The student can provide concise and complete information. The student has the specific terminology of the field, so he is in a position to discuss with counterparts who have both a chemical and a physical/engineering background. He has a "problem-solving" attitude.

Learning skills

The student can extend what he has learned in the lectures to case studies not covered during the course. In particular, he can independently manage the vast literature dedicated to conjugated materials. He knows the search tools of the dedicated literature, including patents.

Contents

Elements of molecular design and identification of components in a conjugated material. Non-covalent interactions, aggregates and molecular solids: dipole-dipole, ion-dipole, hydrogen bond, coordinative bond and interactions between walls. Examples of guest-host interactions in solution: crown ethers, coronands, cryptands, calixarenes and resorcinarenes, rotaxanes and catenanes. Recall of light-matter interactions in organic systems. Materials for nonlinear optics: theoretical background. Molecular materials for optoelectronics. Push-pull derivatives and BLA model. Thin films (polar and sol-gel polymers, Langmuir-Blodgett films, self-assembled superlattices). Two-photon absorbing materials and their applications (lasers and imaging, optical limiting, 3D microfabrication). Synthesis and characterisation of organic semiconductors. Transport properties in charge-transfer complexes. Conducting polymers (polyacetylene, PPV, polyheterocycles). Electrochemical and oxidative polymerisations. Cross-coupling polymerisations.
Electrochromic materials and devices: basic and design criteria for molecular and polymeric materials. Specific problems with device assembly. Materials for displays and lighting: operating principle and architecture of OLEDs. Polymeric materials and molecular materials. Solid-state conversion devices. Materials for organic and hybrid solar devices. Organic rechargeable batteries and redox-flow systems. Elements of organic materials for bioimaging and photodynamic therapy.

Detailed program

The course is organized into classroom activities, guided reading activities, and interactive classroom activities based on molecular design analysis.

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

•Electrochromic materials
•Organic Field Effect Transistors
•Photodynamic therapy
•Organic solar cells (DSSC, perovskite, bulk heterojunction)
•Charge transfer complexes
•Organic light emitting devices

Guided readings activites of relevant literature works.
Design and critical analysis of molecular structures: the work will be carried out in groups in the classroom and specific structures of molecules will be proposed and analysed. The structures will then be modified cooperatively to modify their intended properties.

Prerequisites

Molecular based materials require an interdisciplinary approach. Elements of
•Materials science
•Organic chemistry
•Inorganic chemistry
•Physical chemistry

Teaching form

Teaching with different teaching approaches:

18 two-hour lectures, in person, Delivered Didactics
3 two-hour practical classes in person in delivered mode in the initial part aimed at involving students interactively in the next part. Mixed teaching.

Textbook and teaching resource

Textbooks:

- Introduction to Organic Electronic and Optoelectronic Materials and Devices. Sam-Shajing Sun and Larry R. Dalton (editors), 2017, Taylor & Francis Group
- Molecular Electronics: From Principles to Practice. Michael C. Petty, 2007, John Wiley & Sons
- Rechargeable Organic Batteries: Materials, Mechanisms, and Prospects. Yongzhu Fu, Xiang Li, Shuai Tang, Wei Guo, 2024 WILEY-VCH GmbH

Annotated slides (on Moodle)
Registration of standard classes (on Moodle)

Semester

Second semester (March-June)

Assessment method

INTERVIEW ON THE TOPICS DEVELOPED IN LESSONS ON THE EXAM TEXTS.

During the exam, the student will have to answer 3 general questions on the topics discussed in the lectures. The questions will focus on the ability to reorganize the concepts discussed in the lectures. Students will be encouraged to reason about the possible use of their notions in practical examples/applications. The exam will include a first question on a topic of the student's choice, and the other two questions will derive from the extension of the concepts exposed and reported on other topics covered in the course.

Grade < 18
Insufficient grade; minimum level of preparation not reached.

Score 18-21
Preparation on a limited number of topics from the course syllabus, with poor ability to discuss and analyze independently which only emerge in the oral exam as a result of the Lecturer's help and questions; presentation skills occasionally uncertain, vocabulary not always clear and accurate, sometimes incorrect, with very limited critical elaboration.

Score 22-24
Preparation on a good number of topics from the course syllabus, although not homogeneous, with sufficient ability to discuss and analyze independently, sometimes prompted by the Lecturer's questions; presentation skills sufficiently clear, generally correct vocabulary, although sometimes not accurate or clear, limited critical elaboration capabilities.

Score 25-27
Preparation on a wide range of topics covering the course syllabus, ability to conduct discussions and critical analysis with good autonomy and ability to apply knowledge to real cases, use of correct vocabulary and competence in the use of disciplinary language.

Score 28-30L
Complete and exhaustive preparation on the subjects of the course syllabus, ability to independently discuss and critically analyze the principal topics, ability to connect themes to real cases and to different contexts and disciplines, excellent capacity for critical and independent thinking, full mastery of disciplinary vocabulary, rigorous and articulate presentation skills, argumentation skills.

Office hours

9:30-12:30, on appointment.

Sustainable Development Goals

AFFORDABLE AND CLEAN ENERGY | INDUSTRY, INNOVATION AND INFRASTRUCTURE | RESPONSIBLE CONSUMPTION AND PRODUCTION | CLIMATE ACTION