60452 - Catalysis

Información del Plan Docente

Academic Year	2016/17
Academic center	100 - Facultad de Ciencias
Degree	543 - Master's in Molecular Chemistry and Homogeneous Catalysis
ECTS	6.0
Course	1
Period	First semester
Subject Type	Compulsory
Module	---

1.Basic info

1.1.Recommendations to take this course

A mastery of the basic concepts of chemical bonding, structure and reactivity of organic and inorganic compounds is recommended. Class attendance along with continued work facilitates to pass the course.

1.2.Activities and key dates for the course

The subject of Catalysis will be taught during the first semester as well as the other compulsory subjects of this Master and the optional subjects *Fundamental methodologies in synthesis* and *Bibliographic resources and databases* . Throughout the course control-exams and individual or team-works will be performed. The dates of the control-exams and deadlines for the presentation of the works will be communicated well in advance.

The experimental practices of the course of *Catalysis* together with those corresponding to other subjects of the Module *Molecular Chemistry and Catalysis* constitute an integrated block. The laboratory sessions will be performed during the second half of the semester, the schedule and the laboratory will be announced well in advance.

2.Initiation

2.1.Learning outcomes that define the subject

The student must identify the importance of catalysis in the development of sustainable chemicals processes.

The student must know the different types of catalysts, their mode of action, advantages and disadvantages, as well as their principal applications.

The student should evaluate the activity, selectivity and environmental impact of the catalytic processes.

The student must identify key reactions in organometallic catalysis.

The student must know the main homogeneous reactions catalyzed by transition metal complexes and their reaction mechanisms.

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The student should describe the different types of heterogeneous catalysts and the different strategies of immobilisation of molecular catalysts.

The student should describe the different types of homogeneous reactions organocatalyzed and its applications.

The student must identify the current research lines in catalysis and its contribution to the scientific and technological development.

2.2.Introduction

The course focuses on the study of the basic concepts of catalysis, the different types of catalysts, their mechanism of action and their applications. The course is divided into several different blocks: i) basic catalytic reactions, mechanisms and applications of organometallic catalysts in homogeneous phase, ii) principles, classification and applications of heterogeneous catalysts, iii) the design and the mechanism of action of organocatalysts. In the last part of the course, we present a selection of some of the cutting-edge research in catalysis and their potential to meet the new challenges for sustainable development.

3.Context and competences

3.1.Goals

The global objective of the course is to provide the student with an advanced training in Catalysis related to the principles, mechanisms and applications of the different types of catalysts that operate both in homogeneous phase, such as organometallic catalysts and organocatalysts, and in heterogeneous phase.

3.2.Context and meaning of the subject in the degree

The course is part of the mandatory module entitled *Molecular Chemistry and Catalysis* . It is a mandatory subject that is taught during the first semester of the course and it has a workload of 6 ECTS credits. The course provides an advanced training for understanding the basic principles in the design of catalysts for synthetic transformations following an efficient and selective manner. Since the development and optimization of catalysts is one of the main goals of many research groups at the ISQCH, this is a fundamental subject for the realization of the *Master's Degree Final Project* in this field of research.

3.3.Competences

To be able to apply newly trained skills to the study and search of new catalytic transformations.

To be able to apply concepts acquired in the field of inorganic, organic and organometallic chemistry to the design of catalysts.

To be able to apply the basics of catalysis to the synthesis of chemicals following sustainable and environmentally friendly procedures.

To identify and use the most useful literature sources in the scientific research field of catalysis.

To appreciate the potential of the catalysis to face up the new challenges for a sustainable development

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To be able to communicate conclusions of a scientific research work in the field of catalysis.

3.4.Importance of learning outcomes

Trained skills in this course should provide the student with an overall view of the main scientific research lines in catalysis and their importance in the development of new catalytic processes.

The design of new catalysts and the optimization of catalytic processes are key steps on the way to ensure access to affordable, reliable, sustainable and modern energy.

4.Evaluation

The evaluation of this course is based on the following activities, weighted as indicated:

1.- Control questions and problem solving tests (25 %).

2.- Elaboration and oral presentation of a supervised individual or team-based practical work on a scientific paper.

3.- Global Exam: Written theoretic and problem solving test, to be performed within the global evaluation period (50 %).

Final numerical mark will be the best of the following:

Mark 1 = 0.25 x mark of control tets + 0.25 x mark of practical work + 0.50 x global exam.*

Mark 2 = Mark of the global exam.*

* The written global exam will include some questions related to the laboratory work.

The number of official examination calls per registration and their use will be subjected to the statements of the *Regulation of Permanence in Master Studies and* *Regulation of the Learning Assessment* . The latest document will also regulate the general design and scoring criteria of the assessment activities, as well as the exam schedules and timetable for the post-examination review.

5.Activities and resources

5.1.General methodological presentation

1.- Interactive lectures (4 ECTS)

2.- Seminar and problem-solving sessions (1.5 ECTS)

3.- Laboratory work (0.5 ECTS)

5.2.Learning activities

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Training activity focused on acquisition of advanced knowledge in catalysis. The lessons will last 40 one-hour interative lectures.

Seminars and problem-solving sessions. The activity includes 15 classroom hours in which the students will work individually or in small groups several case studies and scientific papers related with the subject's content.

Academic tutoring. Students will own 3 hours per week for individualized tutoring.

Laboratory work. The activity consists in 5 hours of compulsory attendance. The laboratory work will be shared with other subjects of *Molecular Chemistry and Catalysis* module.

5.3.Program

The course contents are divided into the following thematic blocks:

Basic concepts in Catalysis

Catalysis: general concepts. Catalysis and green chemistry. Classification of catalysts: homogeneous catalysts, heterogeneous catalysts and biocatalysts. Homogeneous catalysis: acid-base catalysis, organometallic catalysis, organocatalysis. Activity and selectivity of the catalysts. Quantification of the environmental impact. Economic importance of catalysis.

Organometallic Catalysis

Mechanisms of organometallic catalysts. Ligands and catalyst design. Reaction mechanisms: thermodynamic and kinetic aspects. Elementary steps: substitution, oxidative addition, reductive elimination, migratory insertion, b -elimination and nucleophilic attack. Catalytic reactions: hydrogenation, transfer hydrogenation, hydrofunctionalization, carbonylation, C-H functionalization, C-C coupling, olefin metathesis, olefin oligomerization and polymerization. Catalytic processes of industrial significance.

Heterogeneous Catalysis

Principles and concepts of heterogeneous catalysis. Classification of heterogeneous catalysts: structure and composition. Supported catalysts. Anchoring strategies: covalent and non-covalent immobilization. Non-covalent immobilization: adsorption, electrostatic interaction, hydrogen bonding, encapsulation. Nanocatalysis. Heterogeneous catalytic processes of industrial and environmental significance.

Organocatalysis

Introduction to asymmetric organocatalysis. Activation pathways in organocatalysis: covalent bond formation, hydrogen bonding, weak interactions, phase-transfer catalysts. Mechanism of action and representative examples.

Frontiers in Catalysis

Activation and functionalization of carbon dioxide. Bio-inspired catalysis. Molecular catalysts for water oxidation.

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Applications of dendrimers in catalysis. Multistep processes: multifunctional catalysts and dual catalysis.

5.4.Planning and scheduling

The information about schedules, calendars and exams is available at the websites of the Sciences Faculty, https://ciencias.unizar.es/calendario-y-horarios , and the Master, http://masterqmch.unizar.es . The presentation of practical works will be done according to the scheluded to be announced well in advance.

The students will be provided with diverse teaching material either at reprography or through the University's web tool: https://moodle2.unizar.es/add .

5.5.Bibliography and recomended resources

Basic bibliography

- Rothenberg, Gadi. Catalysis : concepts and green applications / Gadi Rothenberg Weinheim : Wiley-VCH, cop. 2008
- Hartwig, John F.. Organotransition metal chemistry : from bonding to catalysis / John F. Hartwig Sausalito, Ca. : University Science Books, 2010
- Fundamentos y aplicaciones de la catálisis homogénea / editado por Luis A. Oro y Eduardo Sola . 2ª ed. Zaragoza : Luis A. Oro y Eduardo Sola, 2000
- Leeuwen, Piet W. N. M. van. Homogeneous catalysis : understanding the art / Piet W.N.M. van Leeuwen Dordrecht [etc.] : Kluwer Academic Publishers, 2004
- Ross, Julian R. H.. Heterogeneous catalysis : fundamentals and applications / Julian R. H. Ross Amsterdam [etc.] : Elsevier, cop. 2012 [i.e. 2011]
- Berkessel, Albrecht. Asymmetric Organocatalysis : from biomimetic concepts to applications in asymmetric synthesis / Albrecht Berkessek, Harald Gröger . - 1st ed., 1st repr. Weinheim : Wiley-VCH, 2005

Complementary bibliography

- Sheldon, Roger A.. Green chemistry and catalysis / Roger Arthur Sheldon, Isabel Arends, and Ulf Hanefeld Weinheim : Wiley-VCH, cop. 2007
- Behr, Arno. Applied homogeneous catalysis / Arno Behr and Peter Neubert Weinheim : Wiley-VCH, cop. 2012
- Hegedus, Louis S.. Transition metals in the synthesis of complex organic molecules / Louis S. Hegedus . - 3rd ed. Sausalito, California : University Science Books, cop. 2010
- Metal-catalysis in industrial organic processes / edited by Gian Paolo Chiusoli, Peter M. Maitlis Cambridge : Royal Society of Chemistry, cop. 2006
- Hagen, Jens. Industrial catalysis : a practical approach / Jens Hagen. - 2nd completely rev. and extended ed. Weinheim : Wiley-VCH, cop. 2006
- Barbaro, P.. Heterogenized Homogeneous Catalysts for Fine Chemicals Production: Materials and Processes. Ed. Springer, 2010
- Serp, P.. Nanomaterials in Catalysis. Wiley-VCH, 2013
- Pihko, P.M.. Hydrogen Bonding in Organic Synthesis. Wiley-VCH, 2009