UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Chemistry of Molecular Materials

2526-2-F5401Q051

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:

1. Understands the concept of conjugation in organic materials and correlates the extent of conjugation with optical, electrical and optoelectronic properties
2. 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
3. Can distinguish between electron donors and acceptors residues in organic molecules. Can reason about their influence on electrical, optical and optoelectronic properties.
4. 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:

1. 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.
2. Can independently collect additional information on any of the topics described during the lessons.
3. 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. Elements of organic materials for bioimaging and photodynamic therapy.

Detailed program

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

•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

Students are inveted to take part to guided readings activites thus organized:

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.

Practical laboratory activity

• The work will be carried out in groups in the laboratory and some activities related to the preparation and characterization of devices will be proposed, experimenting with some techniques seen during the classroom lessons.

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

Teaching with different teaching methods:

13 two-hour lecture, in person, Delivered Didactics
4 two-hour practical classes in person in delivered mode in the initial part aimed at involving students interactively in the next part. Mixed teaching.
3 lab activities for a total of eight-hour, in person, Interactive 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)
•H. Tian, G. Boschloo, A. Hagfeldt, Molecular Devices for Solar Energy Conversion and Storage, Springer, 2018 (https://doi.org/10.1007/978-981-10-5924-7)

•Annotated slides (on moodle)
•Registration of standard classes (on moodle)
•Video lessons (on moodle)

Semester

second semester.

Assessment method

•INTERVIEW ON THE TOPICS DEVELOPED IN LESSONS, ON THE EXAM TEXTS AND DISCUSSION ON THE LABORATORY ACTIVITIES.

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.

The following level of judgment is applied in relation to the following parameters:

1. Conceptual knowledge and understanding ability
2. Ability to apply knowledge and understanding
3. Communication and argumentation skills
4. Learning, self-assessment and self-regulation skills

Grade < 18
Knowledge and Understanding
The student only partially identifies the characteristics of the concepts. The connections between the concepts are fragmented and poorly supported by theoretical knowledge.
Ability to apply knowledge and understanding
The student identifies only some relevant elements in a phenomenon, without being able to integrate them into an organic analysis.
Communication and argumentation skills
In the oral exam, the student develops an essential argument, lacking logical articulation and characterized by numerous expository inaccuracies.
Learning, self-assessment and self-regulation skills
The student is able to reconstruct only some aspects of his/her learning and professional development path.

Score 18-22
Knowledge and Understanding
The student recognizes and returns most of the conceptual characteristics and is able to provide a relatively coherent explanation, although with some inaccuracies. Theoretical references are present but not always rigorously.
Ability to apply knowledge and understanding
The student is able to recognize a significant number of elements and provide a partial explanation, although highlighting some gaps in the analysis.
Communication and argumentation skills
In the oral exam, the student constructs a basic argument, with a minimal structure but with some inaccuracies.

Learning, self-assessment and self-regulation skills
The student demonstrates a basic awareness of his/her learning path, managing to trace essential connections between the formative experiences, although with some inaccuracies.

Score 23-27
Knowledge and Understanding
The student demonstrates an in-depth understanding of the conceptual characteristics. In the oral exam, the explanations are well-structured and supported by an adequate use of theoretical references.
Ability to apply knowledge and understanding
The student accurately identifies the essential elements of a phenomenon. The application of knowledge occurs with a methodological rigor that is not always solid.
Communication and argumentative skills
In the oral exam, the student develops a coherent and well-organized argument, demonstrating good command of the language and a solid logical-argumentative structure. Communication is clear and effective.
Learning, self-assessment and self-regulation skills
The student analyzes his/her learning path in a clear and structured way, highlighting significant relationships between the different evolutionary stages and demonstrating a good capacity for critical reflection.

Score 28-30
Knowledge and Understanding
The student demonstrates a complete mastery of the concepts, articulating complex connections and providing exhaustive explanations. Theoretical references are used with relevance and rigor.
Ability to apply knowledge and understanding
The student demonstrates an advanced ability to analyze a phenomenon, identifying and interpreting all the salient elements in an exhaustive manner. The application of knowledge occurs with methodological rigor, supported by a solid and articulated argument.
Communication and argumentative skills
In the oral exam, the student develops a solid and articulated argument, with a rigorous logical structure and a high level of textual coherence. The speech is fluid and well-structured.
Learning, self-assessment and self-regulation skills
The student demonstrates an advanced ability to self-reflect, developing a detailed and in-depth analysis of his/her own learning and professional development path. The connections between training experiences and theoretical concepts are clear, coherent and rigorous.

Office hours

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

Sustainable Development Goals

QUALITY EDUCATION | AFFORDABLE AND CLEAN ENERGY | INDUSTRY, INNOVATION AND INFRASTRUCTURE