COURSE DATA

Data Subject	
Code	44614
Name	Advanced materials
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2019 - 2020

Study (s)

Degree	Center	Acad. year	Period
2218 - M.U. en Química	Faculty of Chemistry	1	First term

Subject-matter

Degree	Subject-matter	Character
2218 - M.U. en Química	9 - Advanced materials	Optional

Coordination

Name	Department
ORTI GUILLEN, ENRIQUE	315 - Physical Chemistry

SUMMARY

The course name, Advanced Materials, refers to polymeric and molecular materials used in the field of Molecular Electronics for the development of organic-based electronic and optoelectronic devices. The field of Molecular Electronics emerges in the 1970s as a consequence of the discovery of electrically conducting polymeric and molecular organic materials and nowadays it represents a real alternative to conventional electronics based on metallic and semiconducting inorganic materials. Organic electroactive materials have the advantage that they combine the benefits of molecular systems (nanoscopic size, low specific weight, high synthetic versatility, transparency, plasticity, processability, biocompatibility, …) with the electrical and optical properties of inorganic metals and semiconductors.

The objective of the course is to provide a general view of:

1) The different types of electrically conducting conjugated organic materials (both, molecular and polymeric). These materials include: a) complexes and charge transfer salts, b) pi-conjugated oligomers and polymers, mainly conducting polymers such as polyacetylene or polythiophene, c) pi-conjugated macrocycles, such as phthalocyanines, and d) carbon nanostructures that include materials such as fullerenes, nanotubes and graphene.

2) The structural, electronic, optical, and charge transport properties of these materials. To facilitate the understanding of these properties, some concepts will be reviewed: a) the electronic structure and chemical bond in carbon-based, pi-conjugated systems, ranging from orbitals in molecular systems to the band theory in polymeric systems, b) the interaction with light and, specially, electronic spectroscopy, and c) the supramolecular organization and the intermolecular interactions.

3) The main applications in electronic/optoelectronic devices that derive from these materials. The principles that govern the electroluminescent devices and transform electricity in light (OLEDs), and the different types of solar cells used to transform light in electrical energy will be explained. Nowadays, OLEDs are a commercial reality because they are present in screens of electronic devices of all types, such as mobile phones and TVs. Organic or hybrid (combining organic and inorganic materials) solar cells are being intensely researched as a realistic alternative to silicon cells.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

Prior knowledge of chemistry is required, at the level taught in the qualifications listed in the recommended profile for admission of candidates to the Masters Degree.

OUTCOMES

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- 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.
- Be able to solve complex chemistry problems, whether in the academic, research or industrial application areas at a specialization or masters-level.
- Possess the necessary skills to develop multidisciplinary activities within the field of chemistry at the master's level.
- Be able to design, perform, analyse and interpret experiences and complex data in the environment of chemistry at a specialization level.
- Acquire advanced knowledge to assess the importance of chemistry in health, the environment, new materials and energy.
- Acquire the necessary advanced knowledge to assess the importance of chemistry in economic and social development in a context of specialization.

LEARNING OUTCOMES

- Be able to assess the role of Chemistry in the design and preparation of new molecular and polymeric materials with technologic applications in important economic and social areas such as the generation and saving of energy.
- Identify the different types of molecular and polymeric materials exhibiting electrical properties, as well as their synthetic methods and their applications.
- Know the requirements that organic semiconductors should fulfill and the structural and electronic properties they exhibit.
- Know the structure and properties of the diferent carbon nanoforms: fullerenes, nanotubes, graphene, etc.
- Understand the structure-property relations that determine the potential of organic semiconductors as electrical and optically active materials.
- Identify the molecular interactions that determine the supramolecular organization of polymeric and molecular materials, and know the implications of such organization in the charge transport properties.
- Know the different types of mechanisms that regulate the charge transport in organic semiconductors.
- Know the architecture, the components, the functioning, and the basic principles of OLED-type electroluminescent devices and solar cells as main applications of organic semiconductors.

DESCRIPTION OF CONTENTS

0. Introduction: Main applications

Objectives of the subject. Molecular electronics: historical development. Organic semiconductors Presentation of the main applications. Devices to save energy and to generate energy.

1. Polymeric materials

Introduction. Definition of polymer. History of polymers. Types of polymers according to their structure and properties. Mechanisms of polymerization: step by step or chain polymerization. Applications.

2. Electronic structure of organic semiconductors

Basic concepts: Atomic orbitals. Multielectronic atoms: the orbital model. The carbon atom. Electronic molecular structure. Molecular orbitals: pi-conjugated systems. Electronic states: singlet and triplet states. Band theory.

3. Interaction with light

General concepts. Potential energy curves. Electronic spectroscopy. Photo-physical processes. Photo-physical parameters. Types of luminescence.

4. Molecular conductors

Historical development. Electron donors: TTF and analogous systems. Electron acceptors: TCNQ and analogous systems. Charge transfer salts. Molecular metals. Molecular superconductors.

5. Electroactive molecular materials

Types of organic conductors. Pi-conjugated oligomers and polymers. Electron donor/acceptor systems (HTMs/ETMs). Metalomacrocycles: Phthalocyanines and other macrocycles. Molecular orbitals: A useful tool. Structural and vibrational properties. Redox properties: charge injection. Optical properties: Absorption and emission of light.

6. Supramolecular organization and transport properties

Non-covalent interactions: intermolecular forces. Supramolecular aggregates: optical properties. Supramolecular polymers. Liquid crystals. Transport properties.

7. Carbon nanostructures

Introduction: carbon structures and nanostructures. Fullerenes: structure and properties. Carbon nanotubes: structure and properties. Other types of carbon nanostructures. Graphene. Functionalization. Applications.

8. Conducting polymers

Synthesis and molecular design. Electronic structure of conjugated polymers. Defects and charge carriers. Interaction with light: optical properties. Transitions and excited states in pi-conjugated polymers. Excitations in aggregates. Electro-luminescence and stimulated emission. Solid state structure: conformation, flexibility, crystallinity, morphology. Structure of organic-inorganic perovskites.

9. Charge transport

Basic concepts. Charge injection. Charge carriers: mobility. Theory of conduction: transport models. Photo-conductivity. Conductivity in doped-polymers. Applications of conducting polymers in bioelectronics.

10. Applications and devices

Solar cells: cell types and functioning principles. Electro-luminescent devices: light-emitting diodes (LEDs). Lasers: basic principles and functioning. Polymer lasers.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Tutorials	5,00	100
Seminars	5,00	100
Development of individual work	10,00	0
Study and independent work	35,00	0
Readings supplementary material	10,00	0
Preparation of evaluation activities	20,00	0
TOTAL	**125,00**	

TEACHING METHODOLOGY

The course will be taught using the following methodology:

- Interactive lectures. In these lectures the basic concepts of the course will be introduced. Active involvement of the students will be promoted through the raising of issues related with the application of concepts and previous knowledge of the students.
- Tutorials. These are raised as discussion forums of the concepts discussed or of the resolution of the proposed exercises. They will be used to assess the comprehension of the subject by the student.
- Seminars. These will cover the explanation of specific topics by the professors of the course or invited professors. Moreover, they will be used to show and discuss the individual or group tasks proposed to the students.

EVALUATION

Fist call:

The grading of the course will be obtained by the weighted average of the marks obtained in a final exam (75%), which will include concepts and knowledge taught during the course, and the marks obtained in the activities of ongoing evaluation made along the course (25%). The minimum grade to be obtained in these two parts of the evaluation must be equal to or greater than 4.0 to carry out the weighted average.

The grading of the ongoing evaluation will be based on the active participation and critical spirit demonstrated in the discussions raised, and on the results obtained in the tasks and activities raised.

The minimum overall grade for passing the course will be 5.0.

Second call:

The grading of the course in the second call will be obtained applying the same criteria stablished for the first call.

REFERENCES

Basic

- A. Köhler, H. Bässler, Electronic Processes in Organic Semiconductors. An Introduction, Wiley-VCH 2015
- M. C. Petty, M. R. Bryce, D. Bloor, (eds), Introduction to Molecular Electronics, Blackwell, 1995
- K. Müllen, G. Wegner, (eds), Electronic Materials: The Oligomer Approach, Wiley-VCH, 1998
- H.S. Nalwa, (ed), Handbook of Organic Conductive Molecules and Polymers Vol. 1-4, John Wiley & Sons, 1977
- T. A. Skotheim, J. R. Reynolds, (eds), Handbook of Conducting Polymers (3rd ed.) Vol. 1 & 2, CRC Press, 2007
- M. S. Dresselhaus, G. Dresselhaus, P. C. Eklund, (eds), Science of Fullerenes and Carbon Nanotubes, Academic Press, 1996.
- J.H. Warner, F. Schäffel, A. Bachmatiuk, M.J. Rümmeli, Graphene: Fundamentals and Applications, Elsevier, 2012

Additional

- I. F. Perepichka, D. F. Perepichka, (eds), Handbook of Thiophene-Based Materials. Applications in Organic Electronics, Vol. 1 & 2, Wiley, 2009.
- P. A. Cox, The Electronic Structure and Chemistry of Solids, Oxford University Press, 1987
- M. C. Petty, Molecular Electronics. From Principles to Practice, Wiley, 2007
- Durante el curso se dará bibliografía especializada basada en artículos de revisión publicados en revistas científicas. Durant el curs es facilitarà bibliografia especialitzada basada en articles de revisió publicats en revistes científiques. During the course, specialized bibliography based on review articles published in scientific journals will be given.

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

English version is not available