UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Chemistry of Molecular Materials

2425-1-FSM01Q006

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 optoelectronical 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 optoelectronical 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 optoelectronical 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 ang 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 walls interactions. Examples of host guest interactions in solution: crown ethers, coronands, criptands, calixarenes and resorcinarenenes, rotaxanes and catenanes. Materials for nonlinearoptics: 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-phonton 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 devices assembly. Materials for displays and lighting: Working principle and device architecture of OLEDS. Molecular materials polymeric materials. Solid state down converting devices. Materials for organic solar cells. 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 laboratory activities.

•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
•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:

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

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:

11 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 four-hour lab activities, 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)
•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