

DEPARTAMENT DE QUÍMICA FÍSICA

NÚMERO	TEMA	TUTOR(S) ACADÈMIC(S) (si un és d'un altre departament, posa'l entre parèntesi)	TUTOR EXTERN (si escau)
4	Photoactivated acids: theoretical study of the photoinduced hydrogen abstraction in orto-nitrobenzaldehyde	Angelo Giussani / Javier Segarra Martí	
9	Design of selective enzyme inhibitors by means of computational simulations.	Jose Javier Ruiz Pernía / Iñaki Tuñón García de Vicuña	
11	Synthesis and Characterization of New Iron(II) Spin Crossover Coordination Polymers	Carlos Bartual Murgui /(José Antonio Real Cabezas de Química Inorgánica)	
13	Mineralization of water pollutants by advanced oxidation techniques and spectroelectrochemical monitoring.	Jerónimo Agrisuelas Vallés / José Juan García Jareño	
15	Generation of reactive oxygen species (ROS) on steel/poly(phenothiazines) electrodes and their application.	Jerónimo Agrisuelas Vallés / José Juan García Jareño	
16	Electrogeneration and characterization of poly(phenosafranine) on stainless steel.	José Juan García Jareño / Jerónimo Agrisuelas Vallés	
17	Electroplating of copper on composite materials of the screen printed carbon electrodes for their possible use in sensors.	Jerónimo Agrisuelas Vallés / José Juan García Jareño	
21	Guest Modulation of Spin-Crossover in Porous Iron(II) Metal–Organic Framework with Periodic DFT Studies	Neyvis Almora Barrios / Salvador Cardona Serra	
23	Lignin extraction from agricultural pruning waste for hydrogels preparation	Mario Culebras Rubio / Francisco Pérez Pla	
26	Encapsulation of Phase Change Materials through Valorization of Lignocellulosic Waste	Mario Culebras Rubio / Rafael Muñoz-Espí	
27	Application of Functionalized Polymer Nanoparticles in Asymmetric Catalysis	Rafael Muñoz-Espí / Francisco F. Pérez-Pla	
28	Polysaccharide-Based Hybrid Particles as Magnetically Separable Catalysts	Rafael Muñoz-Espí / Francisco F. Pérez-Pla	
32	Photoactive Nanoparticles Prepared by Miniemulsion Polymerization	Rafael Muñoz-Espí / María González Béjar (Química Orgànica)	
33	Synthesis and Validation of Essential Oil-Based Antimicrobial Systems with Controlled Release via Molecular Gates	M.Carmen Martínez Bisbal	Lucía González Bermúdez
37	Theoretical study of the photophysical properties of heteroleptic Ir(III) complexes	Enrique Ortí Guillem / Angelo Giussani	

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Angelo Giussani

ACADEMIC TUTOR (if needed): Javier Segarra Martí

EXTERNAL TUTOR (if needed): _____

Department: Department of Physical Chemistry

TITLE (Mandatory in English)

Photoactivated acids: theoretical study of the photoinduced hydrogen abstraction in orto-nitrobenzaldehyde

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

The following three main objectives are envisage:

- Characterize the UV-vis accessible electronic excited states of orto-nitrobenzaldehyde
- Study the main non-reactive photophysical path of orto-nitrobenzaldehyde
- Determine the photoinduced mechanism leading to the hydrogen abstraction in orto-nitrobenzaldehyde

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The study will be based on computational calculations using the following two ab-initio wave-function electronic structure methods:

- Complete active space self-consistent field (CASSCF) method.
- Complete active space second-order perturbation method (CASPT2) method

All calculation will be performed using the OpenMolcas software in our local cluster



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VNIVERSITAT (ò*) E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Jose Javier Ruiz Pernía

ACADEMIC TUTOR (if needed): Iñaki Tuñón García de Vicuña

EXTERNAL TUTOR (if needed): _____

Department: Química Física

TITLE (Mandatory in English)

Design of selective enzyme inhibitors by means of computational simulations.

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Construcción de un modelo representativo del centro activo de la enzima en estudio.
Optimización del modelo reducido de una conformación o estructura de rayos X de la enzima.
Estudio del mecanismo de reacción de la enzima en presencia de un inhibidor, estableciendo las diferentes etapas y las barreras de energía potencial.
Determinación de las barreras de energía libre.
Comparación de las propiedades cinéticas del modelo construido con los datos experimentales disponibles.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

Se utilizarán métodos de cálculo de Química Cuántica.
Fundamentalmente programa Gaussian, aunque se podrían utilizar también ORCA. Además se usarán programas de visualización de estructuras, tal como: Molden, Gaussview fundamentalmente y VMD puntualmente.
Localización de los posibles estados de transición del proceso catalítico.
Determinación de la constante de velocidad para cada uno de las etapas de la reacción analizadas.



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VNIVERSITAT (ò*) E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Carlos Bartual Murgui (Dpto. Química Física)

ACADEMIC TUTOR (if needed): José Antonio Real Cabezas (Dpto. Química Inorgánica)

EXTERNAL TUTOR (if needed): _____

Department: Química Física

TITLE (Mandatory in English)

Synthesis and Characterization of New Iron(II) Spin Crossover Coordination Polymers

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

El objetivo de este TFG es introducir los conceptos fundamentales del fenómeno de transición de espín en compuestos de hierro(II) y realizar la síntesis y caracterización físico-química de nuevos polímeros de coordinación 2D con ligandos axiales pi-aceptores

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

Realización de un estudio bibliográfico, preparación y caracterización de los complejos $[\text{Fe}(\text{L})_2[\text{M}(\text{CN})_4]]$ con $\text{M} = \text{Ni}(\text{II}), \text{Pd}(\text{II}), \text{Pt}(\text{II})$ y siendo L el ligando axial pi-aceptor.



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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Jerónimo Agrisuelas Vallés

ACADEMIC TUTOR (if needed): José Juan García Jareño

EXTERNAL TUTOR (if needed): _____

Department: Química-Física

TITLE (Mandatory in English)

Mineralization of water pollutants by advanced oxidation techniques and spectroelectrochemical monitoring.

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Use of reusable electrodes for electrochemical removal of pollutants.
Approach to the study of advanced oxidation processes.
Optimization and monitoring of the process by spectroelectrochemical techniques.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

1. Bibliographic study
2. Introduction to the electrochemical techniques.
3. Electrode preparation.
4. Design of electrochemical experiments.
5. Analysis of obtained results and discussion.
6. Writing the TFG report.



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VNIVERSITAT (ò*) E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: José Juan García Jareño

ACADEMIC TUTOR (if needed): Jerónimo Agrisuelas Vallés

EXTERNAL TUTOR (if needed): _____

Department: Química-Física

TITLE (Mandatory in English)

Corrosion rate study of steels. Effect of protective polymeric films.

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Measuring corrosion rate of steels in different aggressive media.
Coating of steel electrodes with protective layers.
Measuring corrosion rate on coated steels in different aggressive media.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

1. Bibliographic study.
2. Introduction to the electrochemical techniques.
3. Electrode preparation.
4. Design of electrochemical experiments.
5. Analysis of obtained results and discussion.
6. Writing the TFG report.



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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Jerónimo Agrisuelas Vallés

ACADEMIC TUTOR (if needed): José Juan García Jareño

EXTERNAL TUTOR (if needed): _____

Department: Química-Física

TITLE (Mandatory in English)

Generation of reactive oxygen species (ROS) on steel/poly(phenothiazines) electrodes and their application.

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Generation of reactive oxygen species in aqueous media on reusable electrodes.
Effect of the medium on the generation of reactive oxygen species.
Optimization and monitoring of the process by spectroelectrochemical techniques.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

1. Bibliographic study
2. Introduction to the electrochemical techniques.
3. Electrode preparation and generation of the polymer.
4. Design of electrochemical experiments.
5. Analysis of obtained results and discussion.
6. Writing the TFG report.



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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: José Juan García Jareño

ACADEMIC TUTOR (if needed): Jerónimo Agrisuelas Vallés

EXTERNAL TUTOR (if needed): _____

Department: Química-Física

TITLE (Mandatory in English)

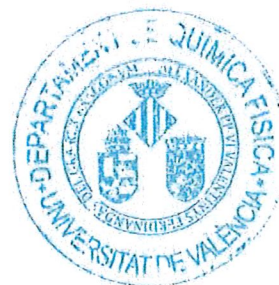
Electrogeneration and characterization of poly(phenosafranine) on stainless steel.

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Preparation of electrodes for electrodeposition.
Polymerization of poly(phenosafranine) on steel electrodes.
Correlate electrochemical data and spectroelectrochemical surface color changes.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

1. Bibliographic study
2. Introduction to the electrochemical techniques.
3. Electrode preparation.
4. Design of electrochemical experiments recorded on digital video.
5. Analysis of obtained results and discussion.
6. Writing the TFG report.



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VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Jerónimo Agrisuelas Vallés

ACADEMIC TUTOR (if needed): José Juan García Jareño

EXTERNAL TUTOR (if needed): _____

Department: Química-Física

TITLE (Mandatory in English)

Electroplating of copper on composite materials of the screen printed carbon electrodes for their possible use in sensors.

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Optimization of conditions for copper deposition on screen-printed electrodes.
Monitoring of metal layer growth by spectroelectrochemical techniques.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

1. Bibliographic study
2. Introduction to the electrochemical techniques.
3. Electrode preparation for metal deposition.
4. Design of electrochemical experiments.
5. Analysis of obtained results and discussion.
6. Writing the TFG report.



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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Neyvis Almora Barrios

ACADEMIC TUTOR (if needed): Salvador Cardona Serra

EXTERNAL TUTOR (if needed): _____

Department: Química Física

TITLE (Mandatory in English)

Guest Modulation of Spin-Crossover in Porous Iron(II) Metal–Organic Framework with Periodic DFT Studies

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

1. Realizar cálculos periódicos usando métodos de funcionales de densidad para investigar las propiedades magnéticas de las redes metal-orgánicas de Fe(II) (Fe-MOF).
2. Establecer una correlación entre las temperaturas críticas experimentales (T_c) y la brecha energética LS-HS calculada, validando la concordancia entre los resultados teóricos y experimentales.
3. Estudiar las interacciones específicas entre el huésped y el Fe-MOF a través de cálculos de energía de absorción y las modificaciones en la transición de spin. Comparar estas propiedades con las del compuesto original.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

1. Revisión bibliográfica: Materiales metal-orgánico (Fe-MOFs), específicamente los que presentan transiciones de espín.
2. Análisis Estructural: Cálculos periódicos de optimización de la geometrías del los cristales para los estados de alto espín (HS) y bajo espín (LS) de los Fe-MOFs. Se empleará el programa SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) o VASP (The Vienna Ab initio Simulation Package).
3. Interacciones Específicas: Determinar la energía de absorción entre el huésped con los Fe-MOF y la variación de en la estabilidad del alto y bajo espín.
4. Correlación Experimental y Teoría: Validar la concordancia entre los resultados teóricos y experimentales.



VNIVERSITAT (ò*) E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Mario Culebras Rubio

ACADEMIC TUTOR (if needed): Francisco Pérez Pla

EXTERNAL TUTOR (if needed): _____

Department: QUÍMICA FÍSICA

TITLE (Mandatory in English)

Lignin extraction from agricultural pruning waste for hydrogels preparation

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Extracción de lignina mediante procesos de fraccionamiento de biomasa. Obtención de hidrogeles y membranas en base a lignina mediante modificación química. Caracterización estructural mediante medidas de peso molecular, morfológica y mecánica de los hidrogeles obtenidos.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

La metodología a utilizar implicará:

1. El empleo de rutas sintetizar para producir hidrogeles a partir de fracciones de biomasa (lignina)
2. El uso de métodos de fraccionamiento de biomasa basados en los procesos "kraft" y "organosolv"
3. Análisis mecánico mediante medidas de compresión.
4. Análisis térmico mediante calorimetría diferencial de barrido modulada y termogravimetría
5. Análisis morfológico mediante microscopía electrónica de barrido y transmisión
6. Análisis estructural mediante FTIR y GPC.



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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Mario Culebras Rubio

ACADEMIC TUTOR (if needed): Rafael Muñoz-Esp

EXTERNAL TUTOR (if needed): _____

Department: Química Física

TITLE (Mandatory in English)

**Encapsulation of Phase Change Materials through
Valorization of Lignocellulosic Waste**

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Preparation of lignin nanocapsules loaded with paraffinic phase change materials (PCMs) for application in thermal energy storage.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The methodology to be used will involve:

1. The use of nanostructuring techniques based on soft templating methods.
2. Thermal analysis using differential scanning calorimetry (DSC) and thermogravimetry (TGA).
3. Morphological analysis using scanning and transmission electron microscopy (SEM/TEM).
4. Structural analysis using infrared spectroscopy (FTIR).
5. Evaluation of the applicability of the materials in thermal energy storage.



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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Rafael Muñoz-Esp

ACADEMIC TUTOR (if needed): Francisco F. Pérez Pla

EXTERNAL TUTOR (if needed): _____

Department: Physical Chemistry

TITLE (Mandatory in English)

Application of Functionalized Polymer Nanoparticles in Asymmetric Catalysis

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

- Preparation of polymer nanoparticles functionalized with organic or organometallic moieties, with ability to catalyze asymmetrically organic reactions.
- Evaluation of the catalytic activity of the prepared materials.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The catalytic moieties will be supported on polymer nanoparticles prepared by colloidal methods (typically, miniemulsion polymerization). The colloidal characterization of the systems will be performed using dynamic light scattering (DLS) and zeta potential measurement. The morphology of the materials will be evaluated using electron microscopy (SEM and TEM). Thermogravimetric analysis (TGA) will be used for thermal characterization.

The catalytic activity and the stereoselectivity will be studied by using liquid chromatography (HPLC).



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DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Rafael Muñoz-Esp

ACADEMIC TUTOR (if needed): Francisco F. Pòrez Pla

EXTERNAL TUTOR (if needed): _____

Department: Physical Chemistry

TITLE (Mandatory in English)

Polysaccharide-Based Hybrid Particles as Magnetically Separable Catalysts

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

- Preparation of polysaccharide particles for complexation of metal ions, so that they can be used in model catalytic reactions.
- Evaluation of the catalytic activity of the prepared materials.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The preparation of the macroscopic particles will take place by ionotropic gelation according to the methods previously developed in our laboratory. Magnetite nanoparticles will be integrated in the system.

Metal ions will be incorporated into the systems either in situ during the preparation of the particles or by post-loading. The metal ions can be reduced to obtain metallic particles on the surface of the particles.

The catalytic activity will be evaluated by UV-vis spectroscopy and/or by chromatography.



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VNIVERSITAT (ò*) E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: **Rafael Muñoz-Esp**

ACADEMIC TUTOR (if needed): Mar a Gonzàlez Bøjar (Department of Organic Chemistry)

EXTERNAL TUTOR (if needed): _____

Department: Physical Chemistry

TITLE (Mandatory in English)

Photoactive Nanoparticles Prepared by Miniemulsion Polymerization

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

- Selection and, if appropriate, preparation of organic compounds with chromophore ability that can be fixed on the surface of polymeric nanoparticles.
- Preparation and characterization of nanoparticles functionalized with the chosen photoactive groups.
- Application of the systems prepared in photocatalysis.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The work will begin with the preparation of photocatalytic compounds that can be incorporated into the surface of polymeric nanoparticles prepared by miniemulsion polymerization. There are two possible strategies: either the ligands incorporate a polymerizable group, or they incorporate a group capable of reacting with functional groups present on the surface of the previously prepared nanoparticles.

In the second phase, nanoparticles incorporating the photoactive compounds of the previous stage will be prepared.

Synthetic parameters will be optimized and the compounds and particles prepared will be characterized by using the appropriate analytical techniques.

The photocatalytic activity of the systems for model reactions of interest will be evaluated.



VNIVERSITAT (Ò*) E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Maria del Carmen Martínez Bisbal

ACADEMIC TUTOR (if needed):

EXTERNAL TUTOR (if needed): Lucía González Bermúdez

Department: Química Física

TITLE (Mandatory in English)

Synthesis and Validation of Essential Oil-Based Antimicrobial Systems with Controlled Release via Molecular Gates

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

The main focus of the project is the development of new antimicrobial systems that utilize essential oils. These systems will be synthesized, characterized, and validated for their antifungal and antibacterial properties. The project emphasizes the controlled release of these antimicrobial agents using molecular gates that respond to the presence of microorganisms.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

This project focuses on the development of novel antimicrobial systems utilizing essential oils, which are encapsulated and released in a controlled manner through molecular gates. The methodology involves synthesizing suitable encapsulation materials, incorporating essential oils, and integrating responsive molecular gates that activate in the presence of specific microbial triggers. Detailed characterization of the encapsulated systems is performed using techniques such as SEM, TEM, DLS, and FTIR to assess stability, size distribution, and surface properties. In vitro release studies are conducted to evaluate the release profiles of the essential oils, followed by antimicrobial efficacy testing against various fungal and bacterial strains. Optimization and validation of the encapsulation and release parameters ensure consistent performance. This project aims to create effective antimicrobial agents with enhanced stability and targeted delivery, providing a promising approach to combating microbial infections.



VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT

CHEMISTRY DEGREE

ACADEMIC TUTOR: Enrique Orti Guillen

ACADEMIC TUTOR (if needed): Angelo Giussani

EXTERNAL TUTOR (if needed): _____

Department: Physical Chemistry

TITLE (Mandatory in English)

Theoretical study of the photophysical properties of heteroleptic Ir(III) complexes

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

The project intend to:

- initiate the student to the use of theoretical and computational methods of quantum chemistry, and the corresponding software
- study the electronic structure and photophysical properties of ionic transition metal complexes with potential applications for electroluminescent devices
- characterize the properties of the excited states of the complexes

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

Ionic transition metal complexes based on Ir(III) are employed as electroluminescent materials, due to their ability to transform electrical energy into luminous energy. The TFG will consist in the characterization of the properties of such materials, which translates in the following tasks:

- 1) bibliographic research of the photophysical properties of Ir(III) complexes
- 2) determination of the structural and electronic properties of reference Ir(III) complexes in their ground state and emitting triplet states, using quantum chemistry methods and software
- 3) analysis of the obtained results using graphical interfaces, and comparison with the available spectroscopy data from the literature
- 4) writing of the final report

